Jet Fragmentation at the LHC

by

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Abstract

Run II at the LHC is pushing the energy and luminosity frontiers, and challenging the theory community to develop new tools both to increase the precision of our predictions and to expand their scope to match measurements of a more diverse set of observables. In this work, we describe the use of a new class of non-perturbative functions called Generalized Fragmentation Functions (GFFs) as a step towards these goals. This theoretical framework enables the calculation of a broad set of semi-inclusive jet observables. We explore known observables whose distributions can now be calculated using GFFs, and construct a new class of non-associative "fractal observables" which can be described with GFFs. As an important application, we calculate the spectrum of track-assisted mass, which can be measured experimentally with much better angular resolution than ordinary jet mass, including the effect of Soft-Drop grooming. In order to make connections to frameworks for describing Quantum Chromodynamics, we discuss the relationship between GFFs and the Generating Functional Approach (GFA).

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Contents

1 Introduction
   1.1 Perturbative QCD .................................. 22
      1.1.1 Cross Sections and Factorization .............. 22
      1.1.2 Deep-Inelastic Scattering ......................... 25
      1.1.3 Parton Distribution Functions ...................... 27
   1.2 Fragmentation ........................................ 32
      1.2.1 Single-Hadron Fragmentation ....................... 32
      1.2.2 Dihadron Fragmentation ............................. 35
   1.3 Jets at the LHC ..................................... 37
      1.3.1 Tagging ............................................ 37
      1.3.2 Grooming .......................................... 38
   1.4 Overview ............................................. 43

2 Generalized Fragmentation Functions and Fractal Observables 53
   2.1 Introduction ......................................... 54
   2.2 Formalism ............................................. 58
      2.2.1 Review of Standard Fragmentation .................. 58
      2.2.2 Introducing Generalized Fragmentation ............. 61
      2.2.3 Introducing Fractal Observables .................... 64
   2.3 Fractal Observables via Clustering Trees ............... 66
      2.3.1 Construction ....................................... 66
      2.3.2 Requirements ...................................... 68
      2.3.3 Evolution Equations ................................ 69
2.4 Weighted Energy Fractions ........................................ 71
  2.4.1 Associativity .................................................. 72
  2.4.2 Extraction of GFFs ............................................ 73
  2.4.3 Evolution of GFFs ............................................. 75
  2.4.4 Limits ......................................................... 81
  2.4.5 Moment Space Analysis ....................................... 83
2.5 Tree-Dependent Observables ....................................... 87
  2.5.1 Node Products ................................................ 88
  2.5.2 Full-Tree Observables ....................................... 92
2.6 Application in Quark/Gluon Discrimination ....................... 93
2.7 Fractal Observables from Subjets ................................ 98
2.8 Conclusions ........................................................ 101

3 Aspects of Generalized Track-Assisted Mass 103
  3.1 Introduction ..................................................... 103
  3.2 Exploration of Generalized Track-Assisted Mass ................ 108
    3.2.1 Observable and Statistic Definitions ...................... 108
    3.2.2 Parton Shower Results .................................... 111
  3.3 Track-Assisted Mass in $e^+e^-$ Annihilation .................. 115
    3.3.1 Defining Track-Based Observables ......................... 116
    3.3.2 Resummed Calculation ..................................... 118
    3.3.3 Insights at Fixed Coupling ................................ 122
    3.3.4 Fixed-Order Corrections ................................... 124
    3.3.5 Extension to Generalized Track-Assisted Mass .......... 127
    3.3.6 Non-Perturbative Corrections ................................ 127
    3.3.7 Best Fit Parameters ....................................... 130
  3.4 Impact of Soft-Drop Grooming .................................. 135
    3.4.1 Track-Assisted Grooming .................................. 135
    3.4.2 Parton Shower Study ....................................... 136
    3.4.3 Analytic Calculation with Grooming ....................... 137
A.5.3 Full-Tree Observables ...................................... 193

B Details of Generalized Track-Assisted Mass Calculation 197
  B.1 Pure Quark and Gluon Ensembles ............................... 197
  B.2 Details of Resummed Calculation ............................... 200
  B.3 Details of Fixed-Order Matching ............................... 204
    B.3.1 Matrix Elements ............................................. 204
    B.3.2 Comparison of Matching Schemes ............................ 208
  B.4 Alternative Soft-Drop Implementation ........................... 210
List of Figures

1-1 Cross section for $e^+e^-$ annihilation to hadrons as a function of the center-of-mass energy $Q$ (GeV) [287]. ........................................... 23

1-2 Deep-inelastic scattering of an electron with momentum $k$ against a proton with momentum $P$. The electron transfers space-like momentum $q$ to a parton carrying momentum $xP$. ........................................... 26

1-3 The structure function $W_2^{2P}$ extracted from data taken in multiple experiments at two values of $Q^2$, 6.5 GeV$^2$ and 90 GeV$^2$. Taken from Ref. [287]. ....................................................... 28

1-4 (a) Quark/gluon discrimination ROC curves for the CMS tagger, showing the effect of the individual observables as well as the combined discrimination power. Taken from Ref. [24]. (b) Similar ROC curves for the ATLAS tagger, as well as a ROC curve for a tagger based on a convolutional neural network taking low-level jet data as its inputs. Taken from Ref. [27]. ....................................................... 39

1-5 Comparison of energy correlation function $C_1^{(\alpha=2)}$ distributions from PYTHIA 8 and analytic calculations, computed for soft-drop groomed jets with various values of the grooming parameter $\beta$. Taken from Ref. [254]. ....................................................... 41

1-6 Radiation contributing to NGLs for light hemisphere jet mass. Taken from Ref. [137]. ....................................................... 42
1-7 (a) CMS measurement of the distribution of $p_T^D$ in $Z+$jet events, and
(b) ATLAS measurement of the first moment of the weighted jet charge
distribution with parameters $\kappa = 0.3, 0.5$, and $0.7$ on up-type and
down-type jets. Taken from (a) Ref. [125] and (b) Ref. [38].

1-8 Gluon GFFs for (a) the node-product observables with $w_a = 0$ and
$\kappa = 4$ and (b) the full-tree fractal observable defined with $\kappa = 2$ and
$\xi = 2$ on only charged particles. These are extracted from VINCIA at
$\mu = 100$ GeV. The tree dependence of these observables is parametrized
by the generalized-$k_t$ exponent, with $p = -1$ (anti-$k_t$, red dashed),
$p = 0$ (C/A, green), and $p = 1$ ($k_t$, blue dotted).

1-9 The $\Delta$ statistic in the two-dimensional $(\kappa, \lambda)$ space, for jets with $p_{T,\text{calo}} > 300$ GeV. The minimum of $\Delta$ occurs at $\kappa = 0.54$, $\lambda = 0.50$.

1-10 GTAM distributions for (a) gluon jets and (b) down-quark jets in $e^+e^-$
collisions. The benchmark observable $M_{TA}^{(0.5,0.5)}$ is a very close match
to the calorimeter jet mass.

1-11 Matched distributions for rescaled jet mass $\rho_{\text{calo}}$ (solid curves) and
rescaled track-assisted mass $\rho_{TA}$ (dashed curves) after soft-drop grooming
for (a) gluon jets and (b) down-quark jets. Shown are soft-drop grooming parameters $z_{\text{cut}} = 0.1$ and $\beta = \{0, 1, 5, \infty\}$.

2-1 Fractal jet observables are defined recursively on binary clustering
trees. In each recursive step, the value $x$ for the mother is expressed
in terms of the momentum fraction $z$ and the value $x_1$ and $x_2$ of the
observable for the daughters.

2-2 Tree structure for fractal observables. Each leaf node has a starting
weight $w_a$. Each edge has a momentum value $p_i$, which is used to cal-
culate the momentum fraction $z$ of the splitting at each non-leaf node.
The observable values at the non-leaf nodes are given by the $\hat{x}(z, x_1, x_2)$
recursion relation. The final value of the observable measured on the
tree as a whole is the value obtained at the root node.
2-3 The three binary trees which could be constructed by clustering three particles. For associative observables studied in Sec. 2.4, the order of the clustering does not affect the final observable. The ordering of the clustering will matter for the non-associative observables studied in Sec. 2.5.

2-4 Gluon and quark-singlet GFFs for weighted energy fractions with (top) \( \kappa = 0.5 \) and (bottom) \( \kappa = 2 \), with all particles given starting weight 1. These distributions were extracted at the scale \( \mu = 100 \) GeV. The left column shows results from the VINCIA parton shower, with uncertainty bands from varying \( R = \{0.3, 0.6, 0.9\} \) while keeping \( \mu \) fixed. The right column shows the fixed jet radius \( R = 0.6 \), with uncertainty bands from testing three different parton showers: PYTHIA, VINCIA, and DIRE. In this and subsequent figures, (Quark) always refers to the quark-singlet combination \( S(x, \mu) \) defined in Eq. (2.30).

2-5 Gluon GFFs of weighted energy fractions with (top row) \( \kappa = 0.5 \), (middle row) \( \kappa = 1 \), and (bottom row) \( \kappa = 2 \). Shown are distributions involving (left column) all particles, (middle column) just charged particles, and (right column) charged particles weighted by their charge. The GFFs extracted from parton showers at \( \mu = 100 \) GeV are shown in solid red. The result of evolving these initial conditions to \( \mu = 4 \) TeV are plotted in solid orange, to be compared to the average distribution obtained from parton showers at that value, plotted in dashed orange. The uncertainties come from both varying \( R \) and the choice of parton shower (i.e. both variations shown in Fig. 2-4).

2-6 Same as Fig. 2-5 but for quark-singlet GFFs, where the distributions extracted from parton showers at \( \mu = 100 \) GeV are shown in solid blue, the evolved distribution are shown in solid light blue, and the distributions extracted at \( \mu = 4 \) TeV are shown in dashed light blue.
2-7 Error bars on the GFF evolution for weighted energy fractions with (top) $\kappa = 0.5$ and (bottom) $\kappa = 2.0$, for (left) gluons and (right) quark singlets. The dark curves come from evolving Eq. (2.18) from $\mu = ER = 100$ GeV to 4 TeV, and the dark bands are the envelope obtained by starting the evolution at $0.5\mu = 50$ GeV and $2\mu = 200$ GeV.

2-8 Gluon GFFs for (a) the modified weighted energy fractions from Eq. (2.31) in the $\kappa \to 1$ limit, and (b) the $\kappa$-th root of the weighted energy fractions from Eq. (2.33) in the $\kappa \to \infty$ limit. The solid lines show the GFFs extracted from VINCIA at $\mu = 100$ GeV, while the dashed lines show the evolution of these GFFs to $\mu = 4$ TeV. The fact that the limits are smooth is a consistency check on the evolution code.

2-9 The two eigenvalues of the matrix in Eq. (2.39), as a function of $\kappa$. This matrix governs the evolution of the first moment of weighted energy fraction GFFs. Only for $\kappa = 1$ is there a zero eigenvalue.

2-10 Evolution of the first and second moments of (top row) the gluon GFFs and quark-singlet GFFs and (bottom row) the $u$-$d$ quark-non-singlet GFFs. Shown are the first and second GFF moments for weighted energy fractions of charged particles with (left column) $\kappa = 0.5$, (middle column) $\kappa = 1$, and (right column) $\kappa = 2$. The initial conditions at $\mu = 100$ GeV are obtained from parton showers as described in Sec. 2.4.2, with uncertainty bands from varying $R$ and changing the parton shower. The values from the parton shower average at $\mu = 4$ TeV are shown as dots (diamonds) for the first (second) moments.

2-11 Gluon GFFs for the node-product observables with $w_a = 0$, taking (a) $\kappa = 1$, (b) $\kappa = 2$, and (c) $\kappa = 4$. These are extracted from VINCIA at $\mu = 100$ GeV. The tree dependence of these observables is parametrized by the generalized-$k_t$ exponent in Eq. (2.22), with $p = -1$ (anti-$k_t$, red dashed), $p = 0$ (C/A, green), and $p = 1$ ($k_t$, blue dotted). For $\kappa = 2$ in (b), there is no tree dependence, as this observable is identical to $2(1 - p_T^D)$ (black dot-dashed).
2-12 Evolution of the gluon GFFs for node products with (top row) \( \kappa = 1 \) and (bottom row) \( \kappa = 4 \), comparing (left column) \( p = -1 \), (center column) \( p = 0 \), and (right column) \( p = 1 \). Shown are the gluon GFFs extracted from parton showers at \( \mu = 100 \text{ GeV} \) (red solid), the GFFs evolved to \( \mu = 4 \text{ TeV} \) (orange solid), and the GFFs extracted from parton showers at \( \mu = 4 \text{ TeV} \) (orange dashed). The evolution agrees qualitatively with parton shower predictions, though the agreement is somewhat worse for \( p = -1 \).

2-13 Same as Fig. 2-11, but for the full-tree fractal observable in Eq. (2.45) defined with \( \kappa = 2 \) on only charged particles, for (a) \( \xi = -2 \), (b) \( \xi = 0 \), and (c) \( \xi = 2 \). Recall that full-tree observables with \( \xi = 0 \) are the same as weighted energy fractions, so panel (b) is the same as the 100 GeV curve in Fig. 2-5h, which is plotted as a dash-dotted black line for comparison.

2-14 Same as Fig. 2-12, but for the full-tree fractal observable in Eq. (2.45) defined with \( \kappa = 2 \) on only charged particles, for (top row) \( \xi = -2 \) and (bottom row) \( \xi = 2 \).

2-15 GFFs for two strong quark/gluon discriminants based on C/A trees: (a) the node-product observable with \( \kappa = 1 \), and (b) the full-tree observable with \( \kappa = 2 \) and \( \xi = 4 \) with all particle weights one. Shown are the gluon GFF (red solid), quark-singlet GFF (blue solid), down-quark GFF (light-blue dashed), and bottom-quark GFF (violet dotted) as extracted from VINCIA at \( \mu = 100 \text{ GeV} \).

2-16 Quark/gluon ROC curves from VINCIA for the node-product observables at (a) \( \mu = 100 \text{ GeV} \) and (b) \( \mu = 4 \text{ TeV} \). The curves correspond to \( \kappa = 1 \) (dark green solid), \( \kappa = 2 \) (green dashed), and \( \kappa = 4 \) (light green dotted). Note that the \( \kappa = 2 \) case has the same ROC curve as \( p_T^D \), and the gray dashed line represents an observable with no discrimination power.
2-17 Evolution of the ROC curves for node-product observables with (a) \( \kappa = 1 \), (b) \( \kappa = 2 \) (equivalent to \( p_D^T \)), and (c) \( \kappa = 4 \). Shown are the ROC curves extracted from parton showers at 100 GeV (light purple band) and 4 TeV (dark purple, dashed), as well as the ROC curve obtained from evolving the GFF from \( \mu = 100 \) GeV to 4 TeV (medium purple band). The spread of these curves is obtained from calculating the ROC curves from the spread of distributions, as described in Sec. 2.4.2.

2-18 Same as Fig. 2-16 but for the full-tree observables with \( \kappa = 2 \) and \( \xi = \{0, 2, 4, 6\} \). Note that the \( \xi = 0 \) case is identical to \( p_D^T \).

2-19 Same as Fig. 2-17 but for the full-tree observables with \( \kappa = 2 \) and (a) \( \xi = 2 \), (b) \( \xi = 4 \), and (c) \( \xi = 6 \). The \( \xi = 0 \) case is identical to \( p_D^T \), shown in Fig. 2-17b.

2-20 Modified fractal jet observables where the recursion relation changes at a characteristic scale \( R_{\text{sub}} \). When using a C/A tree, it is possible to switch the recursion relation from \( \hat{x}_1 \) to \( \hat{x}_2 \) for angular scales \( \theta > R_{\text{sub}} \). This is equivalent to determining the observable \( \hat{x}_1 \) on all subjets of radius \( R_{\text{sub}} \) and then using these as initial weights for the tree with \( \hat{x}_2 \).

2-21 Evolution of the fractal observable defined by equations Eqs. (2.46) and (2.48), where \( \hat{x}_1 \) and \( \hat{x}_2 \) are given by weighted energy fractions measured on all particles with \( \kappa_1 = 1 \) and \( \kappa_2 = 2 \), respectively.

3-1 Distributions of jet mass \( M_{\text{calo}} \) and GTAM \( M_{\text{TA}}^{(\kappa, \lambda)} \) in \( e^+e^- \) collisions, extracted from (a) VINCIA 2.2.2 and (b) NLL+LO calculations convolved with a non-perturbative shape function.

3-2 (a) GTAM distributions for \( p_{T,\text{calo}} > 300 \) GeV with \( \kappa = 0 \) and \( \lambda = \{0, 0.5, 1, 1.5\} \), with ordinary jet mass plotted as a dashed black curve for comparison. (b) \( \Delta(0, \lambda) \) as a function of \( \lambda \), in the \( p_{T,\text{calo}} > 100 \) GeV, \( p_{T,\text{calo}} > 300 \) GeV, and \( p_{T,\text{calo}} > 1000 \) GeV ensembles.

3-3 Same as Fig. 3-2 but (a) with GTAM parameters \( \kappa = \{0, 0.5, 1, 1.5\} \) and \( \lambda = 0 \) and (b) \( \Delta(\kappa, \lambda = 0) \) as a function of \( \kappa \).
3-4 Same as Fig. 3-2 but (a) with GTAM parameters \((\kappa, \lambda) = \{(0, 1), (0.5, 0.5), (1, 0)\}\) and (b) \(\Delta(\kappa, 1 - \kappa)\) as a function of \(\kappa\). ..................................... 113

3-5 (a) The \(\Delta\) statistic in the two-dimensional \((\kappa, \lambda)\) space, for the \(p_{T,\text{calo}} > 300\) GeV sample. The minimum of \(\Delta\) occurs at \(\kappa = 0.54, \lambda = 0.50\). (b) One-dimensional slices of \(\Delta(\kappa, \lambda)\), corresponding to Figs. 3-2b, 3-3b, and 3-4b. ......................................................... 114

3-6 (a) Track functions extracted from PYTHIA 8.230 (see Ref. [158]) for gluons and active quark flavors at a scale of \(\mu = 300\) GeV. (b) Track functions from PYTHIA for gluon jets (red) and down-quark jets (blue) at scales \(\mu = \{100, 300, 1000\} \) GeV. ................................. 117

3-7 An eikonal quark emitting soft, collinear gluons. For the calculation of a track-based observable, each gluon emission, as well as the final quark, must be weighted with the appropriate track function. .... 120

3-8 Resummed distributions at NLL for rescaled jet mass \(\rho_{\text{calo}}\) (dashed curves) and rescaled track-assisted mass \(\rho_{TA}\) (solid curves) with \(R = 1\) for (a) gluon-initiated jets and (b) down-quark-initiated jets. Shown are three different values of the jet energy, \(E_{\text{calo}} = 100\) GeV, 300 GeV, and 1000 GeV. ......................................................... 121

3-9 Top row: Components of the matching calculation for (a) gluons and (b) down quarks. The full matched NLL+LO result is in red, the LO fixed-order distribution is in dark green, and the \(\mathcal{O}(\alpha_s)\) piece of the fixed-order expansion of the NLL resummed distribution is in light green. The NLL distribution is plotted in blue. Bottom row: The corresponding ratios of the \(\mathcal{O}(\alpha_s)\) piece of the NLL distribution over the LO differential distribution, for various values of jet radius \(R\) to highlight the \(R \log R\) residual. ......................................................... 131

3-10 Top row: NLL+LO calculations of the GTAM distribution for (a) gluon jets and (b) down-quark jets, compared to ordinary jet mass. Bottom row: corresponding ratio between GTAM and jet mass. ............. 132
3-11 GTAM distributions computed from VINCIA (stepped histograms) and NLL+LO with non-perturbative corrections (smooth curves). Shown are (a) calorimeter jet mass, (b) track mass, (c) track-assisted mass, and (d) GTAM with $\kappa = 0.5$ and $\lambda = 0.5$.

3-12 Left column: Distribution of $\Delta(\kappa, \lambda)$ computed using the analytic NLL+LO distributions convolved with the shape function $F_{\text{NP}}$ for gluons (top) and down quarks (bottom). The white cross marks the best-fit value, which is $(0.9, 0.1)$ for gluons and $(\kappa, \lambda) = (0.8, 0.1)$ for down quarks. The white dot marks track-assisted mass, $\rho_{\text{TA}} = \rho_{\text{TA}}^{(1,0)}$. Right column: One-dimensional slices of the distributions on the left. The slight offset of the minimum values in (c) from the line $\lambda = 1 - \kappa$ manifests in the red $(\xi, 0)$ curve dipping below the blue $(\xi, 1 - \xi)$ curve in (d) before intersecting again at $\xi = 1$.

3-13 (a) Groomed jet mass and track-assisted mass distributions in VINCIA for $z_{\text{cut}} = 0.1$ and various values of $\beta$. The $\beta = \infty$ curve corresponds to the ungroomed distribution. (b): The statistic $\Delta(\kappa, 1 - \kappa)$ for the same values of $\beta$.

3-14 Matched distributions for rescaled jet mass $\rho_{\text{calo}}$ (solid curves) and rescaled track-assisted mass $\rho_{\text{TA}}$ (dashed curves) after soft-drop grooming for (a) gluon jets and (b) down-quark jets. Shown are soft-dropped grooming parameters $z_{\text{cut}} = 0.1$ and $\beta = \{0, 1, 5, \infty\}$.

3-15 Ratios of the soft-drop groomed $\mathcal{O}(\alpha_s)$ piece of the expanded NLL distributions over the LO $\rho_{\text{TA}}$ distributions. The $\beta = 0$ case is dashed since this calculation is formally only LL order.

4-1 Comparison of analytic distributions of $\Delta z \equiv E_{\text{RSD}} / E_{\text{jet}}$ with PYTHIA 8.223 for (a) initial quarks and (b) initial gluons.

4-2 Evolution comparison between PYTHIA 8.230 and Eqs. (4.3) and (4.4) for (a) initial quarks and (b) initial gluons.
A-1 Sensitivity of the evolution from $\mu = 100$ GeV to 4 TeV on the choice of fine bin width. Shown are the (left) gluon GFF and (right) quark-singlet GFF for the weighted energy fraction with $\kappa = 0.5$. The curves labeled $\Delta n_X$ are the difference between the result using $n_{\text{fine}} = X$ and the result using $n_{\text{fine}} = 1000$. For the default value of $n_{\text{fine}} = 100$ used in this chapter, the results are indistinguishable by eye.

A-2 Downward evolution from $\mu = 4$ TeV to $\mu = 100$ GeV of the (left column) gluon GFF and (right column) quark-singlet GFF with (top row) $\kappa = 0.5$ and (bottom row) $\kappa = 2.0$. The envelopes of the evolved distributions are constructed as in Sec. 2.4.2 by varying the jet radius $R$ and the choice of parton shower, which highlight the numerical instability of downward evolution.

A-3 Moment space evolution of the node-product observables with (top row) $\kappa = 1$ and (bottom row) $\kappa = 4$ for the generalized-$k-t$ clustering trees with (left column) $p = -1$, (middle column) $p = 0$, and (right column) $p = 1$. Shown are the first (solid curves) and second (dashed curves) moments of gluon (red) and quark-singlet (blue) GFFs. The first (second) moments extracted from the parton shower average at $\mu = 4$ TeV are shown as points (diamonds).

A-4 The same as Fig. A-3, except now for the full-tree observables with $\kappa = 2$ measured on charged particles, with (top row) $\xi = -2$ and (bottom row) $\xi = 2$.

B-1 Distribution of $\Delta(\kappa, \lambda)$ for the processes $pp \to gg$ (top) and $pp \to q\bar{q}$ (bottom), to be compared to Fig. 3-12. The full two-dimensional distributions are on the left, and slices of these distributions are shown on the right.

B-2 Feynman rules for $Hgg$, $Hggg$, and $Hgggg$ couplings in the $m_t \to \infty$ EFT, where all momenta are taken to be ingoing.
B-3 Feynman diagrams for (a,b,c) $e^+e^- \rightarrow H \rightarrow ggg$ and (d,e) $e^+e^- \rightarrow H \rightarrow gq\bar{q}$ processes. ................................................. 207

B-4 Comparison of fixed-order/resummed matching schemes for (a) gluon jets and (b) down-quark jets. ................................................................. 210

B-5 Comparison between track-assisted mass with soft-drop grooming for (a) gluon jets and (b) down-quark jets. The solid curves were computed by first grooming the jet and then restricting to charged particles. The dotted lines were computed by reclusterizing only the charged particles and then grooming. ................................................. 213
Chapter 1

Introduction

A multitude of successful comparisons between experiment and theory over almost half a century have indisputably confirmed Quantum Chromodynamics (QCD) as the correct theory of the strong nuclear force [183, 191, 202, 198, 196, 292, 197, 317, 57, 58, 54, 159, 205, 244, 78, 89, 77, 67]. Over this time, theoretical calculations of QCD processes have dramatically increased in sophistication and precision. Perturbative calculations as an expansion in powers of the coupling $\alpha_s$ have been performed to ever higher orders. Large logarithmic corrections arising from processes involving widely separated energy scales or tightly constrained corners of phase space have been computed using resummations of the perturbation series to all orders in $\alpha_s$. Effective field theories including soft-collinear effective theory [68, 70, 69] and heavy quark effective theory [157, 182, 195, 270] have enabled even more precise and systematically improvable calculations.

Despite these improvements to perturbative calculations, confinement and the transition to strong coupling embodied in the running of $\alpha_s$ makes it impossible to make physical predictions without confronting fundamentally non-perturbative problems. This is because the asymptotic states of QCD are not the same degrees of freedom appearing in the Lagrangian, but instead are color neutral bound states. Properties of these states can be calculated from first principles numerically using lattice QCD techniques, but the enormous computational complexity of the problem, especially the cost of computing integrals over the gauge-field configurations, limits
the applicability of these methods. In particular, including non-perturbative effects in scattering processes or in processes with high multiplicity final states requires a different approach. One common method is to use a phenomenological model, as implemented in parton-shower event generators. The other approach is to use factorization theorems to partition calculations into separate pieces corresponding to parts of the physical process which occur at different characteristic scales. Rates for high-scale phenomena can be calculated in perturbation theory. Low-scale, fundamentally non-perturbative effects such as hadronization can then be parametrized by functions which are extracted from fits to experimental data.

The last approach is the one followed in this work. The unifying idea of this thesis is that by defining an appropriate generalized fragmentation function (GFF) to parametrize the non-perturbative hadronization transition and absorb collinear singularities, we can calculate distributions of collinear-unsafe jet observables. In the rest of this chapter, I provide some background material and motivation. I then briefly describe the work that makes up the later chapters, and give some context for it. In Chapter 2, I provide a rigorous theoretical framework for the generalized fragmentation function (GFF) formalism. I use this framework to describe fractal observables, which were inspired by the GFF evolution equation, and explore their potential applications to the problem of quark versus gluon jet discrimination. Chapter 3 studies an observable called generalized track-assisted mass (GTAM), and employs the GFF formalism to perform analytic calculations of its distribution. In Chapter 4, I make connections to a related set of ideas, the generating functional approach (GFA), and investigate the overlap and differences between the two frameworks.

1.1 Perturbative QCD

1.1.1 Cross Sections and Factorization

We consider first the cross section for $e^+e^-$ annihilation into hadrons. This is a fully inclusive process, so at high energies its cross section can be calculated perturbatively,
with a finite result order-by-order in $\alpha_s$. This calculation has been performed [120, 150, 109, 188, 316, 118, 119] up to $N^3$LO order ($\mathcal{O}(\alpha_s^3)$), including corrections for non-zero quark masses up to fourth order ($m_f^4/Q^4$), where $Q$ is the center-of-mass energy of the collision. For massless quarks, the cross section at order $\alpha_s$ is

$$\sigma_{NLO} = \frac{4\pi\alpha^2}{3Q^2} \left( 3 \sum_f e_f^2 \right) \left[ 1 + \frac{3\alpha_s(Q)C_F}{4} + \mathcal{O}(\alpha_s(Q)^2) \right],$$

(1.1)

where the sum runs over all flavors $f$ which are kinematically possible to produce at a center-of-mass energy $Q$. This cross section has been measured to great accuracy across a wide range of energies by many experiments, with impressive agreement between theory and data. Fig. 1-1 [287] shows this comparison including data from multiple experiments.

While the accuracy of this prediction is satisfying, a fully inclusive process can only give limited insight into the physics involved. It cannot even predict the most obvious structure of the final state of a high-energy collision: jets. In order to be calculable order-by-order in perturbation theory, a cross section must be infrared and collinear (IRC) safe. A cross section to produce $m$ jets,

$$\sigma(e^+e^- \rightarrow j_1, j_2, \ldots j_m) = \sum_{N=m}^{\infty} \int_{\text{jet}} d\Phi_N |\mathcal{M}(e^+e^- \rightarrow N \text{ partons})|^2$$

(1.2)
is IRC safe provided the algorithm used to define the jet is IRC safe [311, 102, 162]. The jet algorithm defines the region of phase space included in the integral $\int_{\text{jet}}$ in Eq. (1.2). This requirement states that the addition of an infinitely soft particle or the collinear splitting of a particle does not change the number of jets found by the algorithm. Expanding to a more exclusive quantity, we can compute differential jet cross sections,

$$\frac{d\sigma}{dv}(e^+e^- \rightarrow j_1, j_2, \ldots j_m) = \sum_{N=m}^{\infty} \int_{\text{jet}} d\Phi_N |\mathcal{M}(e^+e^- \rightarrow N \text{ partons})|^2 \delta(\hat{v}\{\Phi_N\} - v).$$

(1.3)

The IRC safety requirement now applies to both the jet algorithm and to the definition of the jet observable $v$. The observable $v$ is IRC safe if arbitrarily soft or collinear emissions do not change its value. This can be expressed by requirements on the function $\hat{v}\{\Phi_N\}$, which expresses the value of the observable for an $N$-parton configuration as a function of the $N$-parton phase space $\Phi_N$. In order to define an IRC safe $\hat{v}\{\Phi_N\}$, we require that [133]

- $\hat{v}$ is a smooth function of the particle momenta $\Phi_N$,
- $\hat{v}$ is a symmetric function of $\Phi_N$,
- For massless particle momenta,

$$\hat{v}\left\{ \frac{p_1}{Q}, \frac{p_i}{Q}, \ldots, \frac{p_{n-1}}{Q}, \frac{\lambda p_i}{Q} \right\} = \hat{v}\left\{ \frac{p_1}{Q}, \frac{(1+\lambda)p_i}{Q}, \ldots, \frac{p_{n-1}}{Q} \right\}. \quad (1.4)$$

So far, we have only discussed cross sections which can be calculated fully perturbatively, up to non-perturbative power corrections which scale as $\Lambda_{QCD}/v$ (for dimensionless observables, $\Lambda_{QCD}/Qv$). The only input needed from experiment to obtain a finite, physical result for any of the calculations above are the values of physical constants (quark masses, $\alpha_s(M_Z)$, etc.). The final states involved are sufficiently inclusive to make predictions without dealing with the effects of confinement in the final state. Instead, these quantities can be calculated perturbatively to high precision, and quark/hadron duality [59, 303, 82] ensures close agreement with data.
To compute even the simplest observables at a hadron collider such as the LHC, we are forced to confront the complexities arising from confinement, since otherwise we cannot even describe the initial state of the collision. Furthermore, in order to connect a parton-level measurement to specific hadronic final states (for any process), hadron structure must also be accounted for in the final state. A differential cross section for the production of a specific (unpolarized) hadron $h$ with momentum $p$ in the final state of a hadron-hadron collision can be written in factorized form as

$$\frac{d\sigma}{d^3 p}(h_1(p_1), h_2(p_2) \rightarrow h(p) + X) = \sum_{i,j,k} \int dx_i \int dx_j f^{i/1}_i(x_i, \mu) f^{j/2}_j(x_j, \mu) \times$$

$$\times \int dz C(x_i p_1, x_j p_2, x_k p_3, x_k p_4, \frac{p}{z}, y_k, \frac{Q^2}{\mu^2}, \alpha_s(\mu))_{i,j\rightarrow k} \times D_{i,k}^{h/k}(z, \mu) + O\left(\frac{\Lambda_{QCD}}{Q}\right).$$

where $y_k$ is the rapidity of parton $k$ and $\mu$ is the renormalization scale. Corrections to this factorized form are suppressed by powers of $\Lambda_{QCD}/Q$, where $Q$ is the characteristic scale of the interaction, for example $Q = p$ or $Q = E_{cm}$ for $e^+e^-$ annihilation. Therefore this approximation will be very accurate for high-energy processes.

The parton distribution functions (PDFs) $f^{a/n}(x, \mu)$ describe the number density of partons of species $a$ inside a hadron of type $n$, carrying a fraction $x$ of hadron $n$'s momentum. Similarly, the fragmentation function (FF) $D_{i,k}^{h/k}(z, \mu)$ describes the number density of hadrons of type $h$ in the particles resulting from the fragmentation and hadronization of a parton of type $k$, with $h$ carrying a fraction $z$ of parton $k$'s original momentum. The functions $C_{i,j\rightarrow k}$ are perturbatively calculable parton-level cross sections for the scattering $i, j \rightarrow k + X$, where $X$ can be any additional final-state particles. Each piece in the factorized cross section also depends on the factorization scale $\mu_F$, which is usually set equal to the renormalization scale $\mu$, as has been done in Eq. (1.5).

1.1.2 Deep-Inelastic Scattering

We now specialize to the deep-inelastic scattering (DIS) of an electron on a proton in order to introduce the main features of the parton distribution functions. This
process is historically important for driving the development of the parton model of hadron structure [83, 85, 84, 101, 168, 192]. If the only measurement made on the final state is the momentum (direction and magnitude) of the electron, then the only hadronic state that must be accounted for is the proton in the initial state. Thus the DIS cross section contains a single PDF (for each parton flavor) and no other non-perturbative functions.

The kinematics of this process are illustrated in Fig. 1-2. Following the standard nomenclature, we write the cross section for the hard scattering of an electron on a proton as

\[ \sigma(e^-(k), P(p) \rightarrow e^-(k'), X(p_X)) = \int \frac{d^3k'}{2|k'|} \frac{1}{q^4} L^{\mu\nu}(k, q) W^{\gamma\rho}_\mu(p, q). \] (1.6)

The (spacelike) momentum transferred from the electron to the proton is \( q = k - k' \), and we define \( Q^2 = -q^2 > 0 \). We neglect possible contributions from Z exchange for simplicity of notation. The leptonic and hadronic tensors \( L^{\mu\nu} \) and \( W^{\gamma\rho}_\mu \) are defined as

\[ L^{\mu\nu} = \frac{e^2}{8\pi^2} tr[k\gamma^\mu k'\gamma^\nu], \] (1.7)

\[ W^{\gamma\rho}_\mu = \frac{1}{8\pi} \sum_{\text{spins}} \sum_X \langle P(p, \sigma)|J_\mu(0)|X \rangle \times \langle X|J_{\nu}(0)|P(p, \sigma)\rangle (2\pi)^4 \delta^4(p_X - q - p). \]
The matrix elements $\langle P|J|X \rangle$ involve hadronic bound states and therefore require non-perturbative information to calculate. Conservation of the electric current requires that $q_{\mu}W^{\mu\nu} = 0$. Using this requirement, we decompose the hadronic tensor into form factors

$$W^{\gamma P}_{\mu\nu} = -\left( g_{\mu\nu} - \frac{q_{\mu}q_{\nu}}{q^2} \right) W_1^{\gamma P}(x, q^2) + \left( p_{\mu} + \frac{q_{\mu}}{2x} \right) \left( p_{\nu} + \frac{q_{\nu}}{2x} \right) W_2^{\gamma P}(x, q^2),$$

where the kinematic variables are $x = Q^2/2p \cdot q$ and $\nu = 2p \cdot q/s$. This decomposition allows us to write the differential cross section in terms of the form factors

$$\frac{d\sigma}{d\Omega d\nu} = \frac{e^4 \cos^2(\theta/2)}{4E_e^2 \sin^2(\theta/2)} \left( 2W_1^{\gamma P} \tan^2(\theta/2) + W_2^{\gamma P} \right),$$

where $d\Omega = \sin \theta d\theta d\phi$ is the solid angle into which the electron scatters and $E_e$ is the energy of the incoming electron in the proton rest frame. Eq. (1.9) makes it clear that $W_1^{\gamma P}$ and $W_2^{\gamma P}$ are experimentally observable quantities. They have been extracted from experimental data at multiple scales and across a wide range of $x$ values, see Fig. 1-3. For $r = 1, 2$ (setting $\mu_F = \mu$), we can write them in the factorized form

$$W_r^{\gamma P}(x, Q^2) = \sum_{i=q, g} \int_x^1 dz \, C_r^{\alpha}(\frac{x}{z}, \frac{Q^2}{z^2}, \alpha_s(\mu)) \, f^{i/P}(z, \mu).$$

The process-dependent coefficient functions $C_r^{\alpha}$ have been calculated for DIS to order $\alpha_s^3$ [332, 325, 279].

### 1.1.3 Parton Distribution Functions

The non-perturbative functions $f^{i/h}$ in Eqs. (1.5) and (1.10) are the parton distribution functions (PDFs), which are used to describe hadronic initial states with partonic degrees of freedom. They can be given proper field-theoretic definitions in terms of light-cone matrix elements. Light-cone coordinates are defined by $\vec{v} = (v^+, v^-, \vec{v}_T)$, where $v^\pm = (v^0 \pm v^3)/\sqrt{2}$. These are a natural set of coordinates to describe pro-

\footnote{A third parity-violating form factor $W_{\alpha\beta}^{\nu P}$ would be required in neutrino deep-inelastic scattering.}
cesses at high-energy colliders, where the beam direction gives a natural choice for the \( \hat{z} \) coordinate. Particles which are highly boosted along the \( \hat{z} \) axis will have one of the \( \pm \) components of their momentum become very large and the other small.

Explicitly, the definition of the quark PDF inside a hadron \( h \) is [129, 130]

\[
  f_{(0)}^{q/h}(x) = \sum_{\text{colors}} \int \frac{dy^-}{2\pi} e^{ixp^+y^-} \langle h|\bar{\psi}^{(0)}_{q}(0,y^-,-\vec{0}_T)W^{(F)}(y^-,0)\frac{\gamma^+}{2}\psi^{(0)}_{q}(0)|h\rangle
\]  

(1.11)

and for a gluon PDF

\[
  f_{(0)}^{g/h}(x) = \sum_{\text{colors}} \sum_{j} \int \frac{dy^-}{2\pi x^P} e^{-ixp^+y^-} \langle h|G_{\alpha}^{(0),\alpha}(0,y^-,-\vec{0}_T)W^{(A)}(y^-,0)\gamma^\mu G^{(0),\beta}_{\mu,j}(0)|h\rangle,
\]  

(1.12)

where the \( (0) \) subscripts denote that the quark and gluon fields in these definitions are non-renormalized. The Wilson lines in Eqs. (1.11) and (1.12) are necessary to make the PDF definitions gauge invariant [130, 131]. The Wilson-line operator in
representation $R$ is defined by

$$ W^{(R)} = P \left\{ \exp \left[ -i g_0 \int_C dx \mu A^{(0)\mu}(x) T^\alpha_{(R)} \right] \right\}, \quad (1.13) $$

where $T^\alpha_{(R)}$ are the SU(3) generator matrices in the $(R)$ representation. Naturally the (anti-)quark PDF involves a Wilson line in the (anti-)fundamental representation, and the gluon PDF requires the adjoint representation.

The matrix elements with a hadronic bound state $|h\rangle$ cannot be calculated perturbatively using partonic degrees of freedom. This requires that these functions be extracted from experimental data.\(^2\) Despite requiring experimental input, the PDFs still have predictive power for two reasons: they are process independent and have a perturbative renormalization-group (RG) evolution.

Process independence means that the PDFs can be used to compute any scattering cross section involving the appropriate hadron in the initial state and the appropriate parton in the hard process. For example, the PDF for a gluon inside a proton is the same whether the proton is participating in deep-inelastic scattering (DIS), $ep$ scattering, or $pp$ scattering. In practice, these functions are computed with global fits to data from multiple experiments [63, 296, 203].

The bare quark and gluon fields in the definitions of the PDFs $f_i^{i/h}$ must be renormalized. This is most commonly done in the $\overline{\text{MS}}$ scheme, which introduces a dependence on the renormalization scale $\mu$. In order to derive the scale dependence of $f_i^{i/h}$, we transform the structure functions in Eq. (1.10) into (Mellin) moment space, where the convolutions become products,

$$ W_r^{xp}(n, Q^2) = \int_0^1 dx \frac{1}{x^{n-1}} W_r^{xp}(x, Q^2). \quad (1.14) $$

Since the structure function is a physically measurable object, it must be independent of the renormalization scale $\mu$. Of course, this still holds after transforming to moment

\(^2\)LQCD methods have been developed for computing these functions from first principles, notably the large momentum effective theory (LaMET) [221, 264, 116, 215], but these are outside the scope of this work.
space, so
\[
\mu \frac{d}{d\mu} W_{\gamma P}(n, Q^2) = \left( \mu \frac{dC_{\gamma i}^{\mu}}{d\mu} \right) f_{i/P}^{\mu}(n, \mu) + C_{\gamma i}^{\mu} \left( \mu \frac{df_{i/P}(n, \mu)}{d\mu} \right) = 0. \tag{1.15}
\]

We can reorganize and undo the transformation to moment space to rewrite this in terms of the perturbatively calculable evolution kernels \( P_{ij} \)
\[
\mu \frac{d}{d\mu} f_{i/P}(x, \mu) = \frac{\alpha_s(\mu)}{\pi} \sum_{j=q,\bar{q},g} \int_x^1 \frac{dz}{z} P_{ij}(z) f_{j/P}(\frac{x}{z}, \mu). \tag{1.16}
\]

These are the well-known DGLAP equations for PDF evolution [193, 265, 151, 49].

The splitting functions \( P_{ij}(z) \) describe the mixing of different parton PDFs by the RG evolution. They can be calculated perturbatively
\[
P_{ij}(z) = P_{ij}^{(0)}(z) + \frac{\alpha_s(\mu)}{2\pi} P_{ij}^{(1)}(z) + \left( \frac{\alpha_s(\mu)}{2\pi} \right)^2 P_{ij}^{(2)}(z) + \ldots. \tag{1.17}
\]

These splitting kernels are fully known up to the \( \mathcal{O}(\alpha_s^3) \) terms\(^3\) \( P_{ij}^{(2)} \) [177, 201, 278, 327], and partial results have been obtained at order \( \alpha_s^4 \) [145]. The lowest-order terms in the splitting functions can be written in terms of a \( 1 \rightarrow 2 \) parton splitting. Here we define this notation for later convenience and give the explicit forms of the leading-order splitting functions.

\[
P_{qq}^{(0)}(z) \equiv P_{q\rightarrow qg}(z) = C_F \left[ \frac{1 + z^2}{1 - z} + \frac{3}{2} \delta(1 - z) \right],
\]

\[
P_{qq}^{(0)}(z) \equiv P_{q\rightarrow qg}(z) = C_F \left[ \frac{1 + (1 - z)^2}{z} \right],
\]

\[
P_{gg}^{(0)}(z) \equiv P_{g\rightarrow qg}(z) = T_F \left[ z^2 + (1 - z)^2 \right],
\]

\[
P_{gg}^{(0)}(z) \equiv P_{g\rightarrow qg}(z) = 2C_A \left[ \frac{1 - z}{z} + \frac{z}{1 - z} + z(1 - z) + \left( \frac{11}{12} - \frac{n_f}{18} \right) \delta(1 - z) \right]. \tag{1.18}
\]

The QCD color factors are \( C_F = \frac{4}{3} \), \( C_A = 3 \), and \( T_F = \frac{1}{2} \), and \( n_f \) is the number

\(^3\)The order of the calculation refers to the power of \( \alpha_s \) appearing in the evolution equation, Eq. (1.16), not Eq. (1.17).
of kinematically-active quark flavors at the relevant scale. The \([+]_+\) distribution is defined by

\[
\int_0^1 dz \frac{f(z)}{[1 - z]_+} = \int_0^1 dz \frac{f(z) - f(1)}{1 - z}
\]

(1.19)

for any smooth function \(f(z)\). This \([+]_+\) function regularization incorporates the effects of virtual diagrams which cancel singularities at \(z = 1\).

The PDFs can be shown to satisfy certain sum rules which are a crucial part of their probability interpretation [130]. The first is that since PDFs represent the number density of partons inside a hadron, they should reproduce the parton-model content of that hadron. For protons, \(h = p\), and this gives

\[
\int_0^1 dx [f_{(0)}^{u/P}(x) - f_{(0)}^{\bar{u}/P}(x)] = 2,
\]

\[
\int_0^1 dx [f_{(0)}^{d/P}(x) - f_{(0)}^{\bar{d}/P}(x)] = 1,
\]

\[
\int_0^1 dx [f_{(0)}^{i/P}(x) - f_{(0)}^{\bar{i}/P}(x)] = 0, \quad i \neq u, d.
\]

There is also a sum rule for total baryon number,

\[
\sum_i \int_0^1 dx [f_{(0)}^{i/P}(x) - f_{(0)}^{\bar{i}/P}(x)] = 3,
\]

(1.21)

and a momentum sum rule

\[
\sum_i \int_0^1 dx x f_{(0)}^{i/P}(x) = 1.
\]

(1.22)

In the valence-number and baryon-number sum rules, the sum runs over only quark flavors. In the momentum sum rule, the sum runs over all quark flavors, anti-quark flavors, and gluons. These sum rules are derived from the canonical commutation relations of the parton-field operators, and so they apply to the bare PDFs \(f_{(0)}^{i/h}\). It can also be shown that the number-density interpretation and sum rules are maintained by renormalization in the \(\overline{\text{MS}}\) scheme [127]. This also leads to sum rules for the
(Mellin-moment space) splitting functions \( \bar{P}_{ij}(n, \mu) \),

\[
\bar{P}_{q_1}(1, \mu) - \bar{P}_{q_1}(1, \mu) = 0,
\]

\[
\sum_i \bar{P}_{ii}(2) = 0.
\]  

1.2 Fragmentation

Suitably inclusive cross sections can be computed to an acceptable accuracy without using non-perturbative objects to describe the final state. However, in order to predict properties of a final state which includes one or more specified hadrons, it is necessary to include information about the hadronization transition. This can be achieved by using fragmentation functions [128, 130], and their extensions to include multiple identified final-state hadrons. We will not specify the physical process for which the FFs are defined in this section, as the results apply to multiple hadronic processes, including DIS and Drell-Yan production.\(^4\)

1.2.1 Single-Hadron Fragmentation

First, we specify the necessary final-state kinematics for the fragmentation of a parton into a single identified final-state hadron \( h \). Working in a frame in which the hadron has no transverse momentum, we define the momentum \( P_h \) of hadron \( h \), the hadron spin vector \( S_h \), and the parton momentum \( k \),

\[
P_h = (P_h^+, P_h^-, \vec{0}_T) = \left( \frac{M_h^2}{2P_h^-}, P_h^-, \vec{0}_T \right),
\]

\[
S_h = (S_h^+, S_h^-, \vec{S}_hT) = \left( -\Lambda_h \frac{M_h}{2P_h^-}, \Lambda_h \frac{P_h^-}{M_h}, \vec{S}_hT \right),
\]

\[
k = (k^+, k^-, \vec{k}_T) = \left( z \frac{k^2 + \vec{k}_T^2}{2P_h^-}, \frac{P_h^-}{z}, \vec{k}_T \right),
\]

\(^4\)An example of a process which violates factorization is the production of back-to-back hadrons at small \( \Delta p_T \) in the process \( h_1 h_2 \rightarrow h_3 h_4 + X \).
where the longitudinal and transverse components of the hadron spin are described by $\Lambda_h$ and $\vec{S}_{hT}$ respectively.

In order to give a field-theoretic definition of FFs analogous to Eqs. (1.11) and (1.12), we define the light-cone fragmentation correlator for a quark $q$ into a spin-0 hadron $h$ to be

\[
\Delta^{h/q}(z, P_h, S_h) = \sum_X \frac{\text{Tr}_{\text{color}}}{3} \int \frac{dy^+}{2\pi} e^{ik^-y^+} \langle 0 | W_1(\infty^+, y^+) \psi_q(y^+, 0^-, \vec{0}_T) | P_h, S_h, X \rangle \times \langle P_h, S_h, X | \psi_q(0^+, 0^-, \vec{0}_T) W_2(0^+, \infty^+) | 0 \rangle ,
\]

(1.25)

where the sum over a complete inclusive set of states for the other particles in the final state is

\[
\sum_X \equiv \sum_X \int \frac{d^3 \vec{P}_X}{(2\pi)^3 2P_X^0} .
\]

(1.26)

The generalization for a spin-$\frac{1}{2}$ hadron only requires multiplying by a factor of two to include the sum over hadron spins. Fragmentation into spin-1 hadrons has also been studied extensively [220, 60, 117]. The correlator $\Delta^{h/q}(z, P_h, S_h)$ is a matrix in Dirac space and depends on the hadron momentum, spin, and longitudinal momentum fraction. As for the PDFs, the Wilson lines required for gauge invariance are defined by Eq. (1.13).

Quark FFs can now be defined by taking traces of $\Delta^{h/q}$ with different Dirac matrices. The FF $D_1^{h/q}(z)$ represents the number density of an unpolarized hadron $h$ inside the unpolarized quark $q$ with momentum fraction $z$. The FFs $G_1^{h/q}$ and $H_1^{h/q}$ are the corresponding number densities for a longitudinally polarized $h$ inside a longitudinally polarized $q$, and a transversely polarized $h$ inside a transversely polarized
respectively. These FFs are defined by the traces\(^5\)

\[
D_1^{h/q} = \frac{z}{4} \text{Tr} [\Delta^{h/q}(z, P_h, S_h)\gamma^-], \tag{1.27}
\]

\[
\Lambda_h G_1^{h/q} = \frac{z}{4} \text{Tr} [\Delta^{h/q}(z, P_h, S_h)\gamma^-\gamma_5], \tag{1.28}
\]

\[
S_{hT}^i H_1^{h/q} = \frac{z}{4} \text{Tr} [\Delta^{h/q}(z, P_h, S_h)i\sigma^i\gamma_5]. \tag{1.29}
\]

The three traces in Eqs. (1.27), (1.28), and (1.29) define the leading-twist (twist-2) quark FFs. The twist of an operator is \(t = d - s\), where \(d\) is the operator dimension and \(s\) the operator spin. Taking the trace of Eq. (1.25) with the remaining thirteen independent Dirac structures give twist-3 and twist-4 FFs. FFs with twist \(n - 2\) are suppressed by a factor of \((M_h/P_h)^{n-2}\) compared to the leading twist (twist-2) operators and therefore have a much smaller impact on high-scale physical observables. A full classification of higher-twist FFs also requires fragmentation correlators with more than two parton fields in addition to Eq. (1.25) [227, 243, 156, 331, 230, 274, 226]. In fact, the twist-3 FFs defined above in terms of two-parton correlators can be redefined using only three-parton correlators [61, 62, 227]. Anti-quark FFs [285, 87, 289] and gluon FFs [130, 284, 127] are defined analogously through the appropriate fragmentation correlators. The Wilson lines in the gluon FFs are defined in the adjoint representation, just like for the gluon PDFs.

The partonic fragmentation functions evolve according to

\[
\frac{d}{d\mu} D_i^{h'}(z, \mu) = \frac{\alpha_s(\mu)}{\pi} \sum_j \int_z^1 \frac{du}{u} P_{ji}(u) D_1^{h/j}\left(\frac{z}{u}, \mu\right). \tag{1.30}
\]

Eq. (1.30) has the same form as Eq. (1.16), the DGLAP equation for PDF evolution, with the replacement \(P_{ji} \to P_{ij}\). The evolution scale in Eq. (1.16) is a space-like momentum scale. The scale in Eq. (1.30) by contrast is time-like, so the splitting functions \(P_{ji}\) appearing in the evolution of parton fragmentation functions are called the time-like splitting functions, and the corresponding initial-state splitting functions are

---

\(^5\)The FFs are defined by the \(\gamma^-\) matrices as opposed to the \(\gamma^+\) matrices in these equations because the frame is chosen such that \(P_h^-\) is the large momentum component instead of \(P_h^+\) as in Eqs. (1.11) and (1.12).
the space-like splitting functions. The space-like and time-like splitting functions are the same at leading order only [193, 194]. The splitting functions for the unpolarized FFs $D^{i/h}$ have been fully calculated at $\alpha_s^2$ [177, 135, 173, 225, 224, 199], and the calculations have nearly been completed at $\alpha_s^3$ [277, 276, 280, 44, 187, 186]. The polarized FFs $G_1^{h/i}$ and $H_1^{h/i}$ have evolution equations with the same structure as Eq. (1.30), but with different evolution kernels $P_{ji}$. These evolution kernels are known to NLO for $G_1^{h/i}$ [313]. For $H_1^{h/i}$ they are known only at leading order, but can in theory be obtained from the space-like splitting functions by analytic continuation [326, 86].

Sum rules analogous to Eqs. (1.20), (1.21), and (1.22) exist for FFs, with the summation over hadrons instead of partons. For example, the momentum sum rule is

$$\sum_{h} \sum_{s_h} \int_0^1 dz \, z \, D_1^{h/q}(z) = 1.$$  \hspace{1cm} (1.31)

### 1.2.2 Dihadron Fragmentation

So far we have discussed fragmentation involving a single identified final-state hadron. This analysis can be extended to final states in which multiple hadrons are identified. In practice, the number of hadrons which can be identified is severely limited by experimental statistics. For this reason, fragmentation studies are usually limited to two identified hadrons, the so called dihadron fragmentation functions (DiFFs).

We denote the momenta and masses of the two identified hadrons as $P_{1,2}$ and $M_{1,2}$, and the invariant mass of the pair $M_h^2 = (P_1 + P_2)^2$. The total and relative hadron momenta are $P_h = P_1 + P_2$ and $R = \frac{1}{2}(P_1 - P_2)$ respectively. With this notation, we can parametrize the hadron momenta with the single parameter $z$,

$$P_1 = \left( \frac{M_1^2 + \vec{R}_T^2}{(1 + z)P_h^-}, \frac{1 + z}{2}P_h^-, \vec{R}_T \right),$$

$$P_2 = \left( \frac{M_2^2 + \vec{R}_T^2}{(1 - z)P_h^-}, \frac{1 - z}{2}P_h^-, -\vec{R}_T \right).$$

We can then define a quark dihadron fragmentation correlator $\Delta^{h_1 h_2/q}(z, P_1, P_2)$. We only consider the case of unpolarized hadrons, since a full classification of DiFFs
including hadron polarization is still incomplete [275]. This correlator has exactly the same form as Eq. (1.25) except that the asymptotic out-states are replaced by states with two identified hadrons, \(|P, X\rangle \rightarrow |P_1, P_2, X\rangle\). The additional final-state hadron leads to a much larger number of DiFFs than single-hadron FFs. Without considering hadron polarization (or quark transverse momentum), there are two DiFFs, 

\[ D_{1}^{h_1 h_2/q}(z_1, z_2, M_h^2) \text{ and } H_{1}^{c h_1 h_2/q}(z_1, z_2, M_h^2), \]

\[ D_{1}^{h_1 h_2/q}(z_1, z_2, M_h^2) = \frac{z}{4} \int d^2 \vec{k}_T \text{Tr} \left[ \Delta_{h_1 h_2/q}(z, \vec{k}_T, P_1, P_2) \gamma^- \right], \]

\[- \frac{\epsilon_{ij} P_{ij}^T}{M_1 + M_2} H_{1}^{c h_1 h_2/q}(z_1, z_2, M_h^2) = \frac{z}{4} \int d^2 \vec{k}_T \text{Tr} \left[ \Delta_{h_1 h_2/q}(z, \vec{k}_T, P_1, P_2) i \sigma^i \gamma_5 \right]. \]

(1.33)

After integrating out the relative transverse momentum \(R_T\) of the two hadrons, only the function \(D_{1}^{h_1 h_2/q}\) is non-zero.

Evolution equations were derived for the DiFFs \(D_{1}^{h_1 h_2/q}(z_1, z_2)\) by Refs. [247, 315, 148]. For parton \(i\) these equations are

\[ \mu \frac{d}{d\mu} D_{1}^{h_1 h_2/i}(z_1, z_2, \mu^2) = \frac{\alpha_s(\mu^2)}{\pi} \left[ \sum_j \int_{z_1}^{1} \frac{du}{u^2} P_{ji}(u) D_{1}^{h_1 h_2/j} \left( \frac{z_1}{u}, \frac{z_2}{u}, \mu^2 \right) \right. \]

\[ \left. + \sum_{jk} \int_{z_1}^{1-z_2} \frac{du}{u(1-u)} \hat{P}_{ji}(u) D_{1}^{h_1/j} \left( \frac{z_1}{u}, \mu^2 \right) D_{1}^{h_2/j} \left( \frac{z_2}{1-u}, \mu^2 \right) \right]. \]

(1.34)

The functions \(\hat{P}_{ji}\) are from splittings \(i \rightarrow jk\) where both \(j\) and \(k\) are real. The identification of multiple hadrons in the final state leads to strikingly different evolution compared to single-hadron FFs. Eq. (1.34) includes a non-linear, non-homogenous term mixing with single-hadron FFs. This structure is necessary to include both the case where parton \(i\) hadronizes into both \(h_1\) and \(h_2\) and the case where parton \(i\) first splits into partons \(j\) and \(k\) which subsequently hadronize into \(h_1\) and \(h_2\). We will return to this point when we discuss the evolution of generalized fragmentation functions and fractal observables in Sec. 1.4 and Chapter 2. Evolution equations for the DiFF \(H_{1}^{c h_1 h_2/q}\) have also been considered by Ref. [108], and contain only the homogeneous term.
1.3 Jets at the LHC

In Sec. 1.1, we described the basic setup of an analytic calculation for a jet observable at a hadron collider. Jets are inescapable at the LHC, since even leptonic observables are produced in association with jets. In addition to calculating total and differential jet cross sections, there are two broad sets of procedures associated with jets: tagging, i.e. identifying jets arising from the decay or fragmentation of a specific particle, and grooming to remove radiation that is not a result of the primary hard process which produced the jet. I give some brief background on these procedures in this section. This is by no means a complete review of jet tagging and grooming methods. Recent comprehensive reviews include Refs. [299, 42, 50, 51, 43, 95, 255, 56].

1.3.1 Tagging

Heavy particles which decay to quarks and gluons, the Higgs, $W^\pm$ and $Z_0$ bosons, and top quarks, can be distinguished by the distinctive topologies of their decay products and possibly by tagging the flavor of the jets or subjets resulting from their decay. There is an extensive literature devoted to this subject, see e.g. Ref. [56] for a recent review. These tagging procedures all require information about the angular distribution of the momenta of the jet constituents. For jets resulting from highly boosted heavy particles, these jet constituents become highly collimated. Particles resulting from a two-body decay of a boosted particle with $p_T > 1$ TeV will be so collimated that hadronic calorimeters cannot distinguish them. This has led to an interest in using charged-particle tracking information to replace angular information from calorimeters in order to improve angular resolution. We will return to this point in Sec. 1.4 with a discussion of track-assisted mass and its generalization.

Distinguishing between jets produced by energetic fragmenting quarks and gluons is an important application of jet-substructure techniques. For two recent in depth studies see Refs. [179, 189]. The primary difference between the two is the associated color factor, $C_A = 3$ for gluons and $C_F = \frac{4}{3}$ for quarks. The probability of a quark or gluon radiating a collinear gluon is proportional to this color factor. Thus
the larger color factor for gluons means that a gluon will produce more collinear radiation [49]. For this reason, the most powerful single discriminant variable is the particle multiplicity of a jet [176]. Most other jet-substructure observables exhibit Casimir scaling at leading-logarithmic order [259, 261], which leads to a ROC curve with a gluon mistag rate of $x^{CA/CF}$, where $x$ is the quark-jet efficiency. This is the approximate practical limit for the quark vs. gluon discrimination power of these observables. Improved discrimination power is possible using a combination of jet-substructure observables. Recently, the effect of using lower-level information about the jet, such as the full momentum four-vector data of all jet components, to train machine learning algorithms has become a quickly growing topic of interest [255]. In practice, the combination of particle multiplicity or a related observable with an observable which exhibits Casimir scaling is enough to produce a nearly optimal quark vs. gluon tagger [245].

The ATLAS [34, 12, 26, 27] and CMS [24, 3, 14, 25] experiments each use quark vs. gluon tagging algorithms based on maximum-likelihood methods. The primary quark vs. gluon tagger for ATLAS uses the number of charged-particle tracks $n_{\text{track}}$ as its multiplicity variable and the jet width as its Casimir-scaling variable [27]. Likewise, CMS uses the combination of the number of particle flow constituents $n_{\text{const}}$, the jet minor-angle opening ($\sigma_2$) in the $\eta - \phi$ plane, and the jet $p_T^D = (\sum (E_i/E_\text{jet})^2)^{1/2}$ as inputs to its tagging algorithm [24].

1.3.2 Grooming

Jets are the experimental signature of both energetic partons and decaying heavy particles. Theoretical calculations can make many clean predictions about their properties and structure. Radiation from unassociated sources degrades the measured precision of jet spectra and complicates the classification of their source. Jet grooming techniques attempt to remove this unassociated radiation from a jet to maintain the resolution of jet measurements [320, 231, 290, 259, 256, 281, 166, 169, 140, 139, 261, 142, 301, 263, 252, 219, 123, 121, 214, 250, 328, 257, 295, 80, 81, 258, 144, 175, 174, 228, 211, 272].
Figure 1-4: (a) Quark/gluon discrimination ROC curves for the CMS tagger, showing the effect of the individual observables as well as the combined discrimination power. Taken from Ref. [24]. (b) Similar ROC curves for the ATLAS tagger, as well as a ROC curve for a tagger based on a convolutional neural network taking low-level jet data as its inputs. Taken from Ref. [27].

At current luminosities at the LHC, a single bunch crossing can result in $n_{pu} \sim 20 - 30$ pp collisions. In the upcoming high luminosity run, this will increase to $n_{pu} \sim 100 - 200$ [40]. A single jet in such an environment can include radiation from many of these collisions, in addition to radiation from the parton forming the hard core of the jet. This pileup contamination is uncorrelated with emissions from the initiating parton, and is distributed roughly uniformly throughout the jet. Additional contamination that is correlated with emissions within the jet can come from the underlying event (UE). At the LHC, the underlying event is not the collision of hard elementary particles but of the remnants of two protons. Radiation from partons in the protons besides the pair involved in the hard interaction can be included in the jet. This introduces unwanted correlations with the initial state of the protons and obscures the interpretation of the jet as a proxy for an elementary particle resulting from a hard interaction. The combination of these sources of noise makes jet grooming an essential tool for making precise experimental measurements and conducting searches for weak signals [114, 33, 237, 112, 4, 38, 35, 8, 37, 39, 22, 11, 12, 13, 17, 28, 172, 288, 2, 113, 5, 6, 238, 239, 36, 31, 30, 29, 19, 9, 10, 16, 18, 240, 21, 20, 15].
Early widely used grooming techniques include filtering [94], trimming [251], and pruning [164]. Filtering takes a wide-angle Cambridge/Aachen (C/A) jet [153, 330] and reclusters its constituents into a C/A tree with the smaller radius $R_{\text{filter}}$. Then the three hardest subjets are kept and recombined to form the groomed jet.

Like filtering, trimming reclusters the jet constituents with a clustering algorithm using a smaller radius $R_{\text{sub}}$. It does not require the use of a particular clustering algorithm, either to define the jet or to recluster it, nor that these algorithms be the same. The subjets of radius $R_{\text{sub}}$ are then kept if they pass the softness criteria $p_{T,jet} > f_{\text{cut}} A_{\text{hard}}$, where $f_{\text{cut}}$ is a dimensionless parameter of the algorithm and $A_{\text{hard}}$ is a hard scale related to the scattering process.

Pruning operates on a jet defined using any jet algorithm. It then reclusters the jet constituents using a recursive algorithm that models the QCD parton shower (mostly the C/A or $k_T$ [103, 162] algorithms). For each step of the reclustering, the algorithm vetos the merger and instead discards the softer subjet if either

$$z = \frac{\min(p_{T,1}, p_{T,2})}{p_{T,1} + p_{T,2}} < z_{\text{cut}}, \quad \Delta R_{ij} > D_{\text{cut}},$$

(1.35)

where $z_{\text{cut}}$ and $D_{\text{cut}}$ are parameters of the algorithm and $\Delta R_{ij}$ is the rapidity-azimuth separation of the two particles (angular separation for $e^+e^-$ collisions).

The modified mass-drop tagger (mMDT) [140] and its generalization to soft-drop grooming [254] draw inspiration from the structure of the QCD parton shower to remove radiation that does not match the soft-collinear singularity structure of QCD. The soft-drop algorithm is as follows:

1. Recluster all jet constituents into a Cambridge/Aachen tree.

2. Starting at the first (widest-angle) splitting, recursively apply the soft-drop condition

$$\frac{\min(p_{T,1}, p_{T,2})}{p_{T,1} + p_{T,2}} > z_{\text{cut}} \left( \frac{\Delta R_{12}}{R_0} \right)^{\beta}.$$  

(1.36)

3. If a splitting fails the soft-drop condition, the softer of the two branches is removed from the jet and the algorithm returns to step 1.
Figure 1-5: Comparison of energy correlation function $C_1^{(a=2)}$ distributions from PYTHIA 8 and analytic calculations, computed for soft-drop groomed jets with various values of the grooming parameter $\beta$. Taken from Ref. [254].

4. When a splitting passes Eq. (4.1), the grooming procedure stops.

In Eq. (1.36), $R_0$ is the radius parameter with which the original jet was defined. The parameters $z_{cut}$ and $\beta$ determine the degree of grooming applied. The modified mass-drop groomer is the same as soft-drop grooming with $\beta = 0$.

In general, the phase-space restrictions imposed by grooming techniques can be difficult to incorporate into analytic calculations. Soft-drop (or mMDT) grooming, on the other hand, substantially simplifies calculations. This is because the recursive declustering procedure is designed to mimic the showering process through which a parton fragments and accumulates the radiation forming a jet. This leads to a very simple phase-space restriction. For a two-parton splitting in the collinear limit, we can write the cross section in the form

$$
\sigma(i \to jk) \sim \frac{\alpha_s}{\pi} \int dz \, P_{i\to jk}(z) \int \frac{d\theta}{\theta} \Theta \left( z - z_{cut} \left( \frac{\theta}{R} \right)^\beta \right).
$$

In a resummed calculation, this structure exponentiates, and the soft-drop phase-space restriction becomes part of the radiator function.

For global event shapes such as thrust or sphericity, radiation in any region of phase space contributes to the observable value. By contrast, for jet-substructure
observables, partons outside of the jet can emit radiation into the jet, as illustrated in Fig. 1-6 from Ref. [137]. The most prominent effects of this non-global radiation are non-global logarithms (NGLs). These were first pointed out for the case of light hemisphere jet mass $m_L$ by Ref. [137], who calculated the leading NGL for $e^+e^-$-collisions at a center-of-mass energy $Q$ to be

$$S_2 = -C_F C_A \frac{\pi^2}{3} \left( \frac{\alpha_s}{2\pi} \log \frac{Q^2}{m_L^2} \right)^2. \quad (1.38)$$

The authors of Ref. [64] developed an evolution equation describing the leading-logarithmic order behavior of NGLs at leading order in the number of colors $N_C$. Substantial progress [143, 55, 329, 297, 65, 235, 209, 210, 234, 236, 204, 242, 200] has been made towards understanding NGLs by exploiting this BMS evolution equation and its extensions. Approaches based on SCET have also been developed for this problem [71, 72, 73, 74]. Despite this progress, an all-orders calculation of NGLs which includes subleading effects in $N_C$ remains an open area of research.

Initial theoretical studies of the mass of groomed jets [140, 139] investigated the effect of grooming on NGLs. Non-global radiation is soft and non-collinear with the jet direction, and therefore it was expected that grooming would be effective at removing it from the jet. The filtering, trimming, and pruning algorithms were found to only partially remove NGLs from jet-mass distributions. This problem spurred the development of the mMDT groomer. It has been shown [140, 254, 174], that the
soft-drop and mMDT grooming procedures remove NGLs at all orders in perturbation theory. This is a major theoretical simplification, which enables complete calculations at next-to-leading logarithmic order without directly calculating the effects of NGLs.

1.4 Overview

In this thesis, I develop the formalism of generalized fragmentation functions (GFFs). I describe their perturbative renormalization-group evolution in terms of a non-linear, DGLAP-like evolution equation, and demonstrate this evolution for a class of observables known as the weighted energy fractions. Motivated by the structure of this equation, I construct a group of non-associative observables called "fractal observables". I apply the GFF formalism to carry out resummed and fixed-order calculations of generalized track-assisted mass (GTAM), and explore the use of this observable as a substitute for ordinary jet mass. Finally, I develop the connection between GFFs and the generating functional approach (GFA).

Standard fragmentation function methods can be used to describe final states with a fixed, and small, number of identified hadrons. In many cases, it is desirable to make measurements using a subset of the particles in a jet labeled by some quantum number such as charge without having to specify the multiplicity of that subset. It is easy to see that such a procedure cannot be collinear safe. The cross section for a gluon splitting into a quark-antiquark pair (or a photon splitting into an $e^+e^-$ pair) changes the number of charged particles and the total momentum carried by charged particles. In order to compute such an observable, which is collinear unsafe at partonic level, a cutoff is required at some small scale. Physically, this cutoff will arise from non-perturbative effects when $\alpha_s$ becomes large. Thus a non-perturbative object like a fragmentation function can be used to render such a measurement well-defined.

In Chapter 2, which is based on Ref. [158], I develop the framework of generalized fragmentation functions (GFFs), which enable this kind of calculation. GFFs describe the distribution of a (soft-safe) quantity among some subset $S$ of the particles in a jet. $S$ can be chosen based on some non-kinematic quantum number (i.e. charge or flavor
but not momentum. Like PDFs and ordinary fragmentation functions, GFFs are non-perturbative objects which must be fit to experimental data. They also have a field-theoretic operator definition, which will be explained in more detail in Chapter 2:

\[
\mathcal{F}_i(x, \mu) = \int dy^+ d^2 y_L e^{i p^- y^+/2} \frac{1}{2N_c} \sum_{S_X} \delta[x - \hat{x}(p^-, S)] \\
\times \text{Tr} \left[ \frac{\gamma^+}{2} \langle 0 | \bar{\psi}_i(y^+, 0, y_L) | S_X \rangle \langle S_X | \bar{\psi}_i(0) | 0 \rangle \right],
\]

(1.39)

\[
\mathcal{F}_g(x, \mu) = -\frac{1}{(d-2)(N_C^2 - 1)p^-} \int dy^+ d^2 y_L e^{i p^- y^+/2} \sum_{S_X} \delta[x - \hat{x}(p^-, S)] \\
\times \langle 0 | G_{-\alpha}^- (y^+, 0, y_L) | S_X \rangle \langle S_X | G_{-\alpha;\lambda}(0) | 0 \rangle.
\]

(1.40)

The Wilson lines required for gauge invariance are suppressed here. Treating the matrix elements \( \langle 0 | \mathcal{O} | S_X \rangle \) partonically, that is replacing the (hadronic) state \( | S_X \rangle \) with a state containing some definite number of quarks, anti-quarks, and gluons, we can calculate Eqs. (1.39) and (1.40) perturbatively. Starting at NLO, this produces phase-space integrals containing both UV and IR singularities. After renormalizing the UV divergences, we are left with an IR-divergent quantity. Explicitly, for a quark GFF this order-\( \alpha_s \) expression is \[110\]

\[
\mathcal{F}^{(1)}_{i, \text{bare}}(x) = \frac{1}{2} \sum_{j,k} \int dz \left[ \frac{\alpha_s(\mu)}{2\pi} \left( \frac{1}{\epsilon_{\text{UV}}} - \frac{1}{\epsilon_{\text{IR}}} \right) P_{i \rightarrow jk}(z) \right] \\
\times \int dx_1 dx_2 \mathcal{F}^{(0)}_j(x_1, \mu) \mathcal{F}^{(0)}_k(x_2, \mu) \\
\times \delta[x - \hat{x}(z, x_1, x_2)],
\]

(1.41)

where the function \( \hat{x}(z, x_1, x_2) \) is the two-parton form of the observable \( x \). The dependence of the GFF on non-perturbative information remains in Eq. (1.41) in the requirement that the leading order GFFs \( \mathcal{F}^{(0)} \) be extracted from data. These IR divergences in Eq. (1.41) are exactly the same as the ones appearing in the NLO parton-level cross section. When we calculate a cross section using a GFF to absorb
collinear divergences, we perform at each order in $\alpha_s$ a matching procedure to cancel these IR singularities. This procedure is an analogue for the equivalent calculation using PDFs or fragmentation functions.

The RG-scale evolution for general GFFs can described by a set of complicated non-linear integro-differential equations that is a generalization of Eq. (1.34). For the most general case, this equation can also mix operators involving different numbers of partons. Schematically, this leading-order evolution can be written as

$$
\mu \frac{d}{d\mu} \mathcal{F}_i(x) = \frac{\alpha_s}{\pi} P_{i\rightarrow jk} \otimes [\mathcal{F}_j(x_1) \otimes \mathcal{F}_k(x_2) + \mathcal{F}_{jk}(x_1, x_2)].
$$

(1.42)

In Chapter 2, we define a specific class of observables called fractal observables whose corresponding GFFs have evolution equations which satisfy a specific, non-linear form of the DGLAP equations for normal fragmentation functions,

$$
\mu \frac{d}{d\mu} \mathcal{F}_i(x, \mu) = \frac{1}{2} \sum_{j,k} \int dz \, dx_1 \, dx_2 \frac{\alpha_s(\mu)}{\pi} P_{i\rightarrow jk}(z) \mathcal{F}_j(x_1, \mu) \mathcal{F}_k(x_2, \mu) \delta[x - \hat{x}(z, x_1, x_2)].
$$

(1.43)

These equations have a self-similar structure (hence the name fractal observables), since only GFFs involving single partons appear on the right side. There is no dependence on multi-parton objects as in Eqs. (1.34) and (1.42). The recursion function $\hat{x}(z, x_1, x_2)$ which defines this equation will be derived below in Chapter 2 for a variety of observables.

Weighted energy fractions (WEFs) are a group of fractal observables defined by [261]

$$
x = \sum_{i \in \text{jet}} w_i z_i^\kappa,
$$

(1.44)

where $z_i = E_i / E_{\text{jet}}$ is the energy fraction of particle $i$, $\kappa$ is a parameter that must be greater than zero for soft safety, and $w_i$ is a weight factor assigned to that particle based on its non-kinematic quantum numbers. For example, the observable\footnote{CMS defined $p_T^D$ as the square root of this quantity.} $p_T^D$ [125] is defined by the weights $w_i = 1$ and $\kappa = 2$, and weighted jet charge [170, 250, 328, 38]
Figure 1-7: (a) CMS measurement of the distribution of $p_T^D$ in $Z+$jet events, and (b) ATLAS measurement of the first moment of the weighted jet charge distribution with parameters $\kappa = 0.3, 0.5,$ and $0.7$ on up-type and down-type jets. Taken from (a) Ref. [125] and (b) Ref. [38].

with exponent $\kappa$ is defined by setting $w_i = Q_i$, the electric charge of particle $i$. The GFFs corresponding to WEFs satisfy Eq. (1.43), with the recursion function

$$\tilde{x}(z, x_1, x_2) = z^\kappa x_1 + (1 - z)^\kappa x_2.$$  \hspace{1cm} (1.45)

These observables are of experimental and phenomenological as well as theoretical interest. The CMS measurement of the $p_T^D$ distribution in $Z+$jet events is shown in Fig. 1-7a [125]. The ATLAS measurement of the first moment of the weighted jet charge distribution with weights $\kappa = 0.3, 0.5,$ and $0.7$ for up-type and down-type jets is shown in Fig. 1-7b [38].

I developed a clustering-tree-based method for constructing fractal observables, which imitates the parton-shower structure of the RG evolution. The weighted energy fractions defined above can be constructed with this procedure, using their recursion function $\tilde{x}(z, x_1, x_2)$. Similarly, other fractal observables can be constructed using recursion functions which are non-associative, that is their value under composition depends on the clustering order. The distribution of these observables then depends
Figure 1-8: Gluon GFFs for (a) the node-product observables with \( w_a = 0 \) and \( \kappa = 4 \) and (b) the full-tree fractal observable defined with \( \kappa = 2 \) and \( \xi = 2 \) on only charged particles. These are extracted from \textsc{Vincia} at \( \mu = 100 \) GeV. The tree dependence of these observables is parametrized by the generalized-\( k_t \) exponent, with \( p = -1 \) (anti-\( k_t \), red dashed), \( p = 0 \) (C/A, green), and \( p = 1 \) (\( k_t \), blue dotted).

As an application of this new type of observable, I performed a quark vs. gluon discrimination study, and found that certain non-associative observables have substantial discrimination power.

For experimental reasons, it is particularly desirable to measure a jet substructure observable using only the momenta of charged particles, for which information from the tracking detector is available. The fundamental jet-substructure observable is the jet mass, which is critical for classifying jets from decaying heavy particles and searching for new resonances. The ATLAS collaboration [126] defined track-assisted
mass
\[ M_{TA} = M_{\text{track}} \left( \frac{PT_{\text{calo}}}{PT_{\text{track}}} \right), \] (1.47)

where the track mass \( M_{\text{track}} \) is the jet mass measured using only the charged particles in the jet and the reweighting factor on the right involves only \( PT_{\text{track}} \), the total transverse momentum carried by charged particles in the jet, and \( PT_{\text{calo}} \), the total transverse momentum of all particles in the jet. I defined the generalized track-assisted mass (GTAM) as a further refinement of this:

\[ M_{TA}^{(\kappa, \lambda)} = M_{\text{track}} \left( \frac{PT_{\text{calo}}}{PT_{\text{track}}} \right)^\kappa \left( \frac{PT_{\text{calo}}}{PT_{\text{track}}} \right)^\lambda. \] (1.48)

The reweighting factors on the right side involve only the total and charged transverse momentum carried by the jet, and carried by an average jet in some appropriately defined ensemble. In Chapter 3, I use parton-shower event generators to study GTAM in \( pp \rightarrow \text{dijet} \) events, and optimize the parameters \( \kappa \) and \( \lambda \) to produce an observable to substitute for jet mass. To quantify the similarity between the \( M_{TA}^{(\kappa, \lambda)} \) and \( M_{\text{calo}} \) distributions, I used the statistic

\[ \Delta(p, q) = \sum_{i \in \text{bins}} \frac{(p_i - q_i)^2}{2(p_i + q_i)}, \] (1.49)

where \( p_i \) and \( q_i \) are the probability mass of distribution \( p \) and \( q \) in bin \( i \). For convenience, we also defined the shorthand notation

\[ \Delta(\kappa, \lambda) \equiv \Delta(M_{TA}^{(\kappa, \lambda)}, M_{\text{calo}}). \] (1.50)

This statistic is shown in Fig. 3-5 over the two-dimensional GTAM parameter space. I found that parameters around \( \kappa = \lambda = \frac{1}{2} \) gave the closest agreement between GTAM and jet mass.

Using the GFF formalism, this observable was calculated to next-to-leading logarithmic order for quark and gluon jets, excluding the effects of non-global logarithms. These resummed distributions were matched to leading-order calculations and con-
volved with a non-perturbative shape function to produce a comparison with parton showers. Specifically, I examined the rescaled, squared jet mass

\[ \rho_{\text{calo}} = \frac{M_{\text{calo}}^2}{E_{\text{jet}}^2 R^2}, \quad \rho_{\text{TA}}^{(\kappa, \lambda)} = \left( \frac{M_{\text{TA}}^{(\kappa, \lambda)}}{E_{\text{jet}}^2 R^2} \right)^2. \]  

(1.51)

Excluding the effects of non-global logarithms, the cumulative distribution of the observable \( \rho_{\text{TA}} \equiv \rho_{\text{TA}}^{(1,0)} \) can be written as

\[ \Sigma_{\text{TA}}(\rho) = \int_0^1 dx_j T_j(x_j) \frac{e^{-\gamma E_{\text{TA}}(\rho, x_j)}}{\Gamma(1 + R_{\text{TA}}(\rho, x_j))} e^{-R_{\text{TA}}(\rho, x_j)} , \]

(1.52)

where the radiator is

\[ R_{\text{TA}}(\rho, x_j) = \int_0^1 dx_k T_g(x_k, \mu) \int_0^1 dz \int_0^R \frac{d\theta}{\theta} \frac{\alpha_s(E_{\text{jet}} z \theta^2)}{\pi} P_i(z) \Theta \left( \frac{x_j z \theta^2}{x_j R^2 - \rho} \right), \]

(1.53)

and \( R'_{\text{TA}} = -dR_{\text{TA}}/d\ln \rho \). The convolutions with the quark and gluon track functions \( T_q \) and \( T_g \) are required to make the overall cross section a collinear-safe quantity.

Due to the importance of grooming procedures that was emphasized in Sec. 1.3.2, theoretical calculations of groomed observables are required for accurate comparisons.
Figure 1-10: GTAM distributions for (a) gluon jets and (b) down-quark jets in $e^+e^-$ collisions. The benchmark observable $M^{(0.5,0.5)}_{TA}$ is a very close match to the calorimeter jet mass.

To experimental data. For this reason, I also performed this NLL+LO calculation with the inclusion of soft-drop grooming. As described in Sec. 1.3.2, these groomed distributions receive no contributions from non-global logarithms, so this calculation is complete to NLL order.

An alternative to incorporating non-perturbative information through an experimentally measured fragmentation function or GFF is to push perturbative calculations to their non-perturbative limit. In the limit that a jet’s radius goes to zero it will contain only a single hadron. By not specifying the hadronic final state of this jet, the calculation can be performed using partonic degrees of freedom. This approach leads to a perturbation series involving large logarithms of the jet radius, $\log(\frac{1}{R})$. In order to avoid spoiling the perturbative expansion, these must then be resummed, which can be accomplished using the generating functional approach (GFA) [138]. In Chapter 4, I make a formal comparison between the GFF and GFA frameworks. I begin with a discussion of differences in the applicability of the two formalisms, which include different information and can be used to describe distinct but overlapping sets
of quantities. Then I compare the evolution equations for the two frameworks, both of which are non-linear DGLAP-like equations. Finally, explicit calculations of observables which can be described by both approaches show the equivalence of GFFs and the GFA in these cases.
Chapter 2

Generalized Fragmentation Functions and Fractal Observables

We introduce a broad class of fractal jet observables that recursively probe the collective properties of hadrons produced in jet fragmentation. To describe these collinear-unsafe observables, we generalize the formalism of fragmentation functions, which are important objects in QCD for calculating cross sections involving identified final-state hadrons. Fragmentation functions are fundamentally nonperturbative, but have a calculable renormalization group evolution. Unlike ordinary fragmentation functions, generalized fragmentation functions exhibit nonlinear evolution, since fractal observables involve correlated subsets of hadrons within a jet. Some special cases of generalized fragmentation functions are reviewed, including jet charge and track functions. We then consider fractal jet observables that are based on hierarchical clustering trees, where the nonlinear evolution equations also exhibit tree-like structure at leading order. We develop a numeric code for performing this evolution and study its phenomenological implications. As an application, we present examples of fractal jet observables that are useful in discriminating quark jets from gluon jets.
2.1 Introduction

Fragmentation functions (FFs) have a long history in QCD for calculating cross sections for collinear-unsafe observables. Ordinary FFs are process-independent nonperturbative objects that describe the flow of momentum from a fragmenting quark or gluon into an identified final-state hadron [184, 282, 160, 135, 47, 128, 130]. Since the momentum of a single hadron is not collinear safe, cross sections for single-hadron observables have singularities beginning at $\mathcal{O}(\alpha_s)$. These collinear singularities are absorbed by the FFs order by order in $\alpha_s$. From this singularity structure, one can derive the renormalization group (RG) evolution for FFs, leading to the well-known DGLAP equations [265, 193, 49, 151]. This evolution is linear, since FFs depend only on the momentum of a single hadron in the final state.

In this chapter, we present a formalism for generalized fragmentation functions (GFFs), which describe the flow of momentum from a fragmenting quark or gluon into subsets of final-state hadrons. Because GFFs depend on correlations between final-state hadrons, their evolution equations are nonlinear and therefore more complicated than in the ordinary FF case. Motivated by the structure of the DGLAP equations, we define fractal jet observables where the evolution, albeit nonlinear, takes a special recursive form that is well-suited to numerical evaluation.\(^1\)

Specifically, we focus on observables defined using hierarchical binary clustering trees that mimic the leading-order tree-like structure of the evolution equations. A fractal jet observable $x$ can then be defined recursively according to Fig. 2-1 as

$$x = \hat{x}(z, x_1, x_2), \quad (2.1)$$

where $x_1$ and $x_2$ are the values of the observable on the branches of a 1 → 2 clustering tree, and $z$ is the momentum sharing between branches, defined by

$$z \equiv \frac{E_1}{E_1 + E_2} \quad (2.2)$$

\(^1\)This should not be confused with "extended fractal observables" recently introduced in Ref. [146], which are based on determining the fractal dimension of a jet.
with $E_i$ the energy of branch $i$. With these definitions, the leading-order evolution equation of the corresponding GFF takes the simplified form

$$
\mu \frac{d}{d\mu} F_i(x, \mu) = \frac{1}{2} \sum_{j,k} \int dz \, dx_1 \, dx_2 \frac{\alpha_s(\mu)}{\pi} P_{i\to j k}(z) F_j(x_1, \mu) F_k(x_2, \mu) \delta[x-\hat{x}(z, x_1, x_2)],
$$

(2.3)

where $F_i(x, \mu)$ is the GFF for parton $i = \{u, \bar{u}, d, \ldots, g\}$, $P_{i\to j k}(z)$ is the $1\to 2$ QCD splitting function, and $\mu$ is the $\overline{\text{MS}}$ renormalization scale. This evolution equation has the same structure as a $1\to 2$ parton shower, which is sufficiently straightforward to implement numerically. It was derived for some specific observables in Refs. [111, 261]. Although we mostly restrict ourselves to lowest order in perturbation theory, our framework allows for the systematic inclusion of higher-order corrections, in contrast to the semi-classical parton shower approach.

The class of fractal jet observables described by Eq. (2.1) is surprisingly rich, allowing for many collinear-unsafe observables to be calculated with the help of GFFs. For example, Eq. (2.3) describes the evolution of weighted energy fractions,

$$
x = \sum_{a \in \text{jet}} w_a \, z_a^\kappa, \quad z_a \equiv \frac{E_a}{E_{\text{jet}}},
$$

(2.4)

where $w_a$ is a weight factor that depends on non-kinematic quantum numbers such as charge or flavor, $\kappa > 0$ is an energy weighting exponent, and the sum extends over all jet constituents. These observables are defined by associative recursion relations, such

---

2While it would be more accurate to call Eq. (2.2) the "energy fraction", we use momentum fraction since that is more common in the fragmentation function literature.
that their value is independent of the choice of clustering tree. Examples of weighted energy fractions include weighted jet charge [170], whose nonlinear evolution was first studied in Ref. [328]; track functions which characterize the fraction of a jet’s momentum carried by charged particles [110, 111]; and the observable $p_T^D$ used by the CMS experiment for quark/gluon discrimination [286, 112], whose nonlinear evolution was first studied in Ref. [261]. While we focus on the case of $e^+e^-$ collisions with jets of energy $E_{\text{jet}}$, our formalism easily adapts to hadronic collisions with jets of transverse momentum $p_T^\text{jet}$.

In addition to performing a more general analysis of weighted energy fractions, we also present examples of fractal observables with non-associative recursion relations. These quantities depend on the details of the clustering tree used to implement Eq. (2.1), providing a complementary probe of jet fragmentation. In particular, while Eq. (2.1) does not involve any explicit angular separation scales, the clustering tree does introduce an implicit angular dependence. Remarkably, the details of the clustering do not affect the leading-order RG evolution in Eq. (2.3) considered in this chapter, beyond the requirement that particles are appropriately clustered in the collinear limit. An example of a non-associative fractal observable is given by node-based energy products,

$$x = \sum_{\text{nodes}} (4z_L z_R)^{\kappa/2},$$  \hspace{1cm} (2.5)

where the observable depends on the momentum fractions carried by the left and right branches at each node in the clustering tree. We also study observables defined entirely in terms of Eq. (2.1), with no obvious simplification. This sensitivity to the tree structure allows non-associative observables to probe parton fragmentation from a different perspective than previously-studied jet observables. As one application, we consider the discrimination between quark- and gluon-initiated jets (see e.g. [179, 180, 259, 261, 81, 53, 167, 245, 189] for recent studies). We find that fractal observables are effective for this purpose, in some cases yielding improved quark/gluon separation power compared to weighted energy fractions.
For clustering trees obtained from the Cambridge/Aachen (C/A) algorithm [153, 330], the depth in the tree is directly related to the angular separation scale between subjets. This opens up the possibility of modifying the recursion relation \( \hat{x} \) in Eq. (2.3) to be a function of angular scale. For example, starting from a jet of radius \( R \), one can introduce a subjet radius parameter \( R_{\text{sub}} \ll R \) such that evolution equation takes a different form below and above \( R_{\text{sub}} \). A particularly simple case is if the weighted energy fraction with \( \kappa = 1 \) is measured on the branches below \( R_{\text{sub}} \), since this effectively amounts to defining fractal observables in terms of subjets of radius \( R_{\text{sub}} \). In this case, the initial conditions for the GFF leading-order evolution is simply given by \( F_i(x, \mu_{\text{sub}}) = \delta(1 - x) \) at the initial scale \( \mu_{\text{sub}} = E_{\text{jet}} R_{\text{sub}} \gg \Lambda_{\text{QCD}} \), such that no nonperturbative input is needed. By evolving the GFFs to \( \mu = E_{\text{jet}} R \), we achieve the resummation of leading logarithms of \( R_{\text{sub}}/R \). Related evolution techniques have been used to resum logarithms of the jet radius \( R \) in inclusive jet cross sections [138, 229, 136].

The formalism of GFFs is reminiscent of other multi-hadron FFs in the literature. This includes dihadron fragmentation functions which describe the momentum fraction carried by pairs of final-state hadrons [315, 324], and fracture functions which correlate the properties of one initial-state and one final-state hadron [323, 190]. In all of these cases, the RG evolution equations are nonlinear. The key difference here is that fractal jet observables are not based on a fixed number of hadrons, but rather allow for arbitrary hadron multiplicities. Depending on the observable, this may require that all hadrons can be consistently labeled by non-kinematic quantum numbers (e.g. charge). As discussed in Ref. [328] for the case of weighted jet charge, the \( n \)-th moment of GFFs can sometimes be related to moments of \( n \)-hadron FFs. At the level of the full distribution, though, GFFs are distinct from multi-hadron FFs, and thereby probe complementary aspects of jet fragmentation.

The rest of this chapter is organized as follows. In Sec. 2.2, we review the theoretical underpinnings of ordinary parton fragmentation and explain how to extend the formalism to generalized fragmentation and fractal observables. We then construct generic fractal jet observables using clustering trees in Sec. 2.3. In Sec. 2.4, we
treat the case of weighted energy fractions, exploring their RG evolution for a range of parameters. We introduce two new sets of non-associative fractal observables in Sec. 2.5—node products and full-tree observables—and motivate their application in quark/gluon discrimination in Sec. 2.6. We briefly explain how our formalism also applies to fractal observables based on subjets rather than hadrons in Sec. 2.7. We conclude in Sec. 2.8, leaving calculational details and a description of the numerical RG implementation to the appendices.

2.2 Formalism

To motivate the definition of fractal jet observables, it is instructive to first review the formalism of standard fragmentation and then generalize it to arbitrary collinear-unsafe observables. We give a general definition of fractal jet observables at the end of this section, which serves as a preamble to the explicit constructions in Sec. 2.3.

2.2.1 Review of Standard Fragmentation

Ordinary FFs, denoted by $D_i^h(x, \mu)$, are nonperturbative objects that describe the number density of hadrons of type $h$ carrying momentum fraction $x$ among the particles resulting from the fragmentation of a parton of type $i$. They are the final-state counterpart to parton distribution functions (PDFs). For any parton flavor $i$, they satisfy the momentum conservation sum rule

$$\sum_h \int_0^1 dx \, x \, D_i^h(x, \mu) = 1.$$  \hspace{1cm} (2.6)

At leading order, the FFs are independent of the factorization scheme (see e.g. [178]).

The field-theoretic definition of the bare unpolarized quark FF is given by [128,
\[
D^h_i(x, \mu) = \frac{1}{x} \int d^2p_\perp^i \int \frac{dy^+ d^2y_\perp}{(2\pi)^3} e^{iy^+ y^+} \sum_x \frac{1}{2N_C} \times 
\times \text{Tr} \left[ \gamma^\perp_2 \langle 0| \psi_i(y^+, 0, y_\perp) | hX \rangle \langle hX | \bar{\psi}_i(0) | 0 \rangle \right],
\]

where we are working in a frame with quark transverse momentum \( p_\perp = 0 \) and using the gauge choice \( A^- = 0 \). The jet-like state \( | hX \rangle \) contains an identified hadron \( h \) of momentum \( p_h \) with \( p^-_h \equiv x p^- \), and \( X \) refers to all other hadrons in that state. The factor \( 1/(2N_C) \), where \( N_C = 3 \) is the number of colors, accounts for averaging over the color and spin of the quark field \( \psi \) of flavor \( i \). Here and in the rest of the chapter, we adopt the following convention for decomposing a four-vector \( w^\mu \) in light-cone coordinates:

\[
w^\mu = w^- n^\mu \frac{n}{2} + w^+ \bar{n}^\mu \frac{\bar{n}}{2} + w^\mu, \quad w^- = \bar{n} \cdot w, \quad w^+ = n \cdot w,
\]

where \( n^\mu \) is a light-like vector along the direction of the energetic parton, and \( \bar{n} \) is defined such that \( n^2 = \bar{n}^2 = 0 \) and \( n \cdot \bar{n} = 2 \). Thus at leading order, \( p^- = 2E_{\text{jet}} \).

Gauge invariance requires adding eikonal Wilson lines in Eq. (2.7) (see e.g. [131]), which we suppress here for notational convenience. An analogous definition applies for the gluon FF.

In the context of \( e^+e^- \) annihilation, FFs are crucial ingredients in the factorization formula for the semi-inclusive cross section at leading power in \( \Lambda_{\text{QCD}}/\sqrt{s} \),

\[
\frac{1}{\sigma^{(0)}} \frac{d\sigma}{dx} (e^+e^- \rightarrow hX) = \sum_i \int_x^1 \frac{dz}{z} C_i(z, s, \mu) D^h_i(x/z, \mu),
\]

where \( x = 2E_h/\sqrt{s} \leq 1 \) is the hadron energy fraction, \( \sigma^{(0)} \) is the tree-level cross section and \( X \) represents all other final state particles in the process.\(^3\) The coefficients \( C_i(z, s, \mu) \) are process-dependent perturbative functions that encode the physics of

\(^3\)In the literature (see e.g. [287]), the cross section \( 1/\sigma^{(0)} d\sigma/dx (e^+e^- \rightarrow hX) = F_h(x, \mu) \) is sometimes referred to as the total FF, in which case \( D^h_i(x, \mu) \) is called the parton FF.
the hard subprocess. The FFs $D_i^h(x, \mu)$ are universal, process-independent functions, which appear (with appropriate PDF convolutions) in related channels such as $ep \to hX$ or $pp \to hX$. Since the coefficients $C_i$ contain logarithms of $s/\mu^2$, in order to avoid terms that could spoil perturbative convergence in Eq. (2.9), the renormalization scale $\mu$ should be chosen close to $\sqrt{s}$.

While computing the FFs themselves requires nonperturbative information about the hadronic matrix elements in Eq. (2.7), their scale dependence is perturbatively calculable. This allows us to, for example, take FFs extracted from fits to experimental data at one scale and evolve them to another perturbative scale. The RG evolution of FFs is described by the DGLAP equations [265, 193, 49, 151],

$$\frac{d}{d\mu} D_i^h(x, \mu) = \sum_j \int_x^1 \frac{dz}{z} \frac{\alpha_s(\mu)}{\pi} P_{ji}(z) D_j^h(x/z, \mu).$$  \hspace{1cm} (2.10)

Here, the splitting kernels $P_{ji}(z)$ can be calculated in perturbation theory,

$$P_{ji}(z) = P^{(0)}_{ji}(z) + \frac{\alpha_s}{2\pi} P^{(1)}_{ji}(z) + \ldots,$$  \hspace{1cm} (2.11)

and are at lowest order the same as the splitting kernels for PDF evolution. The next-order splitting function $P^{(1)}_{ji}$ arises from $1 \to 3$ splittings as well as loop corrections to $1 \to 2$ splittings.

In order to motivate the transition to generalized fragmentation, it is convenient to rewrite the lowest-order splitting function explicitly as a $1 \to 2$ process:

$$P^{(0)}_{ji}(z) \equiv P_{i \to jk}(z),$$  \hspace{1cm} (2.12)

where the parton $j$ carries momentum fraction $z$, e.g. $P_{g \to gg}(z)$ or $P_{q \to gg}(z) = P_{q \to qg}(1-z)$. With this notation, we can rewrite the leading-order DGLAP equation in a sug-
gestive form\textsuperscript{4}

\[
\frac{d}{d\mu} D_i^h(x, \mu) = \frac{1}{2} \sum_{j,k} \int_0^1 dx_1 \int_0^1 dx_2 \int_0^1 dz \frac{\alpha_s(\mu)}{\pi} P_{i \to jk}(z) \\
\times \left( D_j^h(x_1, \mu) \delta[x - zx_1] + D_k^h(x_2, \mu) \delta[x - (1 - z)x_2] \right). \tag{2.13}
\]

Though we have written Eq. (2.13) as an integral over both \(x_1\) and \(x_2\), corresponding to the two final state branches from the \(i \to jk\) splitting, the FFs only require information about one single final-state hadron in each term, so the evolution simplifies to the linear form in Eq. (2.10). This will no longer be the case with generalized fragmentation, which depends on correlations between the final-state hadrons.

### 2.2.2 Introducing Generalized Fragmentation

We now extend the FF formalism to handle the distribution of quantities \(x\) carried by a subset \(S\) of collinear particles, where \(x\) can be more general than the simple momentum fraction and \(S\) is defined by non-kinematic quantum numbers. For example, we will consider observables defined on all particles within a jet, but also on charged particles only. For a given observable \(x\), there is a GFF for each parton species \(i\), which we denote by \(\mathcal{F}_i(x, \mu)\). At lowest order in \(\alpha_s\), the GFF is the probability density for the particles in \(S\) to yield a value of the observable \(x\) from jets initiated by a parton of type \(i\). The GFF automatically includes information about hadronization fluctuations. Being a probability density, the GFFs are normalized to unity for each parton type,

\[
\int dx \mathcal{F}_i(x, \mu) = 1. \tag{2.14}
\]

For any collinear-unsafe (but soft-safe) observable \(x\), we can give an operator definition for GFFs analogous to that for fragmentation functions. A (bare) quark

\textsuperscript{4}Because the splitting functions are divergent as \(z \to 1\) and as \(z \to 0\), plus-function regulators are required at both endpoints when integrating over the entire range \(0 \leq z \leq 1\).
GFF for the gauge choice $A^- = 0$ is defined as

$$
\mathcal{F}_i(x, \mu) = \int dy^+ d^2y_\perp e^{ip^-y^+/2} \frac{1}{2N_C} \sum_{S \times X} \delta[x - \bar{x}(p^-, S)]
\times \text{Tr} \left[ \frac{\gamma^-}{2} \langle 0|\psi_i(y^+, 0, y_\perp)|S X \rangle \langle S X |\psi_i(0)|0 \rangle \right],
$$

(2.15)

to be compared with Eq. (2.7). Here, $|S X\rangle$ is the asymptotic final state divided into the measured subset $S$ and unmeasured subset $X$, and $\bar{x}(p^-, S)$ is the functional form of the quantity being observed, which can depend on the overall jet momentum and any information from $S$. We stress that, in contrast to the standard FFs, a GFF involves a sum over polarizations and a phase-space integration over all detected particles in $S$; if the measured set $S$ consists of a single hadron, then Eq. (2.15) reduces to Eq. (2.7) for a quark FF. The definition for gluon-initiated jets is

$$
\mathcal{F}_g(x, \mu) = -\frac{1}{(d-2)(N_C^2 - 1)p^-} \int dy^+ d^2y_\perp e^{ip^-y^+/2} \sum_{S \times X} \delta[x - \bar{x}(p^-, S)]
\times \langle 0|G_{-a}^\Lambda(y^+, 0, y_\perp)|S X \rangle \langle S X |G_{-a, \Lambda}(0)|0 \rangle,
$$

(2.16)

where $G_{-a}^\Lambda = \bar{\epsilon}^\mu G_{\mu\Lambda}^a$ is the gluon field strength tensor for generator $T^a$, the factor of $1/(d-2)$ comes from averaging over the gluon polarizations in $d$ space-time dimensions, and the factor of $1/(N_C^2 - 1)$ comes from averaging over the color of the gluon.

The definitions in Eqs. (2.15) and (2.16) extend the ones introduced in Ref. [110] for track functions. In the track function case, $x$ is the momentum fraction carried by the charged particles in the final states, irrespective of their individual properties or multiplicities. As mentioned in the introduction, GFFs are reminiscent of multi-hadron FFs [315, 324], with the key difference that multi-hadron FFs describe a fixed number of identified final-state hadrons (i.e. two in the case of dihadron FFs), whereas GFFs allow for a variable number of final-state hadrons in the subset $S$.

With these GFFs in hand, we can calculate the cross section differential in the fractal observable $x$ for an inclusive jet sample with radius parameter $R \ll 1$. Letting
$z_J$ be the fraction of the center-of-mass energy carried by the measured jet ($z_J \equiv 2E_{jet}/E_{cm}$), we have

$$
\frac{1}{\sigma^{(0)}} \frac{d\sigma}{dz_J \, dx} (e^+ e^- \rightarrow \text{jet} + X) = \sum_i \int \frac{dy'}{y'} C_i (z_J/y', E_{cm}, \mu) \times \left\{ \delta (1 - y') F_i (x, \mu) + \sum_j J_{i \rightarrow j}^{(1)} (y', E_{jet} R, \mu) F_j (x, \mu) \right. \\
+ \delta (1 - y') \frac{1}{2} \sum_{j,k} \int dz \, dx_1 \, dx_2 \, J_{i \rightarrow jk}^{(2)} (z, E_{jet} R, \mu) F_j (x_1, \mu) F_k (x_2, \mu) \delta [x - \hat{x} (z, x_1, x_2)] \\
+ \frac{1}{2} \sum_{j,k} \int dz \, dx_1 \, dx_2 \, J_{i \rightarrow jk}^{(1)} (y', z, E_{jet} R, \mu) F_j (x_1, \mu) F_k (x_2, \mu) \delta [x - \hat{x} (z, x_1, x_2)] \\
\left. \right\} + \ldots \right\},
$$

(2.17)

where the ellipsis includes further terms at next-to-next-to leading order and $\sigma^{(0)}$ denotes the tree-level cross section. There is a similar version of Eq. (2.17) for $pp$ and $ep$ collisions with the inclusion of PDFs, where the jet rapidity would appear in the $C_i$ coefficients and $z_J$ would be replaced with $E_{cm}/Q$. As in Eq. (2.9), the effects of the hard interaction producing a parton $i$ are encoded in the coefficients $C_i$, which can be expanded perturbatively and depend on $z_J$ and $E_{cm}$. At leading order, the jet only consists of parton $i$, thus $C^{(0)}_i (z_J) = \delta (1 - z_J)$ and the dependence on the fractal observable $x$ arising from parton production and hadronization is described simply by $F_i$. The perturbatively calculable jet functions $J^{(n)}_{i \rightarrow j}$ and $J^{(n)}_{i \rightarrow jk}$ encode subsequent parton evolution computed at $O(\alpha_s^n)$. For most of the chapter, we restrict ourselves to leading order, though we stress that Eq. (2.17) provides the tools to interface our GFF formalism with fixed-order calculations and to extract GFFs beyond leading order, assuming that a tractable evolution equation can still be derived.

At next-to-leading order in Eq. (2.17), the parton $i$ can undergo a perturbative splitting into partons $j$ and $k$. If only $j$ is inside the jet then $z_J < 1$, as described by the perturbative coefficient $J^{(1)}_{i \rightarrow j}$ that can be derived from ref. [229], and the $x$-dependence is described by $F_j$. If both partons belong to the jet then again $z_J = 1$, but the observable $x$ now follows from combining the values $x_1$ and $x_2$ of the GFFs
for partons \(j\) and \(k\) with the momentum fraction \(z\) of the perturbative splitting described by the \(\mathcal{J}_{i \to jk}^{(1)}\) from ref. [328]. At next-to-next-to-leading order, there are even more contributions, including one with three partons in the jet involving \(\mathcal{J}_{i \to jk}^{(2)}\). In Eq. (2.17), we displayed only the term with two partons belonging to the jet, since it is the first term that directly correlates \(z_j\) and \(z\). The natural scale of the coefficients \(\mathcal{J}_{i \to j}, \mathcal{J}_{i \to jk}, \ldots\), is the typical jet invariant mass \(E_{\text{jet}} R\), so we conclude that the GFFs should be evaluated at \(\mu \simeq E_{\text{jet}} R\) to minimize the effect of higher-order corrections. If \(R \gtrsim 1\), then \(C_i\) and \(\mathcal{J}\) can be combined, and the natural scale to evaluate the GFF would be \(\mu \simeq E_{\text{jet}}\).

It is important to note that Eq. (2.17) really combines two different formalisms. The first is the formalism for GFFs discussed initially in Refs. [328, 110] for track-based observables and further developed here. The second is the formalism for fragmentation in inclusive jet production of Refs. [136, 228], which builds upon work on fragmentation in exclusive jet samples Refs. [294, 216, 266, 217]. Both of these formalisms are needed to perform higher-order jet calculations, though at leading order, the GFF formalism alone suffices. For the interested reader, we provide all details of the matching for \(e^+e^- \rightarrow \text{jet} + X\) at next-to-leading order in App. A.1. As in Refs. [328, 110], we expect that the absorption of collinear divergences by GFFs can be carried out order-by-order in \(\alpha_s\) due to the universality of the collinear limits in QCD.

### 2.2.3 Introducing Fractal Observables

The above generalized fragmentation formalism works for any collinear-unsafe (but soft-safe) observable. The RG evolution for a generic \(\mathcal{F}_i(x, \mu)\), however, can be very complicated. In order to deal with numerically tractable evolution equations, we focus on observables whose RG evolution simplifies to a nonlinear version of Eq. (2.13). Specifically, we want to find the most general form of the function \(\hat{\mathcal{F}}(p^-, S)\) in Eqs. (2.15) and (2.16) such that the RG evolution of \(\mathcal{F}_i(x, \mu)\) depends only on itself and other GFFs for the same observable, and does not mix with other functions. An example of an observable that involves GFF mixing is given in App. A.2, where the
evolution equation is considerably more complicated than considered below.

We define fractal observables as those whose GFFs obey the (leading-order) RG equation in Eq. (2.3), repeated here for convenience:

\[ \mu \frac{d}{d\mu} \mathcal{F}_i(x, \mu) = \frac{1}{2} \sum_{j,k} \int dz \, dx_1 \, dx_2 \, \frac{\alpha_s(\mu)}{\pi} P_{i\to jk}(z) \, \mathcal{F}_j(x_1, \mu) \, \mathcal{F}_k(x_2, \mu) \, \delta[x - \hat{x}(z, x_1, x_2)] , \]

(2.18)

where \( \hat{x}(z, x_1, x_2) \) is a function related to \( \hat{x}(p^-, S) \), which now depends on the momentum \( p \) only through the momentum sharing \( z \). As advertised, the evolution of \( \mathcal{F}_i(x, \mu) \) depends only on GFFs for the same observable \( x \), and no other nonperturbative functions. We leave a detailed discussion of higher-order evolution to future work, and focus primarily on the leading-order evolution here. As a consistency check, the \( \delta \) function in Eq. (2.18) ensures that the RG evolution automatically preserves the GFF normalization,

\[ \mu \frac{d}{d\mu} \int dx \, \mathcal{F}_i(x, \mu) = \frac{1}{2} \sum_{j,k} \int dz \, \frac{\alpha_s(\mu)}{\pi} P_{i\to jk}(z) \int dx_1 \, \mathcal{F}_j(x_1, \mu) \int dx_2 \, \mathcal{F}_k(x_2, \mu) = 0 , \]

(2.19)

where we used the fact that \( \sum_{j,k} \int dz \, P_{i\to jk}(z) = 0 \).

As a simple example of a fractal observable, consider the momentum fraction \( x \) carried by a subset \( S \) of hadrons of a common type. This case has already been studied in the context of track functions [110, 111], where \( S \) corresponded to charged particles. Treating the states \( |SX) \) in Eqs. (2.15) and (2.16) partonically, the next-to-leading-order bare GFF in dimensional regularization with \( d = 4 - 2\epsilon \) satisfies

\[ \mathcal{F}_i^{(1)}(x) = \frac{1}{2} \sum_{j,k} \int dz \, \frac{\alpha_s(\mu)}{2\pi} \left( \frac{1}{\epsilon_{\text{UV}}} - \frac{1}{\epsilon_{\text{IR}}} \right) P_{i\to jk}(z) \times \int dx_1 \, dx_2 \, \mathcal{F}_j^{(0)}(x_1, \mu) \, \mathcal{F}_k^{(0)}(x_2, \mu) \, \delta[x - \hat{x}(z, x_1, x_2)] . \]

(2.20)

Here, the function \( \hat{x}(z, x_1, x_2) \) is the form of \( \hat{x}(p^-, S) \) written in terms of two subjets,

\[ \hat{x}(z, x_1, x_2) = z x_1 + (1 - z) x_2 , \]

(2.21)
where $x_1$ and $x_2$ are the momentum fractions carried by particles belonging to subjets 1 and 2 within $S$, and $z$ is the momentum fraction carried by subjet 1, as defined in Eq. (2.2). Renormalizing the UV divergences in Eq. (2.20) in the $\bar{\text{MS}}$ scheme leads directly to the RG equation in Eq. (2.18). Thus, the momentum fraction $x$ carried by the final-state subset $S$ is indeed a fractal observable.

In the above analysis, we implicitly assumed massless partons, since otherwise the parton mass $m$ would regulate the $1/\epsilon_{\text{IR}}$ divergence. As long as $m \ll E_{\text{jet}}R$, it is consistent to take the $m \to 0$ limit. This also enables us to resum large logarithms of $E_{\text{jet}}R/m$ for charm and bottom quarks and $E_{\text{jet}}/\Lambda_{\text{QCD}}$ for light quarks that arise in the cross section for the fractal observable. At the scales $\mu = m_c$ and $\mu = m_b$, one has to match the GFF evolution onto the appropriate heavy-quark description. At the scale $\mu \gtrsim \Lambda_{\text{QCD}}$, it is necessary to match to chiral perturbation theory.

### 2.3 Fractal Observables via Clustering Trees

We now present a straightforward way to build a broad class of fractal observables that have the desired RG evolution in Eq. (2.18). The idea is to use recursive clustering trees that mimic the structure of the leading-order RG evolution equations. Our construction is based on the following three ingredients, as shown in Fig. 2-2:

1. Weights $w_a$ for each final-state hadron;
2. An IRC-safe binary clustering tree;
3. The recursion relation $\hat{x}(z, x_1, x_2)$.

By implementing the function $\hat{x}$ directly on recursive clustering trees, the resulting observable is guaranteed to have fractal structure.

#### 2.3.1 Construction

For this discussion, we start with a collection of hadrons from an identified jet, found using a suitable jet algorithm, e.g. anti-$k_t$ [97] in the studies below. As the initial
boundary condition for the observable, each final-state hadron within the jet is assigned a weight \( w_a \) (possibly zero) based on some non-kinematic quantum number associated with that hadron. This weight controls how much each type of hadron contributes to the value of the jet observable. For example, to construct an observable that only depends on the charged particles in the jet, all charged particles would be given weight 1 and all neutral particles weight 0. It is crucial that \( w_a \) is independent of the energy and direction of the hadron, otherwise the NLO GFF would not take the form in Eq. (2.20).

These final-state hadrons are then used as inputs to an IRC-safe binary clustering tree, which is in general different from any clustering algorithm used to determine the identified jet. For our studies, we use the generalized-\( k_t \) family of jet clustering algorithms [97], which are designed to follow the leading-order structure of the parton shower. In the context of \( e^+ e^- \) collisions, these algorithms have the pairwise clustering metric

\[
d_{ij} = \min[E_i^{2p}, E_j^{2p}] \Omega_{ij}^2,
\]

where the exponent \( p \) parametrizes the tree-dependence of the observable, with \( p = \)
\{-1, 0, 1\} corresponding to the \{anti-\textit{k}_t [97], C/A [153, 330], \textit{k}_t [103, 162]\} clustering algorithms, and \(\Omega_{ij}^2\) is a measure of the angular separation between two constituent’s momenta scaled by the jet radius parameter \(R\). For any value of \(p\), generalized-\textit{k}_t provides a pairwise clustering structure that directly mimics Eq. (2.18). For \(pp\) collisions, one insteads use a form of Eq. (2.22) based on transverse momenta \(p_T\) and distance \(\Delta R_{ij}\) in azimuthal angle and rapidity.

From this clustering tree, one can determine the observable \(x\) by applying the recursion relation \(\hat{x}(z, x_1, x_2)\) at each stage of the clustering. Specifically, the value of \(x\) at each node depends on the momentum fraction \(z\) given by the \(2 \rightarrow 1\) merging kinematics as well as on the \(x_1\) and \(x_2\) values determined from the corresponding daughter nodes (which might be the initial weights \(w_a\)). When all nodes are contained in a single connected tree, the root node represents the entire jet, and the root value of \(x\) determines the final observable.

Even though the clustering tree is IRC safe, the resulting fractal observable \(x\) is generally collinear unsafe. These collinear divergences are absorbed into the GFFs, and are in fact responsible for the evolution in Eq. (2.3).

### 2.3.2 Requirements

There are a few fundamental limitations on the choice of \(\hat{x}(z, x_1, x_2)\) dictated by the fact that this same function will appear in Eq. (2.18). First, the recursion relation must be symmetric under the exchange \(z \leftrightarrow 1 - z, x_1 \leftrightarrow x_2\), since the assignment of these labels is unphysical. Second, the recursion relation has to be IR safe, since the GFF formalism only regulates collinear (and not soft) divergences. In order that an emission with \(z \rightarrow 0\) does not change the observable, IR safety translates into the conditions

\[
\lim_{z \rightarrow 1} \hat{x}(z, x_1, x_2) = x_1, \quad \lim_{z \rightarrow 0} \hat{x}(z, x_1, x_2) = x_2,
\]  

\[
(z, x_1, x_2)
\]

5Since we start with the constituents of an identified jet, all of the particles are (re)clustered into a single tree. For this reason, the single-particle distance measure and the jet radius parameter \(R\) in the (re)clustering algorithm are irrelevant.

6In the case of jets with heavy flavor, one could use heavy-flavor tags to define asymmetric recursion relations (see e.g. [212]). We do not give a separate treatment of heavy-flavor GFFs in this work, and instead assume to always work in the \(m_{b,c} \ll E_{\text{jet}}R\) limit.
such that an arbitrarily soft branch in the clustering tree has no impact on the values of $x$. Third, the recursion relation has to have unambiguous limits. As a counterexample, $\hat{x}(z, x_1, x_2) = x_1^z x_2^{1-z}$ satisfies Eq. (2.23) when $x_1$ and $x_2$ are non-zero, but not when they vanish. Apart from these limitations, any choice of $\hat{x}(z, x_1, x_2)$ (along with starting weights and a clustering tree) defines a fractal observable.

The tree traversal prescription, along with the requirement in Eq. (2.23), helps ensure IR safety to all $\alpha_s$ orders. As a counterexample, consider the sum over all tree nodes of some function $f(z)$ which vanishes as $z \to 0$ or $z \to 1$. In that case, the resulting observable would receive no contribution from a single infinitely soft splitting, but subsequent finite $z$ splittings that followed the soft one would not be suppressed, violating IR safety. By contrast, Eq. (2.23) requires the contribution from an entire soft branch to be suppressed, as desired.

In this chapter, we mainly focus on recursion relations that do not depend explicitly on the opening angle $\theta$ between branches in the clustering tree. In Sec. 2.7, we do discuss how the recursion relation gets modified if a threshold value for $\theta$ is introduced (i.e. $\theta_{\text{thr}} = R_{\text{sub}} \ll R$). Of course, fractal observables depend indirectly on angular information through the structure of the clustering tree, but as discussed below, the leading-order evolution equations do not depend on the clustering algorithm. When explicit $\theta$-dependence is included in the $\hat{x}$ function, this sometimes results in a fully IRC-safe observable, requiring a different type of evolution equation that is beyond the scope of the present work (see e.g. [176]).

### 2.3.3 Evolution Equations

The generalized-$k_t$ clustering tree has an obvious mapping to a parton branching tree, such that at order $\alpha_s$, the RG evolution is given precisely by Eq. (2.18), with the flavor of the GFF matching the flavor of the jet's initiating parton. More formally, as discussed in Sec. 2.2.3, the NLO calculation of the bare GFF shows that the same recursion relation $\hat{x}(z, x_1, x_2)$ appears in Eq. (2.20), as desired.

In fact, to order $\alpha_s$, the evolution in Eq. (2.18) is insensitive to the clustering tree, as long as it is IRC safe, even if the fractal observable itself depends on the
clustering order. We explicitly test this surprising feature in Sec. 2.5. Note that if the clustering tree is not collinear safe, in the sense that particles with collinear momenta are not clustered with each other first, then the collinear divergences in the GFF will not cancel against the collinear divergences in the hard matching coefficients of Eq. (2.17). If the clustering tree is not IR safe, then the observable \( x \) is not IR safe, and the GFF formalism does not apply.

We stress that the evolution in Eq. (2.18) is only valid to lowest order in \( \alpha_s \). At higher orders in \( \alpha_s \), the evolution of fractal observables is more complicated, but, as discussed more in the paragraph below, still satisfies the property that the evolution of \( \mathcal{F}_i(x, \mu) \) depends only on GFFs of the same observable. Schematically, this can be written as

\[
\frac{d}{d \mu} \mathcal{F}_i = \frac{\alpha_s}{\pi} P_{i \rightarrow jk} \otimes \mathcal{F}_j \otimes \mathcal{F}_k + \left( \frac{\alpha_s}{\pi} \right)^2 P_{i \rightarrow jk\ell} \otimes \mathcal{F}_j \otimes \mathcal{F}_k \otimes \mathcal{F}_\ell + \ldots, \tag{2.24}
\]

where \( \otimes \) represents a convolution. This equation includes \( 1 \rightarrow n \) splittings at order \( \alpha_s^{n-1} \). There is no longer a one-to-one correspondence between pairwise clustering trees and GFF evolution trees, and one has to explicitly carry out the calculation in Eq. (2.20) to higher orders to determine the evolution. In particular, there will be different clusterings of the \( 1 \rightarrow n \) splitting into a binary tree when integrating over phase space, which depend on the choice of clustering algorithm. Because our specific realization of fractal observables in this section is based on recursive clustering trees, this guarantees that Eq. (2.24) depends only on GFFs of the same type as \( \mathcal{F}_i \) at all perturbative orders.

To justify the structure of Eq. (2.24) in a bit more detail, it is instructive to take a closer look at the \( 1/\epsilon_{\text{UV}} \) poles of \( \mathcal{F}_i \). As usual, the anomalous dimension of the GFFs is determined by the single \( 1/\epsilon_{\text{UV}} \) poles. At order \( \alpha_s \), we get \( (1/\epsilon_{\text{UV}})P_{i \rightarrow jk} \), as shown in Eq. (2.20). At order \( \alpha_s^2 \), the \( 1 \rightarrow 3 \) splitting factorizes into a sequence of two \( 1 \rightarrow 2 \) splittings when the angles of the splittings are strongly ordered. This leads to a term like \( (1/\epsilon_{\text{UV}}^2)P_{i \rightarrow jk} \otimes P_{j \rightarrow \ell m} \) which does not contribute to the GFF's anomalous dimension. However, it does justify attaching \( \mathcal{F}_j \) and \( \mathcal{F}_k \) to the external splittings in
Eq. (2.18), as it corresponds to the cross term between a one-loop renormalization factor and one-loop \( \mathcal{F}_j \) (and tree-level \( \mathcal{F}_k \)). Away from the strongly-ordered limit, the \( 1 \rightarrow 3 \) splitting does have a genuine \( 1/\epsilon_{\text{UV}} \) divergence, contributing to the second term in Eq. (2.24). The precise structure of this term depends on how the clustering algorithm maps the three partons to a binary tree. The justification for attaching GFFs to each of the three external partons follows again by considering higher-order corrections with some strong ordering. For example, consider a \( 1 \rightarrow 5 \) splitting that is strongly ordered such that it factorizes in a \( 1 \rightarrow 3 \) splitting, in which two partons undergo \( 1 \rightarrow 2 \) splittings. Such a term would have a \( 1/\epsilon_{\text{UV}}^3 \) divergence, corresponding to the cross term of the renormalization factor for the \( 1 \rightarrow 3 \) splitting term at order \( \alpha_s^2 \) with two one-loop \( \mathcal{F} \)'s and one tree-level \( \mathcal{F} \). Finally, the \( 1/\epsilon_{\text{UV}} \) from the one-loop virtual contribution to the \( 1 \rightarrow 2 \) splitting gives a higher-order correction to the first term in Eq. (2.18). For the remainder of this chapter, we focus on the leading-order evolution, leaving an analysis at higher orders to future work.

### 2.4 Weighted Energy Fractions

The procedure outlined in Sec. 2.3 is very general, but for special choices of \( \hat{\chi}(z, x_1, x_2) \), the definition of a fractal observable can simplify greatly. In this section, we consider the recursion relation

\[
\hat{\chi}(z, x_1, x_2) = x_1 z^\kappa + x_2 (1 - z)^\kappa, \tag{2.25}
\]

where \( \kappa > 0 \) is an energy exponent. As we will see, for any choice of pairwise clustering tree, the resulting observable simplifies to a sum over the hadrons in a jet,

\[
x = \sum_{a \in \text{jet}} w_a z_a^\kappa, \quad z_a \equiv \frac{E_a}{E_{\text{jet}}},
\]

where \( \kappa \) is the same as in Eq. (2.25), and \( w_a \) is the hadron weight factor. We call these observables weighted energy fractions.
Several examples of weighted energy fractions have already been studied in the literature. The weighted jet charge is defined for any $\kappa > 0$ and weights given by the electric charges of final-state hadrons [170, 250, 328]. This quantity has, for example, been used in forward-backward asymmetry measurements at $e^+e^-$ experiments [314, 149], as well as to infer the charge of quarks [75, 92, 41]. Recently, the scale dependence of the average jet charge was observed in $pp \rightarrow$ dijets [38]. Track fractions correspond to the case of $\kappa = 1$, where charged particles are given weight 1 and neutral particles given weight 0 [110, 111]. Jet $p_T^D$ is a weighted energy fraction with $\kappa = 2$ and all particles given weight 1 [112, 286]. Weighted energy fractions with arbitrary $\kappa > 0$ and $w_a = 1$ for all particles were studied in Ref. [261] for applications to quark/gluon discrimination.

### 2.4.1 Associativity

Weighted energy fractions have an associative recursion relation, meaning that the order of the clustering tree does not affect the final observable. To see this, consider the case of just three particles with weights $\{w_1, w_2, w_3\}$ and respective momentum fractions $\{z_1, z_2, z_3\}$. As shown in Fig. 2-3, there are three clustering trees that can be built using only $1 \rightarrow 2$ splittings, labeled as A, B, and C.\(^7\) The corresponding

---

\(^7\)Of course, for a specific choice of kinematics, not all of these trees will be possible from generalized-$k_t$ clustering, particularly in the collinear limit.
observables are

\[ x_A = \hat{x} \left( z_1, w_1, \hat{x} \left( \frac{z_2}{z_2 + z_3}, w_2, w_3 \right) \right), \]
\[ x_B = \hat{x} \left( z_2, w_2, \hat{x} \left( \frac{z_3}{z_3 + z_1}, w_3, w_1 \right) \right), \]
\[ x_C = \hat{x} \left( z_3, w_3, \hat{x} \left( \frac{z_1}{z_1 + z_2}, w_1, w_2 \right) \right). \]  

(2.27)

Using Eq. (2.25) and the fact that \( z_1 + z_2 + z_3 = 1 \), it is straightforward to prove that

\[ x_A = x_B = x_C = w_1 z_1^\kappa + w_2 z_2^\kappa + w_3 z_3^\kappa, \]  

(2.28)

owing to the fact that the recursion relation has homogenous scaling with \( z \). This argument generalizes to an arbitrary numbers of particles, so the weighted energy fractions are indeed independent of the clustering tree.⁸

Of course, there are other observables that have non-associative recursion relations, where the observable does not simplify to a sum over final-state hadrons and the full tree traversal is necessary. We explore some non-associative observables in Sec. 2.5.

### 2.4.2 Extraction of GFFs

In general, to extract GFFs, one has to numerically match the cross section in Eq. (2.17) using perturbatively calculated values for the coefficients \( C_i, J_{i\rightarrow j}, J_{i\rightarrow jk}, \ldots \). For the parton shower studies in this chapter, we limit ourselves to leading order where \( C_i^{(0)}(z_j) = \delta(1 - z_j) \), and we use parton-shower truth information to assign the parton label \( i \). To generate pure samples of quark- and gluon-initiated jets, we use the \( e^+e^- \rightarrow \gamma/Z^* \rightarrow q\bar{q} \) and \( e^+e^- \rightarrow H^* \rightarrow gg \) processes in PYTHIA 8.215 [305], switching off initial-state radiation. We find jets using FASTJET 3.2.0 [99], with the \( ee \)-generalized \( k_t \) algorithm with \( p = -1 \) (i.e. the \( e^+e^- \) version of anti-\( k_t \) [97]) and

---

⁸ Remember that this tree is one obtained from reclustering the particles in the jet. The value of a jet observable of course depends on the choice of initial jet algorithm, which may itself be a clustering algorithm.
then determine the various weighted energy fractions on the hardest jet in the event. At leading order, the normalized probability distributions for the weighted energy fractions directly give the corresponding GFF $\mathcal{F}_i(x, \mu)$.

As discussed in Sec. 2.2.2, for jets of a given energy $E_{\text{jet}}$ and radius $R$, the characteristic scale for GFFs is expected to be

$$\mu = E_{\text{jet}}R,$$  

(2.29)

which is roughly the scale of the hardest possible splitting in the jet. By varying $E_{\text{jet}}$ and $R$ but keeping $\mu$ fixed, we can estimate part of the uncertainty in the extraction of the GFFs. In addition, we assess the uncertainty from using different parton shower models. Here, since our primary interest is in the perturbative uncertainty in different shower evolution equations, we test the native PYTHIA parton shower along with the VINCIA 2.0.01 [185] and DIRE 0.900 [207] parton shower plugins. A further source of uncertainty would be given by the hadronization model, which enters the boundary conditions used for GFF evolution. This is not included in our present study, since we decided to interface all of the showers above with the Lund string model. In the context of an experimental analysis, one would also have statistical and systematic uncertainties from the extraction of GFFs from data.

For each observable $x$, there are 11 GFFs, corresponding to 5 quark flavors $\{u, d, s, c, b\}$, 5 anti-quark flavors, and the gluon. To avoid a proliferation of curves, it is convenient to define singlet (denoted by $\langle\text{Quark}\rangle$ in the figures below) and non-singlet combinations for the quark GFFs, respectively,

$$S(x, \mu) = \frac{1}{2n_f} \sum_{i \in \{u, d, s, \ldots, b\}} \mathcal{F}_i(x, \mu),$$

$$\mathcal{N}_{ij}(x, \mu) = \mathcal{F}_i(x, \mu) - \mathcal{F}_j(x, \mu).$$  

(2.30)

For the observables we study, the anti-quark GFFs are either identical to the quark GFFs or simply involve the replacement $x \rightarrow -x$, due to charge conjugation symmetry. We start by showing numerical results for the gluon GFF and the quark-singlet
combination, postponing a discussion of the non-singlet case to Sec. 2.4.5.

In Fig. 2-4, we show the extracted gluon and quark-singlet GFFs at $\mu = E_{\text{jet}}R = 100$ GeV for the weighted energy fractions with $w_a = 1$, comparing $\kappa = 0.5$ and $\kappa = 2$. Since gluon jets have roughly a factor of $C_A/C_F$ larger hadron multiplicity than quark jets, the mean of the gluon GFF is roughly a factor of $(C_A/C_F)^{1-\kappa}$ higher than the mean of the quark-singlet GFF. In the left column, we show the impact of changing the jet radius $R = \{0.3, 0.6, 0.9\}$, leaving $\mu$ fixed. The envelope from changing $R$ is very small, indicating that $\mu = E_{\text{jet}}R$ is an appropriate definition for the RG scale. In the right column, we show the impact of switching between the PYTHIA, VINCIA, and DIRE parton shower models. The envelope is larger, but still reasonably narrow, giving us confidence in the extraction of the GFFs, at least as far as changing the perturbative shower model is concerned. Though not shown here, we checked that the GFFs for the $\kappa \to 1$ and $\kappa \to \infty$ limits behave sensibly as well (see Sec. 2.4.4 below).

### 2.4.3 Evolution of GFFs

We now use these extracted GFFs as boundary conditions for the RG evolution in Eq. (2.18). In App. A.3, we describe in detail the numeric implementation of the evolution. Formally, the evolution equations work equally well running up or down in $\mu$, but in practice downward evolution is numerically unstable, as discussed further in App. A.4. As a proof of principle for our RG evolution code, we show upward evolution from $\mu = 100$ GeV to $\mu = 4$ TeV, comparing our RG evolution in Eq. (2.18) to that obtained from parton showers. In principle, this evolution could be started at a low scale such as $\mu \sim 1$ GeV to ensure that no large logarithms are present in the GFFs themselves, as is done with PDFs. We chose to begin the evolution at a high scale where the calculation is fully perturbative in order to avoid complications from matching to low-energy effective theories.

In Figs. 2-5 and 2-6, we present the evolution results for gluon and quark-singlet GFFs respectively, for the weighted energy fractions with $\kappa = \{0.5, 1.0, 2.0\}$. We test three different choices for the particle weights: $w_a = 1$ for all particles, $w_a = 1$
Figure 2-4: Gluon and quark-singlet GFFs for weighted energy fractions with (top) $\kappa = 0.5$ and (bottom) $\kappa = 2$, with all particles given starting weight 1. These distributions were extracted at the scale $\mu = 100$ GeV. The left column shows results from the VINCIA parton shower, with uncertainty bands from varying $R = \{0.3, 0.6, 0.9\}$ while keeping $\mu$ fixed. The right column shows the fixed jet radius $R = 0.6$, with uncertainty bands from testing three different parton showers: PYTHIA, VINCIA, and DIRE. In this and subsequent figures, (Quark) always refers to the quark-singlet combination $S(x, \mu)$ defined in Eq. (2.30).
Figure 2-5: Gluon GFFs of weighted energy fractions with (top row) $\kappa = 0.5$, (middle row) $\kappa = 1$, and (bottom row) $\kappa = 2$. Shown are distributions involving (left column) all particles, (middle column) just charged particles, and (right column) charged particles weighted by their charge. The GFFs extracted from parton showers at $\mu = 100$ GeV are shown in solid red. The result of evolving these initial conditions to $\mu = 4$ TeV are plotted in solid orange, to be compared to the average distribution obtained from parton showers at that value, plotted in dashed orange. The uncertainties come from both varying $R$ and the choice of parton shower (i.e. both variations shown in Fig. 2-4).
Figure 2-6: Same as Fig. 2-5 but for quark-singlet GFFs, where the distributions extracted from parton showers at $\mu = 100$ GeV are shown in solid blue, the evolved distribution are shown in solid light blue, and the distributions extracted at $\mu = 4$ TeV are shown in dashed light blue.
(\(w_a = 0\)) for charged (neutral) particles, and \(w_a = Q_a\) with \(Q_a\) being the particle’s electric charge. The initial conditions extracted from the parton showers at \(\mu = 100\) GeV are the same as those shown in Fig. 2-4, with the same color scheme of red for gluon GFFs and blue for quark-singlet GFFs. As described in Sec. 2.4.2, the uncertainty bands are given by the envelope of values obtained both from varying the jet radius/energy (keeping \(\mu\) fixed) and from using different parton showers. The evolved distributions to \(\mu = 4\) TeV are shown in orange for the gluon GFFs and light blue for the quark-singlet GFFs, where the uncertainty bands show the spread in final values due to the spread in initial conditions.

For comparison, we show in dashed lines the GFFs extracted at \(\mu = 4\) TeV, averaged over the three parton showers and three \(R\) values.\(^9\) Overall, our numerical GFF evolution agrees well with parton shower evolution, with both methods giving the same shift in the peak locations. As previously seen in Ref. [328], the two evolution methods agree best for \(\kappa \geq 1\), with larger differences seen in the widths of the distributions when \(\kappa < 1\). This is likely because \(\kappa < 1\) is more sensitive to collinear fragmentation, with larger expected corrections from higher-order perturbative effects. Note the expected \(\delta\)-function when \(\kappa = 1\) and \(w_a = 1\) for all particles, since the sum of the energy fractions for all particles in the jet equals 1. The \(\kappa \to 1\) limit of weighted energy fractions is discussed in Sec. 2.4.4 below.

In Fig. 2-7, we show the evolution of WEF distributions with (top) \(\kappa = 0.5\) and (bottom) \(\kappa = 2.0\) for (left) gluon GFFs and (right) quark-singlet GFFs extracted from \textsc{Pythia} 8.230 at \(\mu = ER = 100\) GeV to \(\mu = 4\) TeV. The error bars on the evolved distributions are obtained by changing the starting RG scale from \(100 \to 50\) GeV and \(100 \to 200\) GeV. The shaded bands are the envelope of these three evolved distributions. This gives an idea of the uncertainty in the evolution due to higher-order terms in the perturbative evolution equation. It is clear that this uncertainty is larger for WEFs with smaller \(\kappa\) values, which are more sensitive to collinear radiation.

\(^9\)The uncertainties from varying the jet radius/energy and changing parton showers at \(\mu = 4\) TeV are similar to the ones shown at \(\mu = 100\) GeV.
Figure 2-7: Error bars on the GFF evolution for weighted energy fractions with (top) $\kappa = 0.5$ and (bottom) $\kappa = 2.0$, for (left) gluons and (right) quark singlets. The dark curves come from evolving Eq. (2.18) from $\mu = ER = 100$ GeV to 4 TeV, and the dark bands are the envelope obtained by starting the evolution at $0.5\mu = 50$ GeV and $2\mu = 200$ GeV.
2.4.4 Limits

There are a few interesting limits of the weighted energy fractions. For the case of $\kappa = 0$, the energy fractions $z_a$ drop out, so $x$ simply counts the hadrons in the final state, weighted by $w_a$. Although hadron multiplicity is IR unsafe, it is possible to calculate the evolution of the average hadron multiplicity using fragmentation functions, see e.g. refs. [269, 268, 88]. This case requires special care, however, because of the soft gluon singularity of the splitting functions. IR-safe variants of multiplicity that have only collinear singularities are explored in a forthcoming chapter [176].

For the case of $\kappa = 1$ with all hadrons assigned weight 1, the weighted energy fraction simply becomes $x = \sum a z_a = 1$. Still, we can expand around the $\kappa \to 1$ limit to find a non-trivial observable [261]. Consider the modified weighted energy fraction and its limit,

$$ x = \frac{1}{\kappa - 1} \left[ \sum_{a \in \text{jet}} z_a^\kappa - 1 \right], \quad \lim_{\kappa \to 1} x = \sum_{a \in \text{jet}} z_a \ln z_a. \quad (2.31) $$

Figure 2-8: Gluon GFFs for (a) the modified weighted energy fractions from Eq. (2.31) in the $\kappa \to 1$ limit, and (b) the $\kappa$-th root of the weighted energy fractions from Eq. (2.33) in the $\kappa \to \infty$ limit. The solid lines show the GFFs extracted from VINCIA at $\mu = 100$ GeV, while the dashed lines show the evolution of these GFFs to $\mu = 4$ TeV. The fact that the limits are smooth is a consistency check on the evolution code.
In the limiting case, the recursion relation becomes

\[
\hat{x}(z, x_1, x_2) = z \ln z + (1 - z) \ln(1 - z) + x_1 z + x_2 (1 - z),
\]

with initial hadron weights of \( w_a = 0 \) (due to the \(-1\) in Eq. (2.31)). This is easy to verify by testing the three clustering trees in Fig. 2-3.\(^{10}\)

The behavior of the evolved GFFs in the \( \kappa \to 1 \) limit offers a non-trivial cross check of our evolution code. Away from the limiting value, the RG evolution can be implemented using the recursion relation in Eq. (2.25). At the limiting value, we have to use a different RG evolution based on the recursion relation in Eq. (2.32). The smooth convergence of the evolved distributions as \( \kappa \to 1 \) is illustrated in Fig. 2-8a, showing the modified weighted energy fraction from Eq. (2.31). The solid curves show the extraction of the corresponding GFFs at \( \mu = 100 \text{ GeV} \) with \( \kappa = 0.99 \) and \( \kappa = 1.01 \), which correctly bracket the \( \kappa \to 1 \) limit.\(^{11}\) The dashed curves show the evolution to \( \mu = 4 \text{ TeV} \), where there is again a smooth approach to \( \kappa \to 1 \).

In the limit that \( \kappa \to \infty \), the most energetic hadron in the jet dominates the sum in Eq. (2.26). We can then take the \( \kappa \)-th root of the weighted energy fraction to have a smooth \( \kappa \to \infty \) limit:

\[
x = \left| \sum_{a \in \text{jet}} w_a z_a^{\kappa} \right|^{1/\kappa}, \quad \lim_{\kappa \to \infty} x = \max_{w_a \neq 0} z_a,
\]

where the maximum is only taken over particles with non-zero weights. The corresponding recursion relation is

\[
\hat{x}(z, x_1, x_2) = \max(|zx_1|, |(1 - z)x_2|),
\]

with modified initial hadron weights of \( \tilde{w}_a = |\text{sign}(w_a)| = \{0, 1\} \). For these modified weights, it is easy to verify that Eq. (2.34) gives an associative recursion relation using

\(^{10}\)Amusingly, the recursion relation in Eq. (2.32) is associative for any choices of initial hadron weights, leading to the fractal observable \( x = \sum_{a \in \text{jet}} z_a (w_a + \ln z_a) \).

\(^{11}\)In practice, we first extract the \( \kappa = 0.99 \) and \( \kappa = 1.01 \) distributions for the unmodified weighted energy fraction, and then do a simple change of variables to match the definition in Eq. (2.31).
In Fig. 2-8b, we show the approach to $\kappa \to \infty$ for the gluon GFFs, considering the case of all particles with equal weight $w_a = 1$. Here, the finite-$\kappa$ evolution equations use the recursion relation in Eq. (2.25) while the $\kappa \to \infty$ limit uses Eq. (2.34), and we plot the $\kappa$-th root of the weighted energy fractions as given in Eq. (2.33). Both the extracted distributions at $\mu = 100$ GeV and the evolved distributions to $\mu = 4$ TeV show a smooth transition from $\kappa = 4$ to $\kappa = 6$ to the final $\kappa \to \infty$ limit. This is again a non-trivial cross check of our evolution code.

### 2.4.5 Moment Space Analysis

To gain further insight into the evolution of the GFFs, it is instructive to examine the evolution equations for the first two moments, which are related to averages and widths of the distribution for the fractal observable. In general, the moments of a GFF are defined as

$$\overline{\mathcal{F}}_i(N, \mu) \equiv \int_{-\infty}^{+\infty} dx \ x^N \mathcal{F}_i(x, \mu),$$

with $N \geq 0$. For the specific case of the weighted energy fractions, it is convenient to introduce a transformed version of the splitting functions

$$\overline{P}_{i\to jk}(\alpha, \beta) \equiv \int dz \ z^\alpha (1 - z)^\beta P_{i\to jk}(z), \quad \overline{P}_{i\to jk}(\alpha) \equiv \overline{P}_{i\to jk}(\alpha, 0).$$

Integrating Eq. (2.18) against $x^N$, the moment space evolution equation for a weighted energy fraction is

$$\frac{d}{d\mu} \overline{\mathcal{F}}_i(N, \mu) = \frac{\alpha_s(\mu)}{2\pi} \sum_{j,k} \sum_{M=0}^{N} \binom{N}{M} \overline{P}_{i\to jk}(\kappa(N-M), \kappa M) \overline{\mathcal{F}}_j(N-M, \mu) \overline{\mathcal{F}}_k(M, \mu),$$

where it is crucial that $N$ is an integer. A derivation of this expression is given in App. A.5.

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12 It is also possible to keep track of the signs of hadron weights by using an alternative recursion relation $\hat{x}(z, x_1, x_2) = \text{signed-max}(zx_1, (1-z)x_2)$, where the signed-max function takes the term (positive or negative) with the largest absolute value. Again, this only yields an associative recursion if the hadron weights are a constant multiple of \{-1, 0, 1\}. 

---
These evolution equations are more compact in the color singlet/non-singlet basis introduced in Eq. (2.30). For the quark-non-singlet pieces, the evolution of the first moment (i.e. the mean) is given by

\[
\mu \frac{d}{d\mu} \mathcal{N}_{ij}(1, \mu) = \frac{\alpha_s(\mu)}{\pi} \mathcal{P}_{q\rightarrow qg}(\kappa) \mathcal{N}_{ij}(1, \mu). \tag{2.38}
\]

Since \( \mathcal{P}_{q\rightarrow qg}(\kappa) < 0 \) for all positive \( \kappa \), Eq. (2.38) implies that the averages of the different (anti-)quark GFFs functions converge to a common value as \( \mu \) evolves upward. This behavior is expected, since QCD branchings only depend on the parton’s color charge, so the low-scale differences between the (anti-)quark flavors, due to e.g. electric charge, get washed out at high scales.

The quark-singlet combination mixes with the gluon GFF. For the first moment this is given by

\[
\mu \frac{d}{d\mu} \left( \frac{\mathcal{S}(1, \mu)}{\mathcal{F}_g(1, \mu)} \right) = \frac{\alpha_s(\mu)}{\pi} \begin{pmatrix} \mathcal{P}_{q\rightarrow qg}(\kappa) & \mathcal{P}_{q\rightarrow gq}(\kappa) \\ 2n_f \mathcal{P}_{g\rightarrow q\bar{q}}(\kappa) & \mathcal{P}_{g\rightarrow gg}(\kappa) \end{pmatrix} \begin{pmatrix} \mathcal{S}(1, \mu) \\ \mathcal{F}_g(1, \mu) \end{pmatrix}. \tag{2.39}
\]

As shown in Fig. 2-9, the matrix in Eq. (2.39) always has one negative eigenvalue for all \( \kappa \), which implies that the first moment of the quark-singlet GFF tries to
track the first moment of the gluon GFF. For example, in the case of $\kappa = 1$, the combination $2C_F \overline{S}(1, \mu) - n_f T_F \overline{F}_g(1, \mu)$ asymptotes to zero at high $\mu$. The second eigenvalue has different signs depending on the value of $\kappa$. For $\kappa < 1$, it is positive, so the first moments of both the quark-singlet and gluon GFF increase with $\mu$. For $\kappa > 1$, the second eigenvalue is negative, so the first moments decrease with $\mu$. For the special case $\kappa = 1$, the second eigenvalue is zero, and the corresponding eigenvector $\overline{S}(1, \mu) + \overline{F}_g(1, \mu)$ stays constant with $\mu$. These broad features agree with the behaviors already seen in Figs. 2-5 and 2-6.

Turning to the second moments, the non-singlet evolution is

$$\frac{d}{d\mu} \overline{N}_{ij}(2, \mu) = \alpha_s(\mu) \left[ \frac{\overline{P}_q \to qq(2\kappa) \overline{N}_{ij}(2, \mu)}{2n_f \overline{P}_q \to qq(2\kappa)} \right] \left[ \frac{\overline{S}(2, \mu)}{\overline{F}_g(2, \mu)} \right] \left[ \frac{\overline{P}_q \to qq(2\kappa) \overline{N}_{ij}(1, \mu) \overline{F}_g(1, \mu)}{2n_f \overline{P}_q \to qq(2\kappa)} \right].$$

(2.40)

Since the splitting function in the first term is negative for all values of $\kappa$, this term pushes the second moment of the non-singlet GFFs towards zero as well. Note, however, that the splitting function in the second term has the opposite sign. For the weighted energy fractions with $\kappa > 1$, which have $\overline{F}_g(1, \mu) \to 0$ as $\mu \to \infty$, this second term is not important, so the different quark GFFs asymptote to the same second moment. For the weighted energy fractions with $\kappa \leq 1$, however, this is not the case. As shown below in Fig. 2-10d for $\kappa = 0.5$, the growth of $\overline{F}_g(1, \mu)$ outpaces the decrease in $\overline{N}_{ij}(1, \mu)$ from the first term, which leads to differences in the widths (but not the means) of the different quark GFFs.

Assuming the asymptotic behavior $\overline{N}_{ij}(1, \mu) \to 0$ for simplicity, the evolution of the second moments of the quark-singlet and gluon GFF can be written as

$$\frac{d}{d\mu} \left( \frac{\overline{S}(2, \mu)}{\overline{F}_g(2, \mu)} \right) = \frac{\alpha_s(\mu)}{\pi} \left[ \frac{\overline{P}_q \to qq(2\kappa)}{2n_f \overline{P}_q \to qq(2\kappa)} \right] \left[ \frac{\overline{S}(2, \mu)}{\overline{F}_g(2, \mu)} \right] + \frac{\alpha_s(\mu)}{\pi} \left( \frac{2\overline{P}_q \to qq(2\kappa) \overline{S}(1, \mu) \overline{F}_g(1, \mu)}{2n_f \overline{P}_q \to qq(2\kappa)} \right).$$

(2.41)

where the assumption allows us to write the nonlinear term as a function of $\overline{S}(1, \mu)$.
instead of individual (anti-)quark contributions. Due to this nonlinear behavior, we now resort to a numerical analysis.

In Fig. 2-10, we show an example of the RG evolution of the first and second moments of the gluon GFFs, quark-singlet GFFs, and $u-d$ quark-non-singlet GFFs. Here, we consider weighted energy fractions where charged particles have weight 1 and neutral particles have weight zero, comparing $\kappa = 0.5, 1, 2$. The evolution starts from GFFs extracted at $\mu = 100$ GeV, as described in Sec. 2.4.2. The GFF moments are then evolved up to $\mu = 10^7$ GeV using the equations above. To connect with the plots in Figs. 2-5 and 2-6, we also indicate the first (second) moments extracted from the parton shower average at $\mu = 4$ TeV with dots (diamonds).

As expected, the first moments evolve in the direction predicted by the eigenvalues in Fig. 2-9, with the $\kappa < 1$ first moment moving to larger values as $\mu$ increases, and the $\kappa > 1$ first moment moving to smaller values. For the boundary case of $\kappa = 1$, the first moment of the gluon and quark singlet GFFs move toward each other, leaving their sum fixed. The second moments roughly evolve in the same direction as first moments, though with different rates. The exception is the $\kappa = 1$ second moment, where both the gluon and quark singlet values decrease (very slowly), as seen already in Figs. 2-5e and 2-6e. The first moment of the non-singlet GFFs approaches zero, as indicated by $\bar{P}_{q \to qg}(\kappa) < 0$. The second moments behave as discussed above, decreasing for $\kappa = 1$ and $\kappa = 2$, and increasing for $\kappa = 0.5$ since $\bar{F}_g(1, \mu)$ grows very large.

We could continue our analysis to third and higher moments, which is a standard way to efficiently solve the DGLAP equations. An interesting difference with the evolution of the ordinary FFs is that we only get the simple expression in Eq. (2.37) for integer moments. In addition, the simple form of Eq. (2.37) does not hold for general fractal observables with more complicated recursion relations. For these reasons, we

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13 For the weighted energy fractions in this study, this approximation is very accurate, giving corrections at the per-mille level.
14 Alternatively, if one assumes that $\bar{F}_g(1, \mu)$ and $\bar{S}(1, \mu)$ have also reached their asymptotic behavior, the equation becomes linear again. This approximation turns out to be even more accurate than the assumption $\bar{N}_{ij}(1, \mu) \to 0$, though for our numerical studies, we make no simplifications.
15 We checked that this agrees with first evolving the full binned distributions and then calculating the first and second moments.
only show the evolution of the first two moments here. Brief moment-space analyses for the non-associative observables in Sec. 2.5 are given in App. A.5.

![Graphs showing the evolution of the first and second moments of weighted energy fractions for charged particles with varying energy and initial conditions.](image)

Figure 2-10: Evolution of the first and second moments of (top row) the gluon GFFs and quark-singlet GFFs and (bottom row) the u-d quark-non-singlet GFFs. Shown are the first and second GFF moments for weighted energy fractions of charged particles with (left column) $\kappa = 0.5$, (middle column) $\kappa = 1$, and (right column) $\kappa = 2$. The initial conditions at $\mu = 100$ GeV are obtained from parton showers as described in Sec. 2.4.2, with uncertainty bands from varying $R$ and changing the parton shower. The values from the parton shower average at $\mu = 4$ TeV are shown as dots (diamonds) for the first (second) moments.

### 2.5 Tree-Dependent Observables

We now study fractal jet observables that do depend on the choice of clustering tree. These are also called non-associative observables, since $x_A \neq x_B \neq x_C$ in the notation of Eq. (2.27). We start in Sec. 2.5.1 with node-product observables, where
the recursion relation simplifies to a sum over internal nodes of the tree. We then
turn to a more general family of non-associative observables in Sec. 2.5.2.

2.5.1 Node Products

Node-product observables are based on the recursion relation

$$\hat{x} = x_1 z^\kappa + x_2 (1 - z)^\kappa + (4z(1 - z))^{\kappa/2}. \quad (2.42)$$

Note that the last term in Eq. (2.42) is independent of $x_1$ and $x_2$, and the factor of 4
is added for convenience, to normalize the contribution of a balanced splitting with
$z = 1/2$ to be 1. It is straightforward to check that this recursion relation is not
associative for generic values of $\kappa$, by considering the three-particle trees in Fig. 2-3.
For the special case of $\kappa = 2$, the recursion relation is associative, yielding an
observable closely related to $p_T^D$ (i.e. the weighted energy fraction with $\kappa = 2$),

$$\kappa = 2 : \quad x = 2 + \sum_{a \in \text{jet}} (w_a - 2) z_a^2. \quad (2.43)$$

For generic values of $\kappa$, this recursion relation simplifies to a sum over the leaves
and nodes in the binary tree,

$$x = \sum_{a \in \text{jet}} w_a z_a^\kappa + \sum_{\text{nodes}} (4z_L z_R)^{\kappa/2}, \quad z_{L,R} = \frac{E_{L,R}}{E_{\text{jet}}}, \quad (2.44)$$

where $z_{L,R}$ are the momentum fractions carried by the two branches at this node,
relative to the whole jet (i.e. $z_L + z_R \neq 1$).\footnote{If $z_L$ and $z_R$ had been relative to the node instead, this observable would not be IR safe, as the contribution from an arbitrary soft gluon that subsequently splits collinearly would not be suppressed; see Eq. (2.23).} To see how this simplification arises, note that the $(4z(1 - z))^{\kappa/2}$ term in Eq. (2.42) adds the product of branch energy fractions to the observable; the $x_1 z^\kappa$ and $x_2 (1 - z)^\kappa$ terms then rescale the energy product to the whole jet momentum. In this way, node products have intermediate
complexity between the weighted energy fractions (with no tree dependence) and
Figure 2-11: Gluon GFFs for the node-product observables with \( w_a = 0 \), taking (a) \( \kappa = 1 \), (b) \( \kappa = 2 \), and (c) \( \kappa = 4 \). These are extracted from VINCIA at \( \mu = 100 \) GeV. The tree dependence of these observables is parametrized by the generalized-\( k_t \) exponent in Eq. (2.22), with \( p = -1 \) (anti-\( k_t \), red dashed), \( p = 0 \) (C/A, green), and \( p = 1 \) (\( k_t \), blue dotted). For \( \kappa = 2 \) in (b), there is no tree dependence, as this observable is identical to \( 2(1 - p_D^2) \) (black dot-dashed).

more general observables (where the full tree recursion is required).

For simplicity, we focus on the case with starting weights of \( w_a = 0 \), such that the node-product observable only depends on non-leaf nodes, as advertised in Eq. (2.5). In Fig. 2-11, we show the distributions for the gluon GFFs for the node products extracted from VINCIA at a jet scale of \( \mu = 100 \) GeV. Here, we take \( \kappa = \{1, 2, 4\} \), testing three different values of the generalized-\( k_t \) clustering exponent \( p = \{-1, 0, 1\} \). The tree dependence of this observable for \( \kappa = 1 \) and \( \kappa = 4 \) is evident. This is particularly true for \( \kappa = 4 \), where the spikes near \( x = 1.1 \) (and \( x = 0.8 \)) come from balanced splittings that are more prevalent in \( k_t \) trees than C/A or anti-\( k_t \) trees. For \( \kappa = 2 \), the node-product observable is independent of \( p \), since it is identical to the associative observable \( 2(1 - p_D^2) \), as shown in Eq. (2.43).

Observables measured on anti-\( k_t \) clustering trees tend to be qualitatively distinct from observables measured on \( p \geq 0 \) trees. This is expected, because C/A and \( k_t \) trees are constructed according to angular and \( k_t \) ordering, respectively, so these observables more directly mirror the singularity structure of QCD and the expected dynamics of the parton shower. By contrast, anti-\( k_t \) trees have a hybrid ordering where angles tend to go from small to large, but energies tend to go from large to
Figure 2-12: Evolution of the gluon GFFs for node products with (top row) $\kappa = 1$ and (bottom row) $\kappa = 4$, comparing (left column) $p = -1$, (center column) $p = 0$, and (right column) $p = 1$. Shown are the gluon GFFs extracted from parton showers at $\mu = 100$ GeV (red solid), the GFFs evolved to $\mu = 4$ TeV (orange solid), and the GFFs extracted from parton showers at $\mu = 4$ TeV (orange dashed). The evolution agrees qualitatively with parton shower predictions, though the agreement is somewhat worse for $p = -1$.

small. Indeed, this reversal in the energy ordering is reflected in Fig. 2-11, where the product $z_L z_R$ tends to be smaller for anti-$k_t$ trees, leading to larger (smaller) values of node-product observable for $\kappa = 1$ ($\kappa = 4$). Because of this hybrid anti-$k_t$ ordering, one might expect higher-order perturbative corrections to be more important for $p < 0$ when evolving the GFFs, but this can only be confirmed by doing an explicit calculation, which is beyond the scope of the present work.

Despite the fact that different values of $p$ lead to different observables, the leading-order evolution equations are independent of $p$. To check whether this is a sensible feature, we evolve the gluon GFFs in Fig. 2-12 for node products with $\kappa = \{1, 4\}$ and
Figure 2-13: Same as Fig. 2-11, but for the full-tree fractal observable in Eq. (2.45) defined with $\kappa = 2$ on only charged particles, for (a) $\xi = -2$, (b) $\xi = 0$, and (c) $\xi = 2$. Recall that full-tree observables with $\xi = 0$ are the same as weighted energy fractions, so panel (b) is the same as the 100 GeV curve in Fig. 2-11b, which is plotted as a dash-dotted black line for comparison.

$p = \{-1, 0, 1\}$. The uncertainty bands in Fig. 2-12 are obtained from the variation of jet radius $R = \{0.3, 0.6, 0.9\}$ and parton shower $PS = \{\text{VINCIA, PYTHIA, DIRE}\}$, as described in Sec. 2.4.2. If the evolution from 100 GeV to 4 TeV would perfectly agree with the extraction at 4 TeV, this would confirm that the evolution is independent of $p$ and all $p$ dependence resides in the initial conditions. Although the agreement is not perfect, the amount of agreement between the evolution from 100 GeV to 4 TeV and the extraction at 4 TeV seems to be fairly independent of $p$, suggesting that this is a reasonable first approximation. Given the interesting features in the node-product observables as a function of scale, this motivates both higher-order calculations of their RG evolution, as well as measurements in data.

For completeness, we show the evolution of the first and second moments for the node-product observables in App. A.5.2.
2.5.2 Full-Tree Observables

As our final example of a fractal observable, we present a recursion relation that depends on the full structure of the clustering tree,

\[ \hat{x} = (z^\kappa x_1 + (1 - z)^\kappa x_2) e^{\xi z(1 - z)}. \]  

(2.45)

This recursion relation satisfies the requirements in Eq. (2.23), making this observable IR (but not collinear) safe. Eq. (2.45) defines a family of fractal observables which depend on the initial particle weights \( w_a \), the generalized-\( k_t \) clustering exponent \( p \), and the parameters \( \kappa \) and \( \xi \). We know of no alternative way to calculate this observable apart from performing the full leaf-to-root recursive traversal of the clustering tree. Of course, for the special value of \( \xi = 0 \), these observables become weighted energy fractions.

The tree dependence of this observable is illustrated in Fig. 2-13 for \( \kappa = 2 \) and \( \xi = \{-2, 0, 2\} \), where charged particles are given weight 1 and neutral particles weights 0. For nonzero \( \xi \), we see that the GFFs depend on the choice of \( p \), with rather different behaviors for anti-\( k_t \) compared to \( k_t \) and C/A. The (associative) observables plotted in Fig. 2-13b are equivalent to the weighted energy fraction with the same weights and \( \kappa = 2 \), shown on this plot for comparison. Corresponding results for the evolution of the gluon GFFs are shown in Fig. 2-14. In this case, it is much clearer that the amount of agreement between the evolution from 100 GeV to 4 TeV and the extraction at 4 TeV is independent of \( p \). Thus, the fact that the leading-order RG evolution is independent of \( p \) seems reasonable, even though the GFFs themselves are tree dependent. This is highlighted by Fig. 2-14d, where the double hump structure at 100 GeV is smoothed out both by the RG evolution equations and the parton shower.

Again for completeness, we discuss the evolution of the first two GFF moments for these full-tree observables in App. A.5.3.
Figure 2-14: Same as Fig. 2-12, but for the full-tree fractal observable in Eq. (2.45) defined with \( \kappa = 2 \) on only charged particles, for (top row) \( \xi = -2 \) and (bottom row) \( \xi = 2 \).

### 2.6 Application in Quark/Gluon Discrimination

Robust and efficient discrimination between quark- and gluon-initiated jets is a key goal of the jet substructure community [42, 50, 51, 43], with applications both in searches for physics beyond the SM and precision tests of QCD (see further discussions in [179, 180, 259, 261, 81, 53, 167, 245, 146, 189]). Weighted energy fractions are already used for quark/gluon discrimination, specifically the \( p_T^D \) observable [286, 112] used by CMS in its quark-gluon likelihood analysis [125]. Here, we explore the potential discrimination power of non-associative fractal jet observables, corresponding to non-associative variants of \( p_T^D \). An alternative application of the GFF formalism to quark/gluon discrimination will be presented in Ref. [176].

It is not immediately obvious that non-associativity should be a valuable feature
Figure 2-15: GFFs for two strong quark/gluon discriminants based on C/A trees: (a) the node-product observable with $\kappa = 1$, and (b) the full-tree observable with $\kappa = 2$ and $\xi = 4$ with all particle weights one. Shown are the gluon GFF (red solid), quark-singlet GFF (blue solid), down-quark GFF (light-blue dashed), and bottom-quark GFF (violet dotted) as extracted from VINCIA at $\mu = 100$ GeV.

to help distinguish quark- from gluon-initiated jets. Compared to $p_T^D$, non-associative observables are of course sensitive to the angular structure of the jet through the clustering tree. Then again, discriminants like the (generalized) angularities [76, 46, 165, 261] and energy correlation functions [259] also encode angular information about particles in the jet, either their angular distance to the jet axis or their pairwise angular distance to each other. As we will see, there are non-associative observables that do exhibit better performance than $p_T^D$, at least in the context of a parton shower study, but we do not (yet) understand the origin of that improvement from first principles.

Here, our primary interest in non-associative observables is for testing the evolution of quark/gluon discrimination power as a function of RG scale $\mu$. As recently studied in Refs. [53, 189], different parton showers exhibit different quark/gluon discrimination trends as a function of jet energy. Therefore, the study of fractal jet observables might help identify which higher-order effects in the parton shower are most important for correctly modeling the radiation patterns of quarks and gluons.
As an initial investigation into non-associative fractal observables for quark/gluon discrimination, we consider some examples of the node-product and full-tree observables from Sec. 2.5. In Fig. 2-15, we show two good quark/gluon discriminants, comparing the gluon GFF distribution to the quark-singlet GFF distribution. We also show the down-quark and bottom-quark GFFs as a cross check. An example of a node-product observable from Eq. (2.44) is shown in Fig. 2-15a, where we take $\kappa = 1$ and $w_a = 0$ on a C/A tree. An example of a full-tree observable from Eq. (2.45) is shown in Fig. 2-15b, where we take $\kappa = 2$ and $\xi = 4$ on a C/A tree with all particles given weight 1. There are noticeable differences between the gluon and quark-singlet GFFs which can be exploited for the purposes of discrimination. Among the observables we tested, these two performed among the best, outperforming, for example, variants using only charged particles.

To evaluate the potential quark/gluon discrimination power more quantitatively, we show ROC (receiver operating characteristic) curves showing the efficiency of identifying quark jets against the mistag rate for gluon jets. These plots are obtained
Figure 2-17: Evolution of the ROC curves for node-product observables with (a) \( \kappa = 1 \), (b) \( \kappa = 2 \) (equivalent to \( p_T^D \)), and (c) \( \kappa = 4 \). Shown are the ROC curves extracted from parton showers at 100 GeV (light purple band) and 4 TeV (dark purple, dashed), as well as the ROC curve obtained from evolving the GFF from \( \mu = 100 \) GeV to 4 TeV (medium purple band). The spread of these curves is obtained from calculating the ROC curves from the spread of distributions, as described in Sec. 2.4.2.

from VINCIA, comparing the discrimination performance at \( \mu = 100 \) GeV to \( \mu = 4 \) TeV. In Fig. 2-16, we show variants of the node-product observables defined on C/A trees for \( \kappa = \{1, 2, 4\} \), recalling that \( \kappa = 2 \) is the same as \( 2(1 - p_T^D) \). The node product with \( \kappa = 1 \) exhibits much better discrimination power than \( \kappa = 2 \), especially at \( \mu = 4 \) TeV. The discrimination power does continue increasing (slowly) with lower \( \kappa \), but approaching the \( \kappa \to 0 \) limit, the observable becomes IR unsafe and the GFF formalism no longer applies.

We can check whether this jet-energy dependence is reasonable using the RG evolution equations, as shown in Fig. 2-17. For \( \kappa = 1 \), the discrimination power does indeed increase with increasing \( \mu \), but not as much as predicted by the parton showers. This could have already been anticipated from the results in Fig. 2-12b, where the RG-evolved gluon GFF does not shift as dramatically as predicted in the parton showers. This could either be a sign that the parton showers are too aggressive in their evolution, or that higher-order terms in the evolution equation are important for getting the proper shape of the \( \kappa = 1 \) distribution. For \( \kappa = 2 \), the evolution of the ROC curves according to Eq. (2.18) does match the evolution in the parton shower,
but this evolution is very slight, less than the spread in the ROC curves at either scale from varying $R$ and the parton shower. For $\kappa = 4$, the discrimination power is poor at all scales, but the evolution matches well between Eq. (2.18) and the parton showers.

We next turn to the full-tree observables in Fig. 2-18, using a C/A tree with $\kappa = 2$ on all particles. We compare $\xi = \{0, 2, 4, 6\}$, where $\xi = 0$ is identical to $p_T^D$. The $\xi = 4$ observable yields comparable performance to $p_T^D$ at $\mu = 100$ GeV, but performs somewhat better than $p_T^D$ at $\mu = 4$ TeV. Note that the quark/gluon discrimination power is not monotonic as a function of $\xi$. We can again check whether this evolution is reasonable using the RG equations, as shown in Fig. 2-19. For all three $\xi$ values, the evolution of the ROC curves in Eq. (2.18) matches the parton shower, but the evolution is extremely slow.

As emphasized in Ref. [261], predicting the quark/gluon discrimination power from first principles is a much more challenging task than predicting the distributions themselves. Because the ROC curve shapes depend sensitively on the overlap between the quark and gluon distributions, small changes in the distribution shapes can lead to large changes in the predicted discrimination power. This is especially evident in
2.7 Fractal Observables from Subjets

As our final investigation into the structure of fractal jet observables, we now consider the possibility that the recursion relation in Eq. (2.1) is modified to depend on the angular scale of the clustering. For simplicity, we only consider observables defined on angular-ordered C/A clustering trees, since in that case the depth in the C/A tree is directly associated with an angular scale $\theta$. This opens up the possibility to define a modified recursion relation with $\theta$ dependence, for example,

$$\hat{x}(z, x_1, x_2) = \begin{cases} 
\hat{x}_1(z, x_1, x_2) & \text{if } \theta < R_{\text{sub}}, \\
\hat{x}_2(z, x_1, x_2) & \text{if } \theta > R_{\text{sub}}.
\end{cases} \quad (2.46)$$

As shown in Fig. 2-20, the nodes as defined by $\hat{x}_1$ become the starting weights for the subsequent nodes defined by $\hat{x}_2$.

It is straightforward to implement the leading-logarithmic resummation of an observable defined by Eq. (2.46). Starting from a low-energy boundary condition, this
Figure 2-20: Modified fractal jet observables where the recursion relation changes at a characteristic scale $R_{\text{sub}}$. When using a C/A tree, it is possible to switch the recursion relation from $\hat{x}_1$ to $\hat{x}_2$ for angular scales $\theta > R_{\text{sub}}$. This is equivalent to determining the observable $\hat{x}_1$ on all subjets of radius $R_{\text{sub}}$ and then using these as initial weights for the tree with $\hat{x}_2$.

This involves an initial evolution to the scale

$$\mu_{\text{sub}} = E_{\text{jet}}R_{\text{sub}}$$

(2.47)

using Eq. (2.18) with the recursion relation $\hat{x}_1$, followed by an evolution to $\mu = E_{\text{jet}}R$ using $\hat{x}_2$ instead. The discontinuity in anomalous dimensions of the evolution equations across the threshold $\mu_{\text{sub}}$ will be compensated by a fixed-order correction at that scale, but this only enters at next-to-leading-logarithmic order.

One interesting case is when the observable defined at small angular scales $\theta < R_{\text{sub}}$ is the weighted energy fraction of all particles with $\kappa = 1$. This observable is simply 1 for each of the branches, so the GFFs at the scale $\mu_{\text{sub}}$ are

$$F_i(x, \mu_{\text{sub}}) = \delta(1 - x),$$

(2.48)

which are then the input for the fractal observable $\hat{x}_2$ for $\theta > R_{\text{sub}}$. This effectively removes the sensitivity to nonperturbative physics, allowing us to calculate fractal observables analytically, as long as the scale $\mu_{\text{sub}}$ is perturbative. An example of this
kind of observable is shown in Fig. 2-21, where the observable is clustered using the recursion relation Eq. (2.25) with $\kappa = 1$ for angles $\theta < R_{\text{sub}}$ and $\kappa = 2$ for $\theta > R_{\text{sub}}$. The spike at $x = 1$ persists in the numerical evolution, even with very fine bins and a large amount of computing time.\footnote{The generating functional approach (see e.g. ref. [161]) provides an alternative implementation of the evolution in Eq. (2.3) that can be used to resum (sub)jet radius logarithms [138]. This approach may be more amenable to an initial condition with a delta function.} This feature is not seen in the \textsc{Vincia} evolution, which at every stage in the parton shower uses a scale closer to $\mu \approx z E_{\text{jet}} \theta$, where $z$ and $\theta$ are the momentum fraction and opening angle of the splitting. Compared to our choice of $\mu = E_{\text{jet}} R$ for the shower as a whole, we would expect the \textsc{Vincia} scale, which corresponds to a larger coupling, to accelerate the depletion of the $\delta$ function in the evolution. It will be interesting to see if this behavior persists with higher-order evolution equations.

An alternative way of viewing the above prescription is that we can build fractal jet observables not just out of hadrons but also out of subjets of radius $R_{\text{sub}}$, thus enlarging the range of applicability of the \textsc{Gff} framework. By taking $R_{\text{sub}}$ not too small, the observable becomes perturbative. On the other hand, we still want $R_{\text{sub}} \ll R$, such that the leading logarithms of $R/R_{\text{sub}}$ dominate the observable and Eq. (2.18)
gives a reliable description of its behavior.

2.8 Conclusions

To date, the bulk of analytic jet physics studies are based on either single-hadron fragmentation functions or IRC-safe jet shapes. In this chapter, we emphasized the intermediate possibility of IR-safe but collinear-unsafe jet observables defined on a subset of hadrons. We started by introducing the framework of Generalized Fragmentations Functions (GFFs), which are applicable to general collinear-unsafe jet observables. The GFFs are universal functions that absorb collinear singularities order by order in $\alpha_s$, which not only restores calculational control, but also implies that the GFFs evolve under a nonlinear version of the DGLAP equations. We then discussed fractal jet observables, defined recursively on an IRC-safe clustering tree with certain initial hadron weights, which satisfy a self-similar RG evolution at leading order given by Eq. (2.18). The higher order evolution is no longer universal, but still self-similar, and has the schematic form in Eq. (2.24).

The simplest fractal jet observables are those with associative recursion relations, whose value does not depend on the choice of clustering tree. This is indeed the case for the weighted energy fractions, studied in Sec. 2.4, which include several observables already in use at colliders, including $p_T^D$, weighted jet charge, and track fractions. More exotic fractal jet observables depend on the clustering sequence, including the node-product and full-tree observables studied in Sec. 2.5. Remarkably, the structure of the RG evolution for these observables is independent of the clustering tree at leading order.

As one potential application of fractal observables, we studied whether non-associative observables could be useful for quark/gluon discrimination. Indeed, we found examples in Sec. 2.6 which do perform better than the weighted energy fraction $p_T^D$ currently used by CMS. Though the GFF formalism does not allow us to predict the absolute discrimination power of collinear-unsafe observables, it does allow us to predict the RG evolution of the discrimination power, a feature that will be further
exploited in Ref. [176]. To gain more perturbative control, one can work with fractal observables defined on subjets (instead of hadrons), as briefly discussed in Sec. 2.7.

Looking to the future, the next step for fractal jet observables is pushing beyond the leading-order evolution equations. This will require computing the bare GFFs to higher orders in $\alpha_s$, as well as extracting GFFs using the matching scheme sketched in Eq. (2.17), and presented in detail at next-to-leading order for $e^+e^-$ collisions in App. A.1. More ambitiously, one would like to study correlations between two or more fractal jet observables, which would require multivariate GFFs. Such correlations are known to be important for improved quark/gluon discrimination [180, 261, 245], though even for IRC-safe jet shapes, there are relatively few multivariate studies [260, 257, 295]. Together with the work in this chapter, higher-order and correlation studies would facilitate a deeper understanding of jet fragmentation, with important consequences for analyses at the LHC and future collider experiments.
Chapter 3

Aspects of Generalized Track-Assisted Mass

Track-assisted mass is a proxy for jet mass that only uses direction information from charged particles, allowing it to be measured at the Large Hadron Collider with very fine angular resolution. In this chapter, we introduce a generalization of track-assisted mass and analyze its performance in both parton shower generators and resummed calculations. For the original track-assisted mass, the track-only mass is rescaled by the charged energy fraction of the jet. In our generalization, the rescaling factor includes both per-jet and ensemble-averaged information, facilitating a closer correspondence to ordinary jet mass. Using the track function formalism in electron-positron collisions, we calculate the spectrum of generalized track-assisted mass to next-to-leading-logarithmic order with leading-order matching. These resummed calculations provide theoretical insight into the close correspondence between track-assisted mass and ordinary jet mass. With the growing importance of jet grooming algorithms, we also calculate track-assisted mass on soft-drop groomed jets.

3.1 Introduction

The Large Hadron Collider (LHC) is currently operating at a collision energy of 13 TeV, allowing it to produce electroweak-scale resonances—like W/Z bosons, Higgs...
bosons, and top quarks—with very high Lorentz boosts. The typical angular separation between the products of a two-body decay $A \rightarrow BC$ is $\Delta R_{BC} \approx 2m_A/p_{T,A}$, so boosted resonances are often reconstructed as a single hadronic jet. At the most extreme kinematics, the decay products can become so collimated that their separation is even below the typical hadronic calorimeter resolution of $0.1 \times 0.1$ in the rapidity-azimuth plane. For example, the products of a decaying $W$ boson would become indistinguishable to a hadronic calorimeter at $p_T \approx 1.5$ TeV.

On the other hand, the charged particle tracking detectors at the LHC experiments offer $10^{-100}$ times better angular resolution than the electromagnetic and hadronic calorimeters [56, 255]. This has motivated the design of jet substructure observables which require direction information from only charged particles [233, 307, 100, 300, 253, 309, 90]. With the goal of improving the mass resolution of boosted objects, the ATLAS collaboration defined the track-assisted mass as [126]

$$M_{TA} = M_{\text{track}} \left( \frac{p_{T,\text{calo}}}{p_{T,\text{track}}} \right),$$

(3.1)

where the track-only mass $M_{\text{track}}$ is computed from charged particle tracking information, while the charged-to-neutral fraction $p_{T,\text{track}}/p_{T,\text{calo}}$ requires input from both tracking and calorimetry. Because of approximate isospin conservation, $M_{TA}$ is a good proxy for ordinary jet mass $M_{\text{calo}}$. In addition, quantities like $M_{\text{track}}$ defined in terms of just charged particles are more resilient to the impact of secondary pileup collisions [56, 255].

In this chapter, we introduce the generalized track-assisted mass (GTAM) and study its properties for ordinary quark and gluon jets. Taking Eq. (3.1) as a starting point...

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1CMS performed a study of vector boson tagging at high $p_T$ and found that the hadronic calorimeter resolution was too coarse to effectively identify vector bosons at $p_T > 1.5$ TeV [7]. This study concluded that momenta reconstructed from the electromagnetic calorimeter would be the key component of high-$p_T$ vector boson tagging, but did not examine a purely track-based measurement.

2Throughout this chapter, we use “track” to refer to just charged particles and “calo” to refer to all particles, even through algorithms like particle flow [32, 304] determine “calo” quantities through a combination of tracking and calorimetry.
point, we define a two-parameter family of GTAM observables,

\[ M_{TA}^{(\kappa,\lambda)} = M_{\text{track}} \left( \frac{P_{T,\text{calo}}}{P_{T,\text{track}}} \right)^\kappa \left\langle \frac{P_{T,\text{calo}}}{P_{T,\text{track}}} \right\rangle^\lambda, \quad M_{TA}^{(1,0)} \equiv M_{TA}, \]  

where \( \langle \cdot \rangle \) denotes an average over an ensemble of jets. The parameters \( \kappa \) and \( \lambda \) determine whether the charged-to-neutral fraction is estimated jet-by-jet or ensemble-by-ensemble. Through a combination of parton shower studies and resummed calculations, we conclude that parameter values around \( \kappa \approx 0.5 \) and \( \lambda \approx 0.5 \) produce an observable which outperforms \( M_{TA} \) as a proxy for jet mass, at least for quark- and gluon-initiated jets. We also study GTAM with soft-drop grooming, and find that it remains a good substitute for jet mass, but with a shift in the optimal parameter values which depends on the degree of grooming.

To preview our results, distributions of jet mass \( M_{\text{calo}} \) and GTAM \( M_{TA}^{(\kappa,\lambda)} \) are plotted in Fig. 3-1 for anti-\( k_t \) jets [97] in \( e^+e^- \) annihilation. Here, we show distributions (a) from the VINCIA 2.2.2 [185, 171] parton shower plugin to PYTHIA 8.230 [306, 305] and (b) from our analytic calculations described below. As expected, \( M_{\text{track}} \) differs

Figure 3-1: Distributions of jet mass \( M_{\text{calo}} \) and GTAM \( M_{TA}^{(\kappa,\lambda)} \) in \( e^+e^- \) collisions, extracted from (a) VINCIA 2.2.2 and (b) NLL+LO calculations convolved with a non-perturbative shape function.
from $M_{\text{calo}}$ by roughly a factor of $2/3$ (corresponding to equal fractions of $\pi^+, \pi^-$, and $\pi^0$). Using standard track-assisted mass $M_{\text{TA}}$ restores the desired peak location, but with some degree of smearing. Our recommended GTAM default of $M_{\text{TA}}^{(0.5,0.5)}$ gets even closer to matching the $M_{\text{calo}}$ distribution. By dimensional analysis, one could already guess that $\kappa + \lambda = 1$ would be preferred, and this intuition is borne out in our analytic calculations. The precise relationship between $\kappa$ and $\lambda$ is sensitive to the details of the event sample and the accuracy of the calculation. Eventually, experimental measurements will be needed to determine whether our recommendation of $\kappa \simeq \lambda \simeq 0.5$ indeed has the best performance as a jet-mass proxy.

The importance of jet mass as a collider observable cannot be overstated. When the decay products of boosted objects become collimated, jet production cross sections cannot distinguish between boosted signal jets and QCD background jets. This challenge has spurred the development of many substructure techniques for tagging highly boosted objects [231, 46, 163, 115, 308, 291, 318, 134, 208, 218, 319, 223, 259, 52, 254, 232, 321, 281, 246]. The most fundamental substructure observable is the jet mass, which has been computed at fixed order, and in resummed calculations to next-to-leading logarithmic (NLL) order [105, 263, 141, 122, 267]. The mass of a boosted signal jet originates primarily from the decaying heavy resonance, while background jets produced by light quarks and gluons gain mass from collinear parton splitting governed by the DGLAP evolution equations [193, 265, 151, 49]. A cut on the value of the jet mass can therefore be an important discriminant between signal and background jets [237, 37], which is why having excellent jet mass resolution is of paramount importance, perhaps achieved through track-assisted measurements.

We now give a detailed outline of the remainder of this chapter. In Sec. 3.2, we review the definition of track-assisted mass and then perform an exploratory parton shower study with VINCIA, using ensembles of quark and gluon jets from $pp$ collisions at $E_{\text{CM}} = 14$ TeV. We compare GTAM and ordinary jet mass for a range of $\kappa$ and $\lambda$ parameters. The closest correspondence between the two occurs for $\kappa \approx 0.5$ and $\lambda \approx 0.5$, where we define the degree of similarity by a symmetric version of the $\chi^2$ statistic. In App. B.1, we repeat this study for pure samples of quark/gluon jets (as
defined by the VINCIA hard process), and find that the optimal GTAM parameters are insensitive to the parton content of the jet.

In Sec. 3.3, we calculate the GTAM spectrum for quark- and gluon-initiated jets in $e^+e^-$ collisions. The use of observables depending on only charged particles is theoretically complicated since these observables are not infrared and collinear (IRC) safe. IRC safety guarantees a finite perturbative expansion order-by-order in $\alpha_s$ [311], whereas the perturbative spectra of unsafe observables exhibit unphysical divergences. Perturbative calculations of cross sections for a large class of collinear-unsafe observables can be performed with the track function formalism, or the broader generalized fragmentation function (GFF) formalism [328, 250, 110, 111, 261, 158]. Just like ordinary fragmentation functions for inclusive single-hadron cross sections [79, 282, 283, 128, 130, 91, 127], these methods absorb collinear singularities from the fixed-order calculation into non-perturbative GFFs, which can be extracted from global fits to experimental data.\footnote{See Ref. [275] for a recent review of these extractions and the experimental datasets used to perform them.}

For the purposes of this study, we used track functions extracted from PYTHIA 8.230 as described in Ref. [158].

The details of the resummed calculation in Sec. 3.3 closely follow those of track thrust in Ref. [111], with additional details provided in App. B.2 and App. B.3. The analytic calculations include resummation to NLL order, excluding the effects of non-global logarithms (NGLs) [137]. To perform leading fixed-order (LO) matching, we use the processes $e^+e^- \rightarrow \gamma^*/Z \rightarrow q\bar{q}g$ and $e^+e^- \rightarrow H \rightarrow ggg(q\bar{q})$. Non-perturbative (NP) effects are modeled by convolution with a shape function [249, 248], giving a final accuracy we call NLL+LO+NP. This calculation broadly supports our conclusions from the VINCIA study and offers additional insight into the correspondence between jet mass and track-assisted mass. Appropriate convolutions with parton distribution functions (PDFs) and the replacement $E \rightarrow p_T$ would allow these results to be translated to the LHC.

We examine the effect of jet grooming in Sec. 3.4, using VINCIA and an NLL+LO calculation to assess the correspondence between groomed GTAM and groomed jet
mass. In the noisy environment of the LHC, jet grooming techniques are essential for removing radiation from sources besides the parton initiating the jet [56, 255]. Pileup contamination in the upcoming high-luminosity runs will make grooming even more indispensable [132, 23]. Soft-drop grooming [254] can be easily incorporated into our analytic calculation, allowing us to compute the spectrum of groomed GTAM. In fact, soft-drop grooming removes radiation associated with NGLs to all perturbative orders [174], greatly simplifying analytic calculations. The absence of NGL contributions to the groomed jet mass distribution also implies that this resummed distribution is a complete NLL calculation. We find that the optimal values of the GTAM parameters $\kappa$ and $\lambda$ have a mild dependence on the values of the soft-drop parameters, so the optional GTAM observable is not entirely independent of the grooming procedure. App. B.4 describes another possibility for track-assisted soft-drop grooming.

Our main conclusions are summarized in Sec. 3.5.

### 3.2 Exploration of Generalized Track-Assisted Mass

#### 3.2.1 Observable and Statistic Definitions

Track mass is the mass of a jet computed only using charged particles,

$$M_{\text{track}} = \sqrt{\left( \sum_{i \in \text{tracks}} E_i \right)^2 - \left( \sum_{i \in \text{tracks}} p_{i}\right)^2} , \quad \quad \quad \quad p_{T, \text{track}} = \sqrt{\left( \sum_{i \in \text{tracks}} p_{T,i}\right)^2} , \quad (3.3)$$

where we have also defined the track transverse momentum. The ordinary jet mass ($M_{\text{calo}}$) and jet transverse momentum ($p_{T,\text{calo}}$) are defined analogously, with the sum running over all particles in a jet. In practice, the energy $E_i$ might be replaced by the magnitude $|p_i|$ if particle mass information is not available.

By using angular information only from charged-particle tracks, measurements of track mass can achieve better angular resolution than for ordinary jet mass. This benefit comes with a clear drawback, though, since the distribution of track mass
for heavy resonance jets will no longer peak sharply at the mass of the decaying resonance. Because of the removal of neutral radiation, the track mass will be shifted to lower values compared to ordinary mass, but such an overall shift could easily be corrected through calibration. More importantly, fluctuations in the fraction of energy carried by charged particles will widen the distribution. For the quark/gluon jet ensemble with \( p_{T,\text{min}} > 300 \) GeV studied below, the fractional standard deviations of the jet mass distributions are

\[
\frac{\sigma_{\text{calo}}}{\langle M_{\text{calo}} \rangle} = 0.48, \quad \frac{\sigma_{\text{track}}}{\langle M_{\text{track}} \rangle} = 0.53, \tag{3.4}
\]

so there is an intrinsic loss of resolution by using charged particles compared to all particles.

An observable that is more closely related to the ordinary jet mass can be constructed using a re-weighting factor involving \( p_{T,\text{calo}} \) and \( p_{T,\text{track}} \). This is the motivation for track-assisted mass in Eq. (3.1) and our generalized version in Eq. (3.2), repeated for convenience:

\[
M_{\text{TA}}^{(\kappa, \lambda)} = M_{\text{track}} \left( \frac{p_{T,\text{calo}}}{p_{T,\text{track}}} \right)^{\kappa} \left( \frac{p_{T,\text{calo}}}{p_{T,\text{track}}} \right)^{\lambda}, \quad M_{\text{TA}}^{(1,0)} \equiv M_{\text{TA}}. \tag{3.5}
\]

If the jet-by-jet fluctuations in the charged-to-neutral mass fraction were identical to the jet-by-jet fluctuations in the charged-to-neutral energy fraction, then just using the per-jet rescaling factor \( p_{T,\text{calo}}/p_{T,\text{track}} \) (i.e. \( \kappa = 1 \) and \( \lambda = 0 \)) would yield a good jet-mass proxy. More generally, one can include charged-to-neutral fraction information from some ensemble of jets \( \mathcal{E} \),

\[
\left\langle \frac{p_{T,\text{calo}}}{p_{T,\text{track}}} \right\rangle = \frac{1}{|\mathcal{E}|} \sum_{\epsilon \in \mathcal{E}} \frac{p_{T,\text{calo}}}{p_{T,\text{track}}}, \tag{3.6}
\]

which has the potential to smooth out jet-by-jet fluctuations to produce a narrower GTAM distribution closer to the width of the ordinary jet mass distribution. In general, the optimal choices of \( \kappa \) and \( \lambda \) will depend on the jet samples of interest, since there can be different correlations between energy and mass for different types
of jets.

To avoid biasing the GTAM distribution, the appropriate ensemble for computing the average in Eq. (3.6) should be as similar as possible to the jets being measured, but still large enough to have acceptable statistical uncertainties. For example, all jets in a relatively narrow \( p_T \) and rapidity range would be a reasonable choice. Fortunately, the charged particle momentum fraction is rather scale insensitive, so averaging over a wide \( p_T \) and rapidity range turns out to not have much of an effect. This is true even accounting for differences in the quark/gluon composition of the ensemble; see further discussion in App. B.1. We also examined the impact of adding a shift parameter \( M_{TA}^{(\kappa, \lambda)} \rightarrow M_{TA}^{(\kappa, \lambda)} + B p_{T,\text{calo}} \), but found that this additional parameter did not improve the correspondence to ordinary jet mass.

To quantify the statistical difference between the distributions of \( M_{TA}^{(\kappa, \lambda)} \) and \( M_{\text{calo}} \), we use the statistic\(^4\)

\[
\Delta(p, q) = \sum_{a \in \text{bins}} \frac{1}{2} \frac{(p_a - q_a)^2}{p_a + q_a}, \quad \Delta \in [0, 1]. \tag{3.7}
\]

The sum is over histogram bins, and \( p_a \) and \( q_a \) are the probability weights of bin \( a \) in the probability distributions \( p \) and \( q \). A value of \( \Delta = 0 \) indicates that the distributions \( p \) and \( q \) are identical, and a value of 1 occurs when they have no overlap. This statistic is appealing because it is simple, symmetric between \( p \) and \( q \), and does not rely on assumptions about the underlying distribution of the data, aside from statistical independence of the samples. In this chapter, we only compare the distributions \( M_{TA}^{(\kappa, \lambda)} \) and \( M_{\text{calo}} \), so for simplicity of notation, we label \( \Delta \) by the \( \kappa, \lambda \) parameters,

\[
\Delta(\kappa, \lambda) \equiv \Delta \left( M_{TA}^{(\kappa, \lambda)}, M_{\text{calo}} \right). \tag{3.8}
\]

It is worth emphasizing that Eq. (3.7) is defined at the level of probability distributions, which is not the same as comparing observables on a jet-by-jet basis. For

\(^4\)Without the normalizing factor of \( \frac{1}{2} \), this is known in the information theory literature as triangular discrimination [1]. In the high-energy physics literature, this is often called the separation power.
single-differential jet mass cross sections, the similarity of the probability distributions is what matters, since that is what is being directly measured. On the other hand, for multi-differential distributions, for calibration purposes, or in the presence of additional jet substructure cuts, the jet-by-jet comparison of GTAM to ordinary jet mass might be more meaningful. Because our analytic calculations in Sec. 3.3 can only handle single-differential distributions, we focus on the statistic in Eq. (3.7), which favors $\kappa \simeq 0.5$ and $\lambda \simeq 0.5$. We have some evidence that the ATLAS default of $\kappa = 1$ and $\lambda = 0$ may be preferable for multi-differential cross sections or when there is a narrow cut on jet mass, but this conclusion depends on the precise statistical metric used.

### 3.2.2 Parton Shower Results

To gain some intuition for the performance of GTAM, we perform a parton shower study relevant for the LHC. We generate the process $pp \rightarrow \text{dijets}$ (including the underlying event) at a center-of-mass energy of 14 TeV, using the VINCIA 2.2.2 [185, 171] parton shower plugin to PYTHIA 8.230 [306, 305]. We verified that similar results could be obtained using the PYTHIA default parton shower as well. Jets are identified using the anti-$k_T$ algorithm [97] with jet radius $R = 0.4$, as implemented by FASTJET 3.3.0 [96, 99]. The jet mass and GTAM are measured on the highest $p_T$ jet in each event. The results are presented for jets with $p_{T,\text{calo}} > 100$ GeV, $p_{T,\text{calo}} > 300$ GeV, and $p_{T,\text{calo}} > 1000$ GeV. Results for separate quark and gluon distributions are provided in App. B.1, where the differences are shown to be small.

As a simple proxy for jet mass, one can rescale the track mass by a constant factor $M_{\text{track}} \rightarrow C \, M_{\text{track}}$. If QCD jets were made entirely of pions with exact isospin symmetry, we would expect $M_{\text{track}}$ to be a rescaling of $M_{\text{calo}}$ by a constant factor of $2/3$, which could be corrected using $C = 3/2$. The jet ensembles considered here have an ensemble-averaged $p_T$ ratio of $\langle p_{T,\text{calo}}/p_{T,\text{track}} \rangle = 1.6$, which is close to the $3/2$ predicted by isospin symmetry. Thus, a useful way to parametrize a constant rescaling is to fix $\kappa = 0$ in Eq. (3.5) and scan over $\lambda$ values, which is the same as rescaling $M_{\text{track}}$ by an overall multiplicative constant. As shown in Fig. 3-2a for
Figure 3-2: (a) GTAM distributions for $p_{T,\text{calo}} > 300$ GeV with $\kappa = 0$ and $\lambda = \{0, 0.5, 1, 1.5\}$, with ordinary jet mass plotted as a dashed black curve for comparison. (b) $\Delta(0, \lambda)$ as a function of $\lambda$, in the $p_{T,\text{calo}} > 100$ GeV, $p_{T,\text{calo}} > 300$ GeV, and $p_{T,\text{calo}} > 1000$ GeV ensembles.

Figure 3-3: Same as Fig. 3-2 but (a) with GTAM parameters $\kappa = \{0, 0.5, 1, 1.5\}$ and $\lambda = 0$ and (b) $\Delta(\kappa, \lambda = 0)$ as a function of $\kappa$. 
$p_T,\text{calo} > 300\text{ GeV}$, this crude rescaling is reasonably successful in practice. Scanning over $\lambda = \{0, 0.5, 1, 1.5\}$, the best correspondence between GTAM and $M,\text{calo}$ is for the thick blue curve with $\lambda = 1$. In Fig. 3-2b, we plot the $\Delta(0, \lambda)$ statistic for jets with $p_T$ cuts of 100 GeV, 300 GeV, and 1000 GeV, where again the best jet-mass proxy is achieved for $\lambda$ close to one.

In the ATLAS approach to track-assisted mass, the track mass is rescaled by the per-jet ratio $p_T,\text{calo}/p_T,\text{track}$. This is equivalent to fixing $\lambda = 0$ in Eq. (3.5). The motivation for this strategy is that the charged-to-total $p_T$ fraction can vary jet by jet, which would leave an imprint on the $M,\text{track}/M,\text{calo}$ ratio. In Fig. 3-3a, we show the distributions of GTAM for $\kappa = \{0, 0.5, 1, 1.5\}$ in the $p_T,\text{calo} > 300\text{ GeV}$ sample. The best fit is obtained from the thick green curve with $\kappa = 1$, which is the value used by ATLAS. We plot $\Delta(\kappa, 0)$ in Fig. 3-3b, where $\kappa = 1$ is preferred in all three $p_T$ ranges considered. Comparing Figs. 3-2b and 3-3b, we see that the per-jet charged $p_T$ fraction is a significantly more effective rescaling factor than the ensemble-average $p_T$ fraction.

As a hybrid of the two above approaches, we can consider $\lambda = 1 - \kappa$. Reweighting the track mass by the per-jet $p_T,\text{calo}/p_T,\text{track}$ ratio does correct for the removal of neutral-particle energies, but it does not account for fluctuations in the angular dist-
Figure 3-5: (a) The Δ statistic in the two-dimensional \((\kappa, \lambda)\) space, for the \(p_{T,\text{calo}} > 300\) GeV sample. The minimum of Δ occurs at \(\kappa = 0.54, \lambda = 0.50\). (b) One-dimensional slices of \(\Delta(\kappa, \lambda)\), corresponding to Figs. 3-2b, 3-3b, and 3-4b.

Distribution of neutral particles. Therefore, one expects that using ensemble-averaged information can help reduce this angular variability. For the \(p_{T,\text{calo}} > 300\) GeV sample, distributions of \(M^{(\kappa, 1-\kappa)}_{\text{TA}}\) are plotted in Fig. 3-4a. Intriguingly, the choice \((\kappa, \lambda) = (0.5, 0.5)\) interpolates between the per-jet rescaling at low mass and the ensemble-averaged rescaling at high mass, giving an overall better correspondence to \(M_{\text{calo}}\). The values of \(\Delta(\kappa, 1-\kappa)\) are shown in Fig. 3-4b, where the overall best fit is close to \(\kappa = 1 - \lambda \approx 0.5\) in all \(p_T\) ranges considered.

The full two-dimensional distribution of Δ as a function of \((\kappa, \lambda)\) is shown in Fig. 3-5a for the \(p_{T,\text{calo}} > 300\) GeV sample. Similar results are obtained in the other \(p_T\) ranges as well. As expected by dimensional analysis, the relationship \(\lambda_{\text{best}} \simeq 1 - \kappa\) holds to an excellent approximation, with the minimum of this \(\Delta(\kappa, \lambda)\) distribution at \(\kappa = 0.54, \lambda = 0.50\). In Fig. 3-5b, we show three one-dimensional slices of the full two-dimensional parameter space, \((\kappa, 0)\), \((0, \lambda)\), and \((\kappa, 1 - \kappa)\), equivalent to the middle curves in Figs. 3-2b, 3-3b, and 3-4b. We conclude that a combination of per-jet and ensemble-averaged charged-fraction information provides a statistically closer proxy to calorimeter jet mass than the original track-assisted definition in Eq. (3.1), motivating further studies of GTAM at the LHC.
It is worth emphasizing that these best-fit values of $\kappa \approx 0.5$ and $\lambda \approx 0.5$ are derived from quark/gluon ensembles. Different optimal parameters may be found for boosted electroweak-scale resonances, though we expect the relation $\lambda_{\text{best}} \simeq 1 - \kappa$ to always hold to an excellent approximation. In preliminary studies, we find that boosted $W$ jets have a $\Delta(\kappa, 1 - \kappa)$ minimum closer to $\kappa = 0.95$, more in keeping with the ATLAS default strategy, though this a relatively shallow minimum. That said, an advantage in $W$ mass resolution might be offset by an increase in QCD background contamination, since larger values of $\kappa$ yield a larger high-side mass tail, as evident from Fig. 3-4a. Moreover, the optimal choice of $\lambda$ and $\kappa$ will be affected by the use of substructure discriminants, so a more detailed study of track-assisted boosted object tagging is warranted.

### 3.3 Track-Assisted Mass in $e^+e^-$ Annihilation

In this section, we perform a first-principles QCD calculation of the GTAM distribution. To avoid the myriad complications from hadronic collisions, we focus on the process $e^+e^- \rightarrow$ hadrons with center-of-mass energy $E_{\text{CM}}$, though many of the results here have a straightforward extension to the LHC. We focus on large radius jets with $R = 1$ such that $E_{\text{calo}} \approx E_{\text{CM}}/2$.

To simplify the presentation, we start with the original track-assisted mass with $(\kappa, \lambda) = (1, 0)$. After defining the necessary quantities in Sec. 3.3.1, we perform a resummed calculation of the $M_{\text{TA}}$ distribution in Sec. 3.3.2, and use this to understand the close correspondence to ordinary jet mass in Sec. 3.3.3. We match to fixed-order calculations in Sec. 3.3.4. Here, we neglect virtual terms, which only contribute to the overall normalization, and fix the normalization at the end of the calculation.

We then extend these calculations to GTAM with general $\kappa$ and $\lambda$ in Sec. 3.3.5. Non-perturbative corrections are included in Sec. 3.3.6 using a shape function. Finally, we present the best-fit values of $\kappa$ and $\lambda$ in Sec. 3.3.7. Details of the resummed calculation appear in App. B.2, and details of the fixed-order calculation appear in App. B.3.
3.3.1 Defining Track-Based Observables

In $e^+e^-$ collisions, a modified version of track-assisted mass is appropriate, with energy replacing transverse momentum,

$$M_{TA} = M_{\text{track}} \left( \frac{E_{\text{calo}}}{E_{\text{track}}} \right).$$

For convenience, we define the dimensionless rescaled (squared) track-assisted mass $\rho_{TA}$ and the equivalent $\rho_{\text{calo}},$

$$\rho_{TA} = \frac{M_{\text{track}}^2}{E_{\text{calo}}^2 R^2} \left( \frac{E_{\text{calo}}}{E_{\text{track}}} \right)^2, \quad \rho_{\text{calo}} = \frac{M_{\text{calo}}^2}{E_{\text{calo}}^2 R^2},$$

which take values in the interval $[0,1].$ For the calculations in this section and Sec. 3.4, we always use a jet radius of $R = 1$ unless otherwise noted.

The track fraction $x_i$ is the fraction of parton $i$’s momentum carried by charged particles after hadronization [261, 111]. At the partonic level, each parton momentum $k_i$ is rescaled by its corresponding track fraction, $k_i^{\mu,\text{charged}} = x_i k_i^\mu + \mathcal{O}(\Lambda_{\text{QCD}}).$ Writing the rescaled track mass then only requires making the replacement $k_i \rightarrow x_i k_i,$ yielding

$$\rho_{TA} = \frac{\left( \sum_{i \in \text{jet}} x_i k_i \right)^2}{\left( \sum_{i \in \text{jet}} x_i E_i \right)^2 R^2}.$$

The track functions $T_i(x_i)$ are the distributions of the track fraction, where there is a process-independent track function $T_i$ for each parton flavor. As shown in Ref. [111], the track functions have well defined field-theoretic definitions. At lowest order in $\alpha_s,$ $T_i(x_i)$ is just the empirical distribution of $x_i$ extracted from a global fit to experimental data, or, as in this work, extracted from the PYTHIA parton shower. Of course, all track functions have support only on $x \in [0,1].$ Some sample track functions are plotted for gluons and active quark flavors in Fig. 3-6a. The anti-quark track functions are the same by charge conjugation invariance. For the remainder of this work we focus on jets initiated by gluons and down quarks. Our calculation for quark-initiated

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5As discussed in Sec. 3.3.4, the upper kinematic boundary for a two parton jet is actually $\approx \frac{1}{4}$. ---
Figure 3-6: (a) Track functions extracted from PYTHIA 8.230 (see Ref. [158]) for gluons and active quark flavors at a scale of $\mu = 300$ GeV. (b) Track functions from PYTHIA for gluon jets (red) and down-quark jets (blue) at scales $\mu = \{100, 300, 1000\}$ GeV.

jets is done in the limit of massless quarks, so the only dependence on the quark flavor comes from these distributions.

While the track functions are non-perturbative objects, they have a perturbative renormalization group evolution [111, 158], which is described by a non-linear version of the DGLAP equations [193, 265, 151, 49]. When applied to a jet of energy $E_{\text{calo}}$, the appropriate scale to evaluate the track function is typically $\mu = E_{\text{calo}}R$. Fig. 3-6b illustrates the scale dependence of the gluon and down-quark track functions. The ordinary jet mass $\rho_{\text{calo}}$ can always be recovered from the track-assisted version simply by setting the track functions to be $T_i(x) = \delta(1 - x)$, which then sets the energy fraction $x$ equal to one in all expressions.

At parton level, for a single splitting $i \rightarrow jk$, we can write the two-parton form of the observable $\hat{\rho}$ in terms of the track fractions $x_j$ and $x_k$, the momentum fraction $z$ carried by parton $k$, and the angle between the splitting products $\theta_{jk}$,

$$
\hat{\rho}_{\text{TA}} = \left( \frac{2x_jx_kz(1 - z)(1 - \cos \theta_{jk})}{x_j^2(1 - z)^2 + 2x_jx_kz(1 - z) + x_k^2z^2} \right) \frac{1}{R^2}.
$$

(3.12)
To perform the resummed calculation for track-assisted mass, we need the soft-collinear limit of this expression. Expanding to lowest order in $z$ and $\theta_{ij} \equiv \theta$, we obtain

$$\hat{\rho}_{TA} \simeq \frac{x_k z \theta^2}{x_j R^2} + \ldots .$$ \hspace{1cm} (3.13)

Subleading terms in this expansion contribute starting at NNLL, beyond the accuracy of our resummed calculation. We expect formally power-suppressed corrections proportional to $R \log R$ arising from this truncation to appear in the fixed-order matching (see Sec. 3.3.4).

### 3.3.2 Resummed Calculation

To resum large logarithms of $\rho$, we must compute the cumulative distribution $\Sigma(\rho)$. Since $\rho$ is an additive observable in the limit $\rho \to 0$, the cumulative distribution can be written in the form

$$\Sigma(\rho) \equiv \int_0^\rho \, dp' \frac{d\sigma}{d\rho'} = C(\alpha_s) \Sigma(\alpha_s, \rho) + D(\alpha_s, \rho).$$ \hspace{1cm} (3.14)

The function $C(\alpha_s)$ can be expanded in powers of $\alpha_s$ and is independent of the observable $\rho$. The remainder function $D(\alpha_s, \rho) \to 0$ as $\rho \to 0$. The large logarithms of $\rho$ appear in the function $\tilde{\Sigma}(\alpha_s, \rho)$, which can be expanded in powers of $\alpha_s$ according to [45]

$$\ln \tilde{\Sigma}(\alpha_s, \rho) = \sum_{n=1}^{\infty} \sum_{m=1}^{n+1} \left( \frac{\alpha_s}{2\pi} \right)^n G_{nm} \ln^m \frac{1}{\rho}$$

\begin{align*}
&= \left( \frac{\alpha_s}{2\pi} \right) \left( G_{12} \ln^2 \frac{1}{\rho} + G_{11} \ln \frac{1}{\rho} \right) \\
&\quad + \left( \frac{\alpha_s}{2\pi} \right)^2 \left( G_{23} \ln^3 \frac{1}{\rho} + G_{22} \ln^2 \frac{1}{\rho} + G_{21} \ln \frac{1}{\rho} \right) \\
&\quad + \left( \frac{\alpha_s}{2\pi} \right)^3 \left( G_{34} \ln^4 \frac{1}{\rho} + G_{33} \ln^3 \frac{1}{\rho} + G_{32} \ln^2 \frac{1}{\rho} + G_{31} \ln \frac{1}{\rho} \right) \\
&\quad + \ldots .
\end{align*}
Our calculation at NLL order accuracy resums terms in $\ln \tilde{\Sigma}$ in the first two columns of Eq. (3.15), that is, terms of the form $(\alpha_s/2\pi)^n G_{nm} \ln^m \frac{1}{\rho}$ for $m = n + 1$ and $m = n$. When combined with fixed-order corrections necessary in the large $\rho$ region, this gives a calculation that is valid for $\alpha_s \ln \frac{1}{\rho} \lesssim 1$, which is much larger than the region $\alpha_s \ln^2 \frac{1}{\rho} \ll 1$.

For a non-track-based observable, we can write this cumulative distribution as [105, 104, 66]

$$\Sigma_{\text{calo}}(\rho) = \frac{e^{-\gamma_E R'_{\text{calo}}(\rho)}}{\Gamma(1 + R'_{\text{calo}}(\rho))} e^{-R_{\text{calo}}(\rho)} N(\rho), \quad R'_{\text{calo}}(\rho) = -\frac{dR_{\text{calo}}(\rho)}{d \ln(\rho)}, \quad (3.16)$$

valid to NLL order. The factor $N(\rho)$ is the result of NGLs [137]. Although progress has been made towards computing this contribution, it still presents a substantial complication to a full NLL calculation of the jet mass. Treating this factor is beyond the scope of this work, though it has been shown [254, 174] that soft-drop grooming removes contributions from NGLs to all orders in $\alpha_s$, so this factor will not be present for the groomed distributions in Sec. 3.4.3.

The radiator $R_{\text{calo}}(\rho)$ can be interpreted as the probability that the hard quark (or gluon) will radiate a gluon such that the mass of the resulting two-parton quark-initiated (gluon-initiated) jet is greater than some value $\rho$. The factor $e^{-R_{\text{calo}}}$ is the exponential of the single-emission probability, and the factors which depend on $R'$ describe the sensitivity of $\rho$ to multiple independent emissions. Explicitly, the radiator for a jet initiated by a parton of flavor $i$ is given by

$$R_{\text{calo}}(\rho) = \int_0^1 dz P_i(z) \int_0^{R_{\text{calo}}} \frac{d\theta}{\theta} \alpha_s \frac{E_{\text{calo}}(z \theta)}{\pi} \Theta(\rho_{\text{calo}} - \rho), \quad (3.17)$$

where $\rho_{\text{calo}}$ is given by Eq. (3.13) with $x_j = x_k = 1$. The reduced splitting functions $P_i$ for $i = q, g$ are given in App. B.2.

To calculate the cross section for a track-based observable, one has to convolve the all-particle results with a track function for each final-state parton [111, 158]. This means that processes with $N$ independent gluon emissions from a parton of flavor $i$
must involve $N$ gluon track functions, plus a single track function for parton $i$, as in Fig. 3-7. Analogous to the calculation for generalized angularities \cite{261}, the gluon track functions will exponentiate with the radiator, while the initiating parton’s track function will not. Therefore for a track-based observable, we include the gluon track function in the definition of the radiator. This leads to the modified cumulative distribution for track-assisted mass

$$
\Sigma_{TA}(\rho) = \int_0^1 dx_j T_j(x_j) \frac{e^{-\gamma E_{R\mu}(\rho, x_j)}}{\Gamma(1 + R_{TA}(\rho, x_j))} e^{-R_{TA}(\rho, x_j)},
$$

where the radiator is

$$
R_{TA}(\rho, x_j) = \int_0^1 dx_k T_g(x_k, \mu) \int_0^1 dz P_t(z) \int_0^R d\theta \frac{\alpha_s(E_{\text{calo}} z\theta)}{\pi} \Theta(\tilde{\rho}_{TA} - \rho).
$$

Both track fractions $x_j$ and $x_k$ appear in the expression of the observable Eq. (3.12), but since the gluon track function $T_g(x_k)$ exponentiates with the radiator, $x_k$ is integrated over in Eq. (3.19). This leaves the radiator as a function of $x_j$, and the integral over $x_j$ is only performed in Eq. (3.18).

To achieve NLL accuracy (neglecting NGLs), it is sufficient to include the running of $\alpha_s$ up to two-loop accuracy in the calculation of Eqs. (3.17) and (3.19). When computing the multiple-emissions prefactor at NLL order, it is sufficient to make the fixed-coupling approximation in $R'$ and only keep the LL terms. Thus, the coupling in $R'$ is evaluated at the hard scale of the interaction, $\mu_{\text{hard}} = E_{\text{calo}} R$. As described above, the track functions have a scale dependence described at leading order ($O(\alpha_s)$) by a nonlinear version of the DGLAP equations. As we shall see in the next section,
Figure 3-8: Resummed distributions at NLL for rescaled jet mass $\rho_{\text{calo}}$ (dashed curves) and rescaled track-assisted mass $\rho_{\text{TA}}$ (solid curves) with $R = 1$ for (a) gluon-initiated jets and (b) down-quark-initiated jets. Shown are three different values of the jet energy, $E_{\text{calo}} = 100$ GeV, 300 GeV, and 1000 GeV.

The radiator in Eq. (3.19) is independent of the track functions at LL, and therefore this running only contributes starting at NNLL. This is beyond the precision of our calculation, and so we freeze all track functions in $\Sigma_{\text{TA}}$ at the scale $\mu_{\text{hard}}$. Pushing the precision of this calculation to NNLL order would require including the evolution of the track functions, evaluated at the scale $E_{\text{jet}}z\theta$.

The differential distribution $\frac{d\sigma}{dp}$ is obtained by numerically taking the $\rho$ derivative of Eq. (3.18). These are plotted in Fig. 3-8 for gluon-initiated jets and for down-quark-initiated jets, with $R = 1$ and $E_{\text{calo}} = 100$ GeV, 300 GeV, and 1000 GeV. The only dependence on the quark flavor comes from the track functions, as illustrated in Fig. 3-6a. The track-assisted mass distributions are similar to the jet mass distributions for both quarks and gluons, but the similarity is much stronger for gluon jets, for reasons which we now explain.
3.3.3 Insights at Fixed Coupling

We can apply the same analysis from Ref. [111] for track thrust to achieve some insight into the close correspondence between track-assisted mass and jet mass. We proceed by examining Eq. (3.18) in the fixed-coupling approximation. The appropriate scale to fix the coupling is the characteristic scale of the jet, which for $e^+e^-$ collisions is just $\mu = E_{\text{calc}}R$. In this approximation, to NLL order in the observable $\rho$, the radiator becomes

$$R_{TA}(\rho, x_j) \equiv \frac{\alpha_s C_i}{\pi} \int_{x_j, \rho}^{\lambda} \frac{dx_k}{x_j, x_k} T_g(x_k) \left[ \frac{1}{2} \ln^2 \left( \frac{\rho}{\rho} \right) + \ln \left( \frac{\rho}{\rho} \right) + \ln \left( \frac{x_k}{x_j} \right) + B_i \right]. \quad (3.20)$$

The factor $B_i$ is $-\frac{3}{4}$ for quark-initiated jets and $-\frac{11}{12} + \frac{T_{\text{F}n}{3} C_A}$ for gluon-initiated jets. The color factors $C_i$ are $C_F = \frac{4}{3}$ for quarks and $C_A = 3$ for gluons.

In choosing to keep only terms with logarithms of $\rho$, we have neglected logarithms of $x_k$ and $x_j$, which become large near the track function endpoint $x \approx 0$. As illustrated in Fig. 3-6, however, the track functions are smooth distributions with most of their probability weight parametrically far from zero. We can parametrize the gluon and down-quark track functions as $T_g(x) \propto x^{\lambda_g}$ and $T_d(x) \propto x^{\lambda_d}$ as $x \to 0$, with $\lambda_g \approx 5.7$ and $\lambda_d \approx 2.4$. In the $x \to 0$ limit where logs of $x$ become large, the integrand $T_k(x) \ln(x) \to x^{\lambda_k} \ln(x) \to 0$. Thus, since the track functions themselves suppress logs of $x_j$ and $x_k$, keeping only logarithms of $\rho$ is justified.

Working to NLL order, from Eq. (3.20) we can compute

$$R''_{TA}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} f^{g, 0}(x_j, 1) \ln \left( \frac{\rho}{\rho} \right), \quad (3.21)$$

defined in terms of the partial logarithmic moments of the track functions

$$f^{i, n}(a, b) = \Theta(\min(b, 1) - a) \int_a^b dx T_i(x) \ln^n(x), \quad f^{i, n} = f^{i, n}(0, 1). \quad (3.22)$$

The zero-th moment is just the normalization of the track function, $f^{i, 0} = f^{i, 0}(0, 1) =$
Since \( x_j \leq 1 \) and we are working in the region where \( \rho \ll 1 \), we can expand the integral around \( x_j \rho \approx 0 \), keeping only the leading term. This amounts to extending the lower endpoint of the integral over \( x_k \) in the radiator to 0.\(^8\) With this approximation, \( R' = R'(\rho) \) is independent of both track fractions, yielding

\[
R_{TA}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} \left[ \frac{1}{2} \ln^2 \left( \frac{1}{\rho} \right) + \ln \left( \frac{1}{\rho} \right) \left( f^{g,1} - \ln(x_j) + B_i \right) \right], \quad R'_{TA}(\rho) = \frac{\alpha_s C_i}{\pi} \ln \left( \frac{1}{\rho} \right).
\]

The explicit expression for the cumulative distribution in this approximation is

\[
\Sigma_{TA}(\rho) = \frac{e^{-\gamma_E R_{TA}}}{\Gamma(1 + R'_{TA})} \exp \left\{ - \frac{\alpha_s C_i}{\pi} \left( \frac{1}{2} \ln^2 \left( \frac{1}{\rho} \right) + \ln \left( \frac{1}{\rho} \right) B_i \right) \right\}
\times \exp \left\{ - \frac{\alpha_s C_i}{\pi} \ln \left( \frac{1}{\rho} \right) f^{g,1} \right\} \times \int_0^1 dx_j T_j(x_j) \exp \left\{ \frac{\alpha_s C_i}{\pi} \ln \left( \frac{1}{\rho} \right) \ln(x_j) \right\}.
\]

We can further simplify the factor involving the down-quark track function with an exponential approximation \(111\),

\[
\int_0^1 dx_j T_j(x_j) \exp \left\{ \frac{\alpha_s C_i}{\pi} \ln \left( \frac{1}{\rho} \right) \ln(x_j) \right\} \approx \exp \left\{ \frac{\alpha_s C_i}{\pi} \ln \left( \frac{1}{\rho} \right) f^{g,1} \right\}.
\]

This exponential approximation holds to within 10% for all parton flavors over the range of energies considered in this chapter down to \( \rho \approx 10^{-6} \). It improves substantially with increasing jet energy and increasing \( \rho \). This provides an approximate expression at NLL order with fixed coupling for the cumulative distribution,

\[
\Sigma_{TA}(\rho) \approx \Sigma_{calo}(\rho) \times \exp \left\{ - \frac{\alpha_s C_i}{\pi} \ln \left( \frac{1}{\rho} \right) (f^{g,1} - f^{d,1}) \right\}.
\]

The gluon and down-quark first logarithmic moments are \((f^{g,1}, f^{d,1}) \approx (-0.53, -0.62)\) at 100 GeV, \((-0.52, -0.59)\) at 300 GeV, and \((-0.51, -0.58)\) at 1000 GeV.

The result above demonstrates why track-assisted mass is numerically so close to

\(^7\)The \( \Theta \)-function and \( \min \) are necessary since the integral bounds are set by the \( \Theta \) functions of the observable (and the soft-drop \( \Theta \) functions in Sec. 3.4).

\(^8\)For \( \rho = 0.1 \), the region \( x_k < \rho \) accounts for only \( \approx 1.2\% \) of the probability weight for down-quark track functions and \( \approx 0.01\% \) for gluon track functions at 300 GeV.
ordinary jet mass, through the approximate cancellation between these two terms. While the cancellation is much more precise for gluon jets, $f^{3,1} = f^{g,1}$, than for quark jets with $f^{3,1} = f^{q,1}$, it is still not exact due to the approximations that we have just described. This is why the agreement in Fig. 3-8 between track-assisted mass and jet mass is closer for gluon jets than for quark jets, but still not perfect. Note that setting $f^{g,1} = f^{q,1} = 0$ recovers the fixed-coupling approximation for ordinary jet mass.

3.3.4 Fixed-Order Corrections

The resummed calculation in Sec. 3.3.2 only holds in the regime $\rho \ll 1$, where terms proportional to $\log^2 \rho$ and $\log \rho$ dominate and terms which are powers of $\rho$ or constants can be neglected. Producing a distribution that is correct over the full kinematic range of $\rho$ requires matching this all-orders distribution to a fixed-order calculation for a specific process. We choose the process $e^+e^- \rightarrow \gamma^*/Z \rightarrow q\bar{q}g$ to match to the resummed quark-jet calculation and $e^+e^- \rightarrow H \rightarrow ggg(q\bar{q}g)$ for the gluon-jet one. Due to the Higgs coupling to gluons only through a quark loop, the process $e^+e^- \rightarrow H \rightarrow ggg(q\bar{q}g)$ is already $O(\alpha_s^2)$ in the Standard Model. To make this computation more tractable, we compute the matrix elements for this process in the $m_t \rightarrow \infty$ limit, as discussed in App. B.3.1. Since the differential distribution $\frac{d\sigma}{d\rho}$ diverges as $\rho \rightarrow 0$ for both processes, we placed a cutoff on the observable, and performed the numerical calculation for $\rho > 10^{-6}$. This allows us to neglect virtual terms which only contribute to a delta function at $\rho = 0$, and also removes contributions from the part of phase space where the matrix elements diverge. Since we are ultimately interested in calculating the statistic in Eq. (3.8), we fix the overall normalization of our distributions to 1.

For a three-parton final state, we can rewrite the observable Eq. (3.12) using the parton energy fractions $y_i = \frac{2E_i}{Q}$, which satisfy $y_1 + y_2 + y_3 = 2$. If partons 1 and 3 are clustered in the same jet, this leads to a new formula for the observable,

$$\hat{\rho}_{TA} = \left(\frac{4x_1 x_3 (1 - y_2)}{(x_1 y_1 + x_3 (2 - y_1 - y_2))^2}\right) \frac{1}{R^2}. \quad (3.27)$$
At this perturbative order, the differential cross section for track-assisted mass is (ignoring contributions proportional to a delta function at $p = 0$),

$$
\frac{d\sigma}{d\rho} = \int dy_1 dy_2 \frac{d\hat{\sigma}}{dy_1 dy_2} \int dx_1 dx_2 T_1(x_1) T_2(x_2) \Theta(R - \theta_{13}) \delta(\hat{\rho}_{TA} - \rho), \quad (3.28)
$$

with $\hat{\rho}_{TA}$ given now by Eq. (3.27). The $\Theta$ function requires that two partons be in the same jet. Explicit expressions for the partonic cross sections $d\hat{\sigma}/dy_1 dy_2$ are given in App. B.3.1. Since track-assisted mass is not IRC safe, the cross section must be convolved with the track functions $T_1(x_1)$ and $T_3(x_3)$ for the two partons in the jet.

To match our all-orders result to the fixed-order calculation, we use the modified log-$R$ matching scheme [104]

$$
\ln \left( \Sigma_{\text{NLL+LO}}(\rho) \right) = \ln \left( \Sigma_{\text{NLL}}(\rho) \right) + \Sigma_{\text{LO}}(\rho) - \Sigma_{\text{NLL},s}(\rho). \quad (3.29)
$$

The cumulative distribution $\Sigma_{\text{NLL},s}$ is obtained by expanding the NLL cumulative distribution in powers of $\alpha_s$ and taking the $O(\alpha_s)$ piece,

$$
\Sigma(\rho)_{\text{NLL}} = 1 - \frac{\alpha_s C_i}{\pi} \int_0^1 dx_j T_j(x_j) \left[ \frac{1}{2} f^{g,0}(x_j \rho, 1) \ln^2 \left( \frac{1}{\rho} \right) \right. \\
+ \ln \left( \frac{1}{\rho} \right) f^{g,0}(x_j \rho, 1) \left[ B_i - \ln(x_j) \right] + f^{g,1}(x_j \rho, 1) \right] + O(\alpha_s^2). \quad (3.30)
$$

The cumulative cross section $\Sigma_{\text{LO}}$ is the integral of the corresponding differential cross section in Eq. (3.28):

$$
\Sigma_{\text{LO}}(\rho) = \int_0^\rho d\rho' \frac{1}{\sigma_0} \frac{d\sigma_{\text{LO}}}{d\rho}. \quad (3.31)
$$

The normalization factors for the quark and gluon fixed-order distributions are the Born-level cross sections

$$
\sigma_0^q = \sum_{\text{colors}} \sum_{f=u, d, b} \frac{4\pi \alpha^2}{3s} Q_f^2, \quad \sigma_0^g = \frac{s^2}{8\pi} \left( \frac{m_e A}{v_{\text{EW}}(s - m_H^2)} \right)^2. \quad (3.32)
$$

Here $Q_f$ is the fermion electric charge, $v_{\text{EW}}$ is the Higgs vacuum expectation value, and $A$ is the effective coupling constant in the $m_t \to \infty$ effective theory [213, 147,
in which the matrix elements for $e^+e^- \rightarrow H \rightarrow ggg(q\bar{q}g)$ were calculated (see App. B.3.2).

We would like our matched NLL+LO distribution to vanish at the upper kinematic endpoint of the LO parton-level process, which is

$$\rho_{\text{max},\text{LO}} = \frac{1 - \cos(R)}{2R^2} \approx 0.23 \ (R = 1).$$

(3.33)

In the modified log-$R$ framework, we enforce this condition with the replacement

$$\frac{1}{\rho} \rightarrow \frac{1}{\rho} - \frac{1}{\rho_{\text{max},\text{LO}}} + e^{-B_i},$$

(3.34)

where $e^{-B_i}$ is the endpoint of the NLL resummed calorimeter mass distribution [272].

In Fig. 3-9, we illustrate the matching procedure described above. In the top row, we plot the gluon and down-quark NLL differential distributions in blue, and LO distributions in dark green. The light green curves are the differential distributions obtained from the $\rho$ derivative of the $\mathcal{O}(\alpha_s)$ piece of Eq. (3.30). As expected, these distributions match the LO distributions in the $\rho \rightarrow 0$ limit, where the fixed-order result is dominated by large logs of $\rho$. With the log-$R$ prescription, this gives us the NLL+LO matched distributions (red curves).

The bottom row of Fig. 3-9 shows the ratio

$$\frac{1 \frac{d\sigma_{\text{NLL},\alpha_s}}{d\rho}}{\sigma_0 \frac{d\sigma_{\text{LO}}}{d\rho}},$$

(3.35)

for $M_{\text{calo}}$ with $E_{\text{CM}} = 300$ GeV and several values of the jet radius $R$. We might naively expect this ratio to approach one as $\rho \rightarrow 0$, since double and single logs of $\rho$ should dominate finite terms in this limit. Instead, the difference between this ratio and unity scales as $R \log R$. This is a power-suppressed effect in the small $R$ limit, as expected since we took the collinear limit of the observable in Eq. (3.13). When we go to the soft-drop groomed distributions in Sec. 3.4.3, this residual will be noticeably smaller since soft drop grooms away wide-angle contributions that contribute to this power correction.
3.3.5 Extension to Generalized Track-Assisted Mass

With the full NLL+LO machinery in place, the extension to GTAM is straightforward for arbitrary values of \( \kappa \) and \( \lambda \). To compute the NLL-resummed GTAM distribution, we first need to rewrite the observable value from Eq. (3.12) for a parton-level splitting \( i \to jk \) as

\[
\hat{\rho}^{(\kappa,\lambda)}_{TA} \simeq \frac{x_k z \theta^2}{x_j^{2\kappa-1} \langle x_i \rangle^{2\lambda} R^2}, \quad \langle x_i \rangle = \int_0^1 dx_i x_i T_i(x_i). \quad (3.36)
\]

The track function in Eq. (3.36) corresponds to the parton initiating the jet, and the expectation value of \( x_i \) gives the ensemble-averaged charged energy fraction for that parton. In terms of the NLL calculation, this just requires the replacement \( R(\rho, x_j) \to R(\rho, x_j^{2\kappa-1} \langle x_i \rangle^{2\lambda}) \) in Eq. (3.18). Similarly, to carry out the fixed-order calculation, we replace Eq. (3.27) with

\[
\hat{\rho}^{(\kappa,\lambda)}_{TA} = \left( \frac{4x_1 x_3 (1 - y_2)(2 - y_2)^{2\kappa-2}}{(x_1 y_1 + x_3 (2 - y_1 - y_2))^{2\kappa}} \right) \frac{1}{\langle x_1 \rangle^{2\lambda} R^2}. \quad (3.37)
\]

The only change to the log-\( R \) matching scheme from Sec. 3.3.4 is

\[
\Sigma_{\text{NLL},\alpha} = - \int_0^1 dx_j T_j(x_j) R(\rho, x_j) \quad \Rightarrow \quad \Sigma_{\text{NLL},\alpha} = - \int_0^1 dx_j T_j(x_j) R(\rho, x_j^{2\kappa-1} \langle x_i \rangle^{2\lambda}). \quad (3.38)
\]

In the top row of Fig. 3-10, we show gluon and down-quark NLL+LO matched distributions for \( \rho_{\text{track}}, \rho_{TA} \), and our recommended GTAM observable \( \rho_{TA}^{(0.5,0.5)} \). To make the comparison between GTAM and jet mass more clear, we plot the ratio of \( \rho_{TA}^{(\kappa,\lambda)} \) over \( \rho_{\text{calo}} \) for these same observables in the bottom row of Fig. 3-10. As expected from the VINCIA study, the \( (\kappa, \lambda) = (0.5,0.5) \) distribution more closely tracks the \( \rho_{\text{calo}} \) shape in the peak region, though a precise comparison needs to include non-perturbative effects, which we now add.

3.3.6 Non-Perturbative Corrections

For low values of \( \rho \), or equivalently low values of \( M \), perturbative all-orders contributions to the cross section are dominated by non-perturbative effects. In par-
ticular, an analytic calculation which does not include non-perturbative information will not correctly predict the location of the peak of the jet mass distribution. As described in App. B.2, the appropriate scale $\mu$ to evaluate the coupling in the radiator functions Eqs. (3.17) and (3.19) is the momentum transfer of the splitting, $\mu = E_{\text{calo}}^2 \theta$. For low $\rho$ values, the lower bounds on the integrals over $z$ and $\theta$ are very small, and $\mu$ can enter the non-perturbative regime. One way to handle this problem is to freeze the coupling at a scale $\mu_{\text{NP}} \simeq \Lambda_{\text{QCD}}$. Non-perturbative effects below this scale can often be handled by convolution with a non-perturbative shape function [271, 154, 249, 248, 298, 262, 206, 273, 312].

These non-perturbative effects will occur with a characteristic scale $E_{\text{NP}} \simeq \Lambda_{\text{QCD}}$, and will therefore be suppressed in a hard interaction with scale $Q$ by powers of $\Lambda_{\text{QCD}}/Q$. The quantity with the appropriate dimensions is

$$\tau_n = \frac{M^2}{E_n} \sim \tau_n^{\text{PT}} + \tau_n^{\text{NP}},$$

where $n = \text{calo}$ or track. We can write the differential cross section including non-perturbative corrections as

$$\left( \frac{d\sigma}{d\rho} \right) = \int_0^{Q^\rho} d\tau F_{\text{NP}}(\tau) \left( \frac{d\sigma(\rho - \tau/Q)}{d\rho} \right)^{\text{PT}},$$

where $Q$ is the scale of the hard interaction. Following Ref. [312], we use a shape function with the parametrized form

$$F_{\text{NP}}(\tau_n) = \frac{4\tau_n}{\Omega^2_n} e^{-\frac{2\tau_n}{\Omega_n}}, \quad n = \text{calo, track},$$

which is normalized to one, falls off exponentially for large $\tau_n$, and goes linearly to zero at small $\tau_n$.

To perform the convolution in Eq. (3.40), we need to identify the appropriate energy scale $Q$ to divide $\tau_n$. For $\tau_{\text{calo}}$, the relevant scale is $Q_{\text{calo}} = E_{\text{calo}} R^2$. For $\tau_{\text{track}},$
we can write

$$\rho^{(\kappa, \lambda)}_{TA} = \frac{M^2_{track}}{E^2_{calo} R^2} \left( \frac{E_{calo}}{E_{track}} \right)^{2\kappa} \left( \frac{E_{calo}}{E_{track}} \right)^{2\lambda} = \left( \frac{\tau_{track}}{E_{calo} R^2} \right) (x_i)^{1-2\kappa} (x_i)^{-2\lambda}. \tag{3.42}$$

In the limit that the track function $T_i$ of the initiating parton is narrow, we can replace the track fraction $x_i$ in Eq. (3.42) with its average value. This gives us the hard scale by which non-perturbative effects are suppressed

$$Q_{\text{track}} = E_{calo} R^2 \langle x_i \rangle^{2\kappa+2\lambda-1} = Q_{\text{calo}} \langle x_i \rangle^{2\kappa+2\lambda-1}. \tag{3.43}$$

Following the reasoning of Ref. [111], we expect that $Q_{\text{track}} \approx \langle x_g \rangle Q_{\text{calo}}$. This should hold in the limit that the matrix element which defines the non-perturbative parameter $Q_{\text{track}}$ in the OPE is dominated by a single gluon emission, and in the limit that the track function of the initiating parton $T_i$ is narrow. We will take the track fraction $\langle x_i \rangle = \langle x_g \rangle = 0.6$ in these relations. The gluon and quark shift parameters should be related by approximate Casimir scaling, $\Omega^g_n / \Omega^q_n \approx C_A / C_F$, as expected for observables which are additive in the soft-collinear limit [259, 189]. As shown in Fig. 3-11, we find a reasonable match between the analytic calculations and VINCIA with the functional form of Eq. (3.41) and the NP parameters

$$\Omega^q_{\text{calo}} = 0.8 \text{ GeV}, \quad \Omega^g_{\text{calo}} = 2.0 \text{ GeV},$$

$$\Omega^g_{\text{track}} = 0.5 \text{ GeV}, \quad \Omega^q_{\text{track}} = 1.2 \text{ GeV}, \tag{3.44}$$

which obey the relations just described. These parameters, which we found by fitting to predictions from a parton shower, must ultimately be extracted from fits to experimental data.

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9 Alternately, one could convolve with a track function. The perturbative cross section in Eq. (3.40) is the NLL+LO matched distribution, so it is not straightforward to assign this track fraction to one of track functions already used in the calculation.

129
3.3.7 Best Fit Parameters

With the complete NLL+LO+NP calculation of the GTAM distributions, we can now compute $\Delta(\kappa, \lambda)$ from first principles. This statistic is plotted in the $(\kappa, \lambda)$ plane for gluons (Fig. 3-12a) and down quarks (Fig. 3-12c), with one-dimensional slices in Figs. 3-12b and 3-12d. Note that we have not attempted to estimate theoretical uncertainties on these distributions.

Compared to the VINCIA $pp$ result in Fig. 3-5a, the analytic calculation of $\Delta(\kappa, \lambda)$ has the same qualitative features, with a broad minimum at $\kappa + \lambda = 1$. The precise value of the minimum is different, though with the NLL+LO+NP result predicting a minimum at $(\kappa = 0.9, \lambda = 0.1)$ for gluons and $(\kappa = 0.8, \lambda = 0.1)$ for down quarks, as compared to $(\kappa = 0.54, \lambda = 0.50)$ for the VINCIA $pp \rightarrow$ dijets study. This is likely due to the fact that the overall degree of agreement between $M_{\text{calo}}$ and $M_{\text{TA}}^{(\kappa, \lambda)}$ is closer in the analytic calculation than in VINCIA, so ensemble-averaged information plays a less effective role.
Figure 3-9: Top row: Components of the matching calculation for (a) gluons and (b) down quarks. The full matched NLL+LO result is in red, the LO fixed-order distribution is in dark green, and the $\mathcal{O}(\alpha_s)$ piece of the fixed-order expansion of the NLL resummed distribution is in light green. The NLL distribution is plotted in blue. Bottom row: The corresponding ratios of the $\mathcal{O}(\alpha_s)$ piece of the NLL distribution over the LO differential distribution, for various values of jet radius $R$ to highlight the $R \log R$ residual.
Figure 3-10: Top row: NLL+LO calculations of the GTAM distribution for (a) gluon jets and (b) down-quark jets, compared to ordinary jet mass. Bottom row: corresponding ratio between GTAM and jet mass.
Figure 3-11: GTAM distributions computed from VINCIA (stepped histograms) and NLL+LO with non-perturbative corrections (smooth curves). Shown are (a) calorimeter jet mass, (b) track mass, (c) track-assisted mass, and (d) GTAM with $\kappa = 0.5$ and $\lambda = 0.5$. 
Figure 3-12: Left column: Distribution of $\Delta(\kappa, \lambda)$ computed using the analytic NLL+LO distributions convolved with the shape function $F_{NP}$ for gluons (top) and down quarks (bottom). The white cross marks the best-fit value, which is $(0.9, 0.1)$ for gluons and $(\kappa, \lambda) = (0.8, 0.1)$ for down quarks. The white dot marks track-assisted mass, $\rho_{TA} = \rho_{TA}^{(0,0)}$. Right column: One-dimensional slices of the distributions on the left. The slight offset of the minimum values in (c) from the line $\lambda = 1 - \kappa$ manifests in the red $(\xi, 0)$ curve dipping below the blue $(\xi, 1 - \xi)$ curve in (d) before intersecting again at $\xi = 1$. 

134
3.4 Impact of Soft-Drop Grooming

In this section, we study track-assisted mass used in parallel with soft-drop grooming [254]. We first discuss different approaches to track-assisted grooming in Sec. 3.4.1. In Sec. 3.4.2, we perform a VINCIA study on groomed jet GTAM at the LHC. In Sec. 3.4.3, we perform an NLL+LO calculation for $e^+e^-$ collisions. The qualitative lessons from the groomed case mirror the ungroomed case, so our discussion here will be relatively brief.

3.4.1 Track-Assisted Grooming

To implement soft-drop grooming on an ordinary jet, the jet is first reclustered into a Cambridge/Aachen tree [153, 330]. Then the soft-drop condition,

$$\frac{\min(p_{T1}, p_{T2})}{p_{T1} + p_{T2}} > z_{\text{cut}} \left( \frac{\Delta R_{12}}{R_0} \right)^\beta,$$

is applied at each splitting in the tree beginning with the widest. If a splitting fails Eq. (3.45), then the softer branch is removed from the jet and declustering continues to the next splitting. When a splitting passes Eq. (3.45), both subjets are kept, and the grooming procedure stops.

We aim to find a track-assisted proxy for groomed jet mass. To do this, we groom the jet first, and then compute GTAM using the groomed jet constituents. In particular, the factors of $p_{T,\text{calo}}$ we use in the definition of the groomed GTAM observable are the $p_T$ of the groomed jet. This approach ensures that the charged particles used to compute $M_{TA}^{(\kappa,\lambda)}$ are the same as the charged particles in the soft-drop groomed jet whose mass we are trying to reproduce.

The drawback to grooming before restricting to only charged particles is that the grooming procedure itself requires angular information. This problem is less serious than the angular resolution problem when computing the mass $M_{\text{calo}}$, in part because the C/A clustering tree mainly relies on the relative angular order between particles, and is therefore less sensitive to the angular resolution. That said, whether
or not an emission passes Eq. (3.45) does depend on absolute $\Delta R_{12}$ information. For this reason, we explore an alternative approach in App. B.4, where we restrict to charged particles before grooming, though this makes it difficult to define $p_{T,\text{calo}}$ for the reweighting factors.

We will only show results for $\beta \geq 0$, where $\beta = 0$ corresponds to the modified Mass Drop Tagger [140]. For $\beta < 0$, the soft-drop algorithm acts like a tagger and completely grooms away all jets without two hard, well-separated prongs. This leads to a bimodal jet mass distribution with a large population near zero mass, a peak closer to the endpoint, and a gap between the two. Our analytic analysis does not give sensible results if the spike near zero mass is included, since $\Delta$ is determined primarily by jets with masses of only a few GeV. Thus, to avoid any confusion about this issue, we will not show any $\beta < 0$ results in this chapter.\footnote{One way to get a sensible result for $\beta < 0$ is to place a cut on the groomed jet mass of $M_{\text{calo}} > 3$ GeV. The fixed-order calculation can then be used to compute the part of the $\beta < 0$ distribution above this small mass cut.}

### 3.4.2 Parton Shower Study

For our groomed parton shower study, we use the same VINCIA event samples as Sec. 3.2.2, taking an ensemble of jets for which the ungroomed jet has $p_{T,\text{calo}} > 300$ GeV. Fig. 3-13a shows distributions of groomed track-assisted mass and groomed jet mass with $z_{\text{cut}} = 0.1$ for a range of $\beta$ values. We see that groomed track-assisted mass continues to accurately reproduce the groomed jet mass distribution for a wide range of soft-drop parameters.

When incorporating soft-drop grooming, we want to compute $\Delta(\kappa, \lambda)$ where both $M_{\text{TA}}^{(\kappa, \lambda)}$ and $M_{\text{calo}}$ are groomed using the same soft-drop parameters $\beta$ and $z_{\text{cut}}$. We checked the full two-dimensional distribution of $\Delta(\kappa, \lambda)$, and found that, as in Fig. 3-5a, the best-fit values obeyed $\kappa + \lambda = 1$. Since this conclusion is unchanged from Sec. 3.2, we fix $\lambda = 1 - \kappa$ and sweep $\kappa$ in this section. Fig. 3-13b shows $\Delta(\kappa, 1 - \kappa)$ as a function of $\kappa$ for the same grooming parameters. We can see that lower values of $\beta$, which correspond to more aggressive grooming, lead to best-fit parameters with
Figure 3-13: (a) Groomed jet mass and track-assisted mass distributions in VINCIA for $z_{\text{cut}} = 0.1$ and various values of $\beta$. The $\beta = \infty$ curve corresponds to the ungroomed distribution. (b): The statistic $\Delta(\kappa, 1 - \kappa)$ for the same values of $\beta$.

a higher $\kappa$ value. Though not shown, we checked that this trend can also be seen by fixing $\beta$ and scanning a range of $z_{\text{cut}}$ values, with higher $z_{\text{cut}}$ leading to more aggressive grooming and higher best-fit $\kappa$. As we argued in Sec. 3.2, the ensemble-averaged reweighting factor controlled by $\lambda$ corrects for fluctuations in the angular distribution of neutral particles. Since grooming removes soft, wide-angle radiation, we expect the impact of these angular fluctuations to be smaller for jets with more aggressive grooming parameters.

3.4.3 Analytic Calculation with Grooming

We can easily adapt the calculations in Sec. 3.3 to handle soft-drop grooming. One of the major benefits of soft-drop grooming from the theoretical perspective is that it removes radiation corresponding to NGLs, which are difficult to calculate and were neglected in Sec. 3.3.

Starting from the NLL resummation, the radiator function in Eq. (3.19) describes the probability of an emission with $\hat{\rho}(z, \theta) > \rho$ and therefore involves an integral over the allowed phase space for this emission. Grooming restricts this allowed phase
space, so the soft-drop condition in Eq. (3.45) must be included in the radiator, which becomes

\[
R_{TA}(\rho, x_j) = \int_0^1 dx_k T_g(x_k) \int_0^1 dz P_1(z) \int_0^R d\theta \frac{\alpha_s(E_{\text{calo}} z \theta)}{\pi} \Theta(\hat{\rho}_{TA} - \rho) \Theta(z - z_{\text{cut}} \left( \frac{\theta}{R} \right)^\beta).
\]

(3.46)

The function \( \hat{\rho} \) is unchanged from Eq. (3.12).11 The track fractions do not appear in the grooming \( \Theta \)-function because grooming is applied to the full jet, as described above; see App. B.4 for an alternate prescription where the grooming is applied to the track-only jet.

Truncating to NLL order and making the fixed-coupling approximation as in Sec. 3.3.3, we can again see the cancellation of the track function logarithmic moments. For \( \beta > 0 \), the radiator in the fixed-coupling approximation becomes (an analogous expression holds for \( \beta = 0 \), see App. B.2)

\[
R_{TA}(\rho, x_j) \overset{\text{F.C.}}{=} \frac{\alpha_s C_i}{\pi} \left\{ \frac{\ln^2(1/\rho)}{2} \left[ \frac{\beta}{2 + \beta} f_{g,0}^{g,0}(y^*, 1) + f_{g,0}^{g,0}(x_j \rho, y^*) \right] + \ln(1/\rho) \left[ B_i f_{g,0}^{g,0}(x_j \rho, 1) - \ln(x_j) \left( \frac{\beta}{2 + \beta} f_{g,0}^{g,0}(y^*, 1) + f_{g,0}^{g,0}(x_j \rho, y^*) \right) \right. \\
+ \frac{\beta}{2 + \beta} f_{g,1}^{g,0}(y^*, 1) + f_{g,1}^{g,0}(x_j \rho, y^*) + \left. \frac{2}{2 + \beta} f_{g,0}^{g,0}(y^*, 1) \ln \left( \frac{1}{z_{\text{cut}}} \right) \right] \right\},
\]

where \( y^* = \min \left( \frac{x_j \rho}{x_{j,\text{cut}}}, 1 \right) \). The terms proportional to \( f_{g,n}^{g,0}(y^*, 1) \) account for the regions of \( x_j, x_k \) phase space where grooming is active, characterized by the boundary \( \frac{x_k \rho}{x_j} < \rho \). The region where grooming is inactive, \( \frac{x_k \rho}{x_j} > \rho \), contributes the terms proportional to \( f_{g,n}^{g,n}(x_j \rho, y^*) \).

Now setting \( x_j \rho \) in the integral endpoints to zero and making the exponential approximation in Eq. (3.25) for the integral over \( x_j \), we obtain the approximate

---

11When one branch of the splitting fails the soft-drop condition, we have simply groomed away the softer particle, without accounting for flavor-changing effects present at finite \( z_{\text{cut}} \). A precise calculation taking this effect into account would have a radiator with matrix structure in flavor space, as described in Refs. [140, 272].
cumulative distribution

\[ \Sigma_{\text{TA}}(\rho) \simeq \exp \left\{ -\frac{\alpha_s C_i}{\pi} \left[ \frac{\beta}{2\gamma} \ln^2(\frac{1}{\rho}) + \ln(\frac{1}{\rho}) \left( \frac{\beta}{2\gamma} \gamma E + B_i + \frac{2}{\gamma} \ln(\frac{1}{\gamma}) \right) \right] \right\} \times \Gamma \left( 1 + \frac{\alpha_s C_i}{\pi} \frac{\beta}{\gamma} \ln(\frac{1}{\rho}) \right)^{-1} \times \exp \left\{ -\frac{\alpha_s C_i}{\pi} \frac{\beta}{\gamma} (f^{g,1} - f^{q,1}) \ln(\frac{1}{\rho}) \right\} . \]

(3.48)

We see that the cancellation between logarithmic moments of the track functions also occurs in the region of phase space where the grooming is active. From this fixed-coupling approximation, we can again predict that in the full calculation, the track-assisted mass will be more similar to the jet mass for gluon jets than for quark jets because of the more complete cancellation. We emphasize that to obtain results which are formally at least NLL order, the full radiator Eq. (3.46) with running \( \alpha_s \) and the accompanying expressions for \( R' \) in App. B.2 are required.

The LO cross section for track-assisted mass measured on soft-drop groomed jets only requires a \( \Theta \) function to implement the grooming,

\[ \frac{d\sigma}{d\rho} = \int dy_1 dy_2 \frac{d\hat{\sigma}}{dy_1 dy_2} \int dx_1 dx_2 T_1(x_1) T_2(x_2) \Theta(R - \theta_{13}) \delta(\rho_{\text{TA}} - \rho) \Theta \left( z - z_{\text{cut}} \left( \frac{\theta_{13}}{R} \right)^\beta \right) . \]

(3.49)

The matching procedure is then exactly the same as in Sec. 3.3.4. It is important that soft-drop grooming with \( \beta \geq 0 \) does not alter the total jet production rate, so the normalization of the fixed-order cross sections is the same as for the ungroomed distribution. The required expressions for the \( \mathcal{O}(\alpha_s) \) piece of the expansion of the resummed distribution, \( \frac{1}{\sigma} \frac{d\sigma_{\text{NLL+LO}}}{dp} \), are given in App. B.2.

Plots of the NLL+LO \( \rho_{\text{calo}} \) and \( \rho_{\text{TA}} \) distributions are shown in Fig. 3-14 for gluon jets and down-quark jets. These distributions have grooming parameters \( z_{\text{cut}} = 0.1 \) and \( \beta = \{0, 1, 5, \infty\} \), where the \( \beta = \infty \) case is the same as the ungroomed observable. As expected from the VINCIA study, we find that the close relationship between track-assisted mass and jet mass holds over a broad range of parameters. This gives a theoretical prediction of the groomed track-assisted mass which can be compared directly to experimental data, without necessitating an unfolding of the track-assisted
mass measurement to ordinary jet mass.

Non-perturbative emissions which contribute to the distribution of $\rho \sim z\theta^2$ must be either soft or collinear. Since Soft Drop changes the relative proportions of soft and collinear radiation, the appropriate non-perturbative parameter $\Omega$ as described Sec. 3.3.6 would depend on the grooming parameters $z_{\text{cut}}$ and $\beta$ [271, 328, 260, 189]. We leave a study of these non-perturbative corrections to future work.

In Fig. 3-15, we again plot the ratio of the $O(\alpha_s)$ piece of the resummed distribution over the fixed-order distribution, this time for groomed jets with $R = 1$, $z_{\text{cut}} = 0.1$, and $\beta = \{0, 1, 5, \infty\}$. For $\beta = \infty$, we recover the $R = 1$ result from Fig. 3-9. With $\beta = 1$ or 5, the two distributions have a much closer match, since the grooming is removing wide-angle radiation that was contributing to the $R \log R$ power correction. The $\beta = 0$ distribution again exhibits a mismatch as $\rho \to 0$, due to constant terms in the radiator which are beyond the order of this calculation. These terms have an effect of the same magnitude as the single logarithmic terms in the $\beta = \infty$ distribution because there are no double-logarithmic terms in the resummed distribution of $\beta = 0$ groomed jet mass [140], so the $\beta = 0$ calculation is formally LL.
Figure 3-15: Ratios of the soft-drop groomed $O(\alpha_s)$ piece of the expanded NLL distributions over the LO $\rho_{TA}$ distributions. The $\beta = 0$ case is dashed since this calculation is formally only LL order.

instead of NLL.
3.5 Conclusions

The different granularity of calorimetry and tracking at the LHC experiments makes it worthwhile to explore proxies for key jet observables like jet mass that can better exploit the fine angular resolution available for charged particle tracks. The original track-assisted mass, as defined by the ATLAS collaboration in Eq. (3.1), is one example of such a proxy, which trades fluctuations in the charged-to-neutral mass fraction for improved track mass resolution. In this paper, we showed that the generalized version of track-assisted mass in Eq. (3.2) can act as an even better proxy for jet mass, by balancing the fluctuations in charged-to-neutral mass fraction against ensemble-averaged information. In the spirit of Ref. [124], this same GTAM philosophy could be applied to situations where both tracking and electromagnetic calorimeter information is used to determine jet mass, but hadronic calorimeter information is only used to determine jet $p_T$. One could even imagine more exotic proxies for jet mass, such as ones that weight higher energy particles more than lower energy ones.

As a step towards a comparison with experimental results, we performed a NLL resummed calculation of the distribution of Eq. (3.10), the rescaled (squared) track-assisted mass, and its generalizations, in $e^+e^-$ collisions. Since track-assisted mass is not an IRC-safe observable, we used the track function formalism to regulate its collinear divergences and regain calculational control. This computation offers some insight into the close correspondence between track-assisted mass and jet mass, as well as the values of the best-fit parameters for GTAM, in terms of the similarity of logarithmic moments of the track functions. We matched our track-assisted mass distributions to the fixed-order processes $e^+e^- \rightarrow q\bar{q}g$ and $e^+e^- \rightarrow H \rightarrow ggg(q\bar{q}g)$ using the log-$R$ matching scheme, and implemented NP corrections using a shape function. We found reasonable agreement between our NLL+LO+NP calculation and distributions obtained from VINCIA. We also explored the impact of soft-drop grooming on track-based observables, where we found that groomed GTAM was effective as a proxy for groomed jet-mass. Though we did not compute contributions from NGLs in this work, these contributions are happily removed by the soft-drop
grooming procedure. It would be interesting to extend our calculations to alternate grooming procedures like recursive soft drop [155].

Future work on this topic would quantify the expected gain in sensitivity to highly collimated decay products at the LHC for generalized track-assisted mass measurements as compared to track-assisted mass and ordinary jet mass using detector simulations. Furthermore, in order to make a quantitative comparison to experimental data, a more precise theoretical calculation is required. Such a calculation would include contributions from NGLs in the ungroomed case, and flavor-changing finite $z_{\text{cut}}$ effects for the soft-drop groomed case. To be competitive with other state-of-the-art jet substructure predictions, the calculation also needs to be pushed to NNLL, including contributions from the RG evolution of the track-functions. The fixed-order corrections have been included only to LO, which is not sufficient for a precision measurement. Lastly, it would be interesting to adapt the machinery developed in Ref. [261] to study the double-differential distribution of $M_{\text{calo}}$ and $M_{\text{T}A}^{(\kappa,\lambda)}$ in order to assess their jet-by-jet correspondence. The use of generalized track-assisted mass as a benchmark jet observable at hadron colliders, with comparisons to precision theoretical calculations, offers the possibility to improve the sensitivity and flexibility of experimental measurements. This will be of vital importance in the high-energy limit at the LHC and at future colliders.
Chapter 4

Comparison of GFF and Generating Functional Frameworks

4.1 Introduction

In this chapter, we compare the generalized fragmentation function formalism with a closely related set of ideas, the generating functional approach (GFA). Generating functionals are a perturbative method with a long history in QCD calculations [247, 225]. They are used to describe the leading-logarithmic-order evolution of quarks and gluons emitting soft-collinear radiation. Ref. [138] derived an evolution equation for quark and gluon generating functionals in terms of the integral over the universal collinear divergence of QCD matrix elements. This evolution equation strongly suggests a close relationship between GFFs and generating functionals. We explore these connections, making both qualitative observations about the differences in structure and applicability between the two methods and explicitly comparing results for observables which are calculable in both frameworks.

First, we give a brief overview of the GFA, focusing on the aspects needed to compare to GFFs, specifically the perturbative evolution of the generating functionals. The two approaches are intrinsically different, so there are many quantities which can be calculated in one framework but not the other. There are however some observables which can be computed in both approaches. Two examples are the energy fraction...
carried by the hardest particle in a jet, and the (moments of) the weighted energy fractions defined in Sec. 2.4, measured on all final-state particles. We explicitly show that these two frameworks are in agreement for these observables. In the second half of this chapter, we develop another connection between the GFF and GFA methods, using the recently developed recursive soft drop (RSD) grooming technique [155]. The fraction of a jet's energy remaining after RSD grooming is an IRC-safe observable only for values of the grooming parameter $\beta > 0$. In this regime, the GFA provides a leading-log resummed calculation of the groomed energy fraction. When $\beta = 0$, the groomed energy fraction becomes collinear unsafe, and the GFF formalism can be applied to regulate this collinear divergence. We make a fixed-order comparison between the two frameworks for the $\beta = 0$ case.

In recent years, building on early work in Refs. [302, 93, 94], a number of novel techniques have been developed to remove unassociated wide-angle radiation from hadronic jets in efficient and robust ways. These techniques have become an essential part of the LHC experiments' toolbox, and have been used in a wide range of contexts.

A drawback of early substructure algorithms is that by imposing hard cuts on subjets, analytic control over jet observables can be spoiled by non-global [137] and clustering logarithms [241, 97, 236]. The modified mass-drop tagger [140, 139] and its extension soft drop [254] resolved this issue by introducing a more theoretically motivated algorithm, leading to groomed jets whose remaining single-logarithmic contributions can be calculated to very high precision [174, 175].

Recursive soft drop, a recently developed recursive extension of the soft drop algorithm, was shown to improve resilience to pileup effects and enhance the jet-mass resolution, while retaining all useful features of mMDT/soft drop. The algorithm proceeds by reclustering a jet with a Cambridge-Aachen (C/A) algorithm [153, 330], and iterating through the clustering tree, removing the softer branch at each step until a node passes the soft-drop condition

$$\min(z, 1 - z) > z_{\text{cut}} \left( \frac{\theta}{R_0} \right)^\beta.$$

(4.1)
At this node, both branches are kept and are ordered in the separation $\Delta R$ of their subjets. The algorithm continues to iterate on the widest remaining subjet until Eq. (4.1) has been satisfied $N$ times, resulting in $N + 1$ subjets, or until the full clustering tree has been processed to its end points. The remaining subjets compose the resulting groomed jet once the algorithm terminates. In the limit that $N \rightarrow \infty$, all soft, wide-angle radiation in the jet is groomed away, leading to jets with a vanishing catchment area [98].

When $\beta > 0$, the fraction of the jet energy retained after grooming is an IRC-safe quantity, since emissions with $\theta < R_0$ will not be groomed, and these emissions set a minimum value on the observable. The GFA can be used to produce an all-orders calculation of the groomed-energy-fraction distribution. We describe this calculation and show plots of the result in Sec. 4.3.2.

In the $\beta \rightarrow 0$ limit, the groomed energy fraction becomes collinear unsafe. This makes all-orders calculations of its distribution using the generating functional technique divergent. The GFF approach can be applied to describe the perturbative renormalization group evolution of the groomed energy fraction at $\beta = 0$. We describe the application of this framework to observables defined with RSD and compare leading fixed-order distributions of the groomed energy fraction from the GFF and GFA approaches.

The layout of the rest of this chapter is as follows. In Sec. 4.2 we make a detailed comparison of the GFF and GFA frameworks. We first review the GFF and GFA formalisms in Secs. 4.2.1 and 4.2.2, and then discuss in general the similarities and differences between GFFs and the GFA in Sec. 4.2.3. We specialize to explicit calculations of the hardest-particle energy fraction in Sec. 4.2.5 and the moment-space weighted energy fractions in Sec. 4.2.4. Sec. 4.3 discusses these tools in the context of jets groomed with recursive soft drop. The GFA for RSD-groomed jets with $\beta > 0$ is described in Sec. 4.3.2. The IRC-unsafe case with $\beta = 0$ is then treated in the GFA in Sec. 4.3.3. RSD with $\beta = 0$ is explored in the GFF formalism in Sec. 4.3.4. Explicit comparisons between the two frameworks for the RSD-groomed energy drop are made at leading order in Sec. 4.3.5. Finally, we conclude in Sec. 4.4.
4.2 Comparison of Generating Functional and GFF Results

4.2.1 Review of the GFF Approach

Generalized fragmentation functions (GFFs) [158] are non-perturbative objects which absorb collinear singularities arising in the calculation of IRC-unsafe observables. A GFF $\mathcal{F}_i(x, \mu)$ encodes the probability that a parton of flavor $i$ at scale $\mu$ will fragment into a jet with a value $x$ of the jet observable. The GFF may be defined using only a subset of the final-state particles resulting from the fragmentation and hadronization of parton $i$. A broad class of observables which can be described using the GFF formalism are the weighted energy fractions (WEFs) [261, 158]. These are defined as

$$ x = \sum_{i \in \text{jet}} w_i \left( \frac{E_i}{E_{\text{jet}}} \right)^\kappa. $$

(4.2)

The exponent $\kappa$ must be $> 0$ to ensure that the WEF is soft safe. The coefficients $w_i$ are weights that can be assigned to jet particles based on any quantum number (except momentum). For example, the weighted jet charge [170] has $w_i = Q_i$, the particle’s electric charge, the track fraction [110, 111] sets $\kappa = 1$ and $w_i = 1$ for charged particles and 0 for neutral particles, and the jet $p_T^D$ [261] sets $w_i = 1$ for all particles and $\kappa = 2$.

The renormalization group evolution of the GFFs due to these divergences is described by the evolution equations

$$ \frac{d}{d\mu} \mu \frac{\mathcal{F}_q(x, \mu)}{\pi} = \int dz dx_1 dx_2 \frac{\alpha_s(\mu)}{\pi} P_{q \rightarrow qg}(z) \mathcal{F}_q(x_1) \mathcal{F}_g(x_2) \delta(x - \hat{x}(z, x_1, x_2)), $$

(4.3)

$$ \frac{d}{d\mu} \mu \frac{\mathcal{F}_g(x, \mu)}{\pi} = \int dz dx_1 dx_2 \frac{\alpha_s(\mu)}{\pi} \left[ \frac{1}{2} P_{g \rightarrow q\bar{q}}(z) \mathcal{F}_q(x_1) \mathcal{F}_q(x_2) ight. $$

$$ + n_f P_{g \rightarrow q\bar{q}}(z) \mathcal{F}_q(x_1) \mathcal{F}_\bar{q}(x_2) \left| \delta(x - \hat{x}(z, x_1, x_2)). \right. $$

(4.4)

---

1An appropriate definition for use at hadron colliders would require the replacement $E_i \rightarrow p_{T,i}$ and $E_{\text{jet}} \rightarrow p_{T,\text{jet}}$.

2The CMS collaboration defines the observable $p_T^D$ as the square root of this quantity [24].
This non-linear version of the DGLAP evolution equations [193, 265, 151, 49] includes a convolution with two GFFs at each parton branching. This is necessary because final-state particles resulting from the hadronization of any parton in the jet can contribute to the value of the observable if they have nonzero weights. In this leading-order evolution equation, it is convenient to write the splitting functions in the notation $P_{i ightarrow jk}$. Higher-order evolution equations would have to include also $1 \rightarrow 3$ splittings. The $\delta$-function enforces the proper evolution of the distribution of the observable $x$, described by the recursion relation $\dot{x}(z, x_1, x_2)$. For example, the recursion relation for the WEFs is

$$\dot{x}(z, x_1, x_2) = z^\times x_1 + (1 - z)^\times x_2.$$  \hspace{1cm} (4.5)

The collinear singularities which GFFs must cancel appear in the perturbative amplitudes for parton-level processes. This implies that they must appear in a parton-level calculation of the GFFs. The field-theoretic GFF operator definition in Ref. [158] includes non-perturbative matrix elements. Treating these matrix elements partonically, the GFFs can be calculated order-by-order in $\alpha_s$. Using dim-reg and $\overline{\text{MS}}$ renormalization obtains at $O(\alpha_s)$

$$\mathcal{F}^{(1)}_{i, \text{bare}}(x) = \frac{1}{2} \sum_{j,k} \int dz \left[ \frac{\alpha_s(\mu)}{2\pi} \left( \frac{1}{\epsilon_{\text{UV}}} - \frac{1}{\epsilon_{\text{IR}}} + 2 \right) P_{i \rightarrow jk}(z) \right]$$

$$\times \int dx_1 dx_2 \mathcal{F}^{(0)}_j(x_1, \mu) \mathcal{F}^{(0)}_k(x_2, \mu) \delta[x - \tilde{x}(z, x_1, x_2)].$$  \hspace{1cm} (4.6)

In this expression, the hadronization information is included in the leading-order GFFs $\mathcal{F}^{(0)}_j$ and $\mathcal{F}^{(0)}_k$, which are just the empirical distribution of the observable $x$ taken from data. From the point of view of perturbative calculations and RG evolution, these empirical distributions merely serve as a boundary condition, which could be changed arbitrarily. Of course, this will give unphysical predictions which do not match data but are useful for a formal comparison to the GFA. The boundary
condition which we will use for the rest of this chapter is

$$F_i^{(0)}(x, \mu) = \delta(1-x).$$  \hspace{1cm} (4.7)

This is the distribution of the observable $x$ for jets consisting of a single parton.

To obtain explicit expressions for a GFF at fixed order in $\alpha_s$, we integrate Eqs. (4.3) and (4.4), obtaining at leading order

$$\int dF_i(x, \mu) = \frac{1}{4} \int d\ln(\mu^2) \sum_{jk} \int dz \frac{\alpha_s(\mu)}{\pi} P_{i\to jk}(z) \int dx_1 dx_2 F_j(x_1) F_k(x_2) \times$$

$$\times \delta(x - \hat{x}(z, x_1, x_2))$$

$$= \frac{1}{4} \sum_{jk} \ln(\mu^2) \int dz \frac{\alpha_s(\mu)}{\pi} P_{i\to jk}(z) \int dx_1 dx_2 F_j(x_1) F_k(x_2) \times$$

$$\times \delta(x - \hat{x}(z, x_1, x_2)) + f(x, \mu_0).$$  \hspace{1cm} (4.8)

In obtaining the second line, we ignored the running of $\alpha_s$, which will make a contribution starting at $O(\alpha_s^2)$, as we will discuss in Sec. 4.2.4. The function $f(x, \mu_0)$ is an integration constant, which we will fix by turning off the perturbative evolution at $\Lambda = 0.2275$ GeV. This requires setting the boundary condition $F_i(x, \Lambda) = F_i^{(0)}(x, \mu) = \delta(1-x)$. Except for the terms from the running coupling, this gives us an expression for the distribution

$$F_i(x, \mu) = \delta(1-x) + \frac{1}{4} \sum_{jk} \ln(\frac{\mu^2}{\Lambda^2}) \int dz \frac{\alpha_s(\mu)}{\pi} P_{i\to jk}(z) \int dx_1 dx_2 F_j(x_1) F_k(x_2) \times$$

$$\times \delta(x - \hat{x}(z, x_1, x_2)).$$  \hspace{1cm} (4.9)

We can then write the GFF for a parton of species $i$ as an expansion in $\alpha_s$,

$$F_i(x, \mu) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{\alpha_s}{2\pi}\right)^n F_i^{(n)}(x, \mu).$$  \hspace{1cm} (4.10)
Inserting this expression into Eq. (4.9), we obtain an iterative solution for $F_i(x, \mu)$.

### 4.2.2 Review of Generating Functional Approach

Generating functional methods have long been known to describe the leading-log emissions of soft and collinear radiation from a fragmenting parton [247, 225]. Their description and derivations of their basic properties can be found in standard textbooks, for example [152, 161]. The collinear evolution equation of Ref. [138] provides a Monte-Carlo based technique for computing jet observables, which is briefly reviewed here.

We introduce the generating functionals for quark and gluon microjets, $Q(x, t)$ and $G(x, t)$ respectively [152, 161, 138], which describe the parton content of a quark or gluon in a hadron with momentum $p_T$, carrying a fraction $x$ of the hadron $p_T$, and probed at a smaller angular scale $t$. Mean numbers of quark and gluon microjets are obtained from the generating functionals by taking functional derivatives

$$\frac{dn_{q(z)}(t)}{dz} = \frac{\delta Q(1, t)}{\delta q(z)} \bigg|_{q(x)=1, g(x)=1}, \quad \frac{dn_{g(z)}(t)}{dz} = \frac{\delta G(1, t)}{\delta g(z)} \bigg|_{q(x)=1, g(x)=1}. \quad (4.11)$$

The generating functionals trivially satisfy the condition

$$Q(x, 0) = q(x), \quad G(x, 0) = g(x), \quad (4.12)$$

where $q(x)$ and $g(x)$ indicate a quark or gluon with momentum fraction $x$ and unit probability.

The angular scale $t$ is defined by integration of $\alpha_s$ over the collinear divergence,

$$t(R, R_0, p_T) = \int_{R_0}^{R} \int_{R^2} \frac{d\theta^2}{\theta^2} \frac{\alpha_s(p_T \theta/R_0)}{2\pi}. \quad (4.13)$$

The evolution of the quark and gluon generating functionals with $t$ can be described
by a set of coupled non-linear differential equations

\[
\frac{dQ(x, t)}{dt} = \int dz p_{qq}(z) [Q(zx, t) G((1 - z)x, t) - Q(x, t)] , \tag{4.14}
\]

\[
\frac{dG(x, t)}{dt} = \int dz p_{gg}(z) [G(zx, t)G((1 - z)x, t) - G(x, t)] \\
+ \int dz p_{qg}(z) [Q(zx, t)Q((1 - z)x, t) - G(x, t)] , \tag{4.15}
\]

where the first term in each integrand corresponds to real emission diagrams and the second term with the opposite sign is the virtual contribution. This real/virtual separation is convenient for the calculations below, and follows the notation in Ref. [138]. Separating the virtual terms in this manner means that plus-function regulators are not needed for the splitting functions. We instead take the real splitting functions

\[
p_{qq}(z) = C_F \left( \frac{1 + z^2}{1 - z} \right) , \tag{4.16}
\]

\[
p_{gg}(z) = 2C_A \left( \frac{z}{1 - z} + \frac{1}{2} z(1 - z) \right) , \tag{4.17}
\]

\[
p_{qg}(z) = n_f T_R (z^2 + (1 - z)^2) . \tag{4.18}
\]

We use this form for the splitting functions in GFA expressions in this chapter.

The evolution equations Eqs. (4.14) and (4.15) can be solved iteratively to obtain \(Q(x, t)\) and \(G(x, t)\) as a series in \(t\),

\[
Q(x, t) = \sum \frac{t^n}{n!} Q_n(x) , \quad G(x, t) = \sum \frac{t^n}{n!} G_n(x) , \tag{4.19}
\]

where \(Q_0(x) = q(x)\) and \(G_0(x) = g(x)\). To obtain an expansion to consistent order in \(\alpha_s\), we expand \(t\) order-by-order in \(\alpha_s\),

\[
t(\theta, R_0, p_T) = \frac{2}{\beta_0} \ln \frac{1}{1 - \frac{\alpha_s(p_T)}{4\pi} \beta_0 \ln \frac{R_T^2}{\theta^2}} = \frac{2}{\beta_0} \sum_{n=1}^{\infty} \frac{1}{n} \left( \frac{\alpha_s(p_T) \beta_0}{4\pi} \ln \frac{R_T^2}{\theta^2} \right)^n , \tag{4.20}
\]

with \(\beta_0 = \frac{11}{3} C_A - \frac{4}{3} T_R n_f\). The angle \(\theta(t)\) is related here to the evolution scale \(t\)
through equation (4.20), which corresponds to

\[
\theta(t) = \exp \left[ \pi \frac{\beta_0}{\alpha_s} \left( e^{-\beta_0 t/2} - 1 \right) \right].
\] (4.21)

Note that due to the Landau pole in \( \alpha_s(p_T, \theta) \), this expression for \( \theta(t) \) does not diverge as \( t \to \infty \). Instead, the evolution variable \( t \) is divergent at finite \( \theta \).

As mentioned above, the GFA can be used to obtain all-orders results by resumming collinear logarithms. This is carried out by recasting equations (4.14) and (4.15) as integral equations

\[
Q(x, t) = \Delta_q(t) Q(x, 0) + \int_0^t dt' \Delta_q(t-t') \int_\epsilon^{1-\epsilon} dz p_{qq}(z) Q(zx, t') G((1-z)x, t'),
\] (4.22)

\[
G(x, t) = \Delta_g(t) G(x, 0) + \int_0^t dt' \Delta_g(t-t') \int_\epsilon^{1-\epsilon} dz \left[ p_{gg}(z) G(zx, t') G((1-z)x, t') + p_{qg}(z) Q(zx, t') Q((1-z)x, t') \right].
\] (4.23)

The Sudakov-like form factors have the explicit definition

\[
\Delta_q(t) = \exp \left( -t \int_\epsilon^{1-\epsilon} dz p_{qq}(z) \right),
\] (4.24)

\[
\Delta_g(t) = \exp \left( -t \int_\epsilon^{1-\epsilon} dz (p_{gg}(z) + p_{qg}(z)) \right).
\] (4.25)

The \( \epsilon \) cutoffs in the integrals are necessary for numerically regulating the endpoint singularities, but in the \( \epsilon \to 0 \) limit, these integrals are convergent and independent of \( \epsilon \).

The form factors can be used as no-splitting probabilities in a Monte-Carlo calculation of partonic distributions which can then be integrated over the appropriate regions of phase-space to obtain perturbative all-orders results for observable distributions. The leading-log precision is formally the same as that obtainable by a parton shower. While parton showers include many additional effects which are not captured
by the generating functional calculation, this approach has the benefit of being more transparent. This allows it to easily be matched to fixed-order calculations.

4.2.3 Setup of GFF/GFA Comparison

In this section, we elaborate on some differences between the GFF and GFA frameworks. The two formalisms have many similarities, as can be seen by comparing the evolution equations for GFFs, Eqs. (4.3) and (4.4), and generating functionals, Eqs. (4.14) and (4.15). Both sets of evolution equations are non-linear versions of the DGLAP [193, 265, 151, 49] equations that describe the RG evolution of parton distribution functions and fragmentation functions. The close resemblance of the GFF and GFA evolution equations makes it clear that the two approaches must be closely related. In fact, they can be used to describe the perturbative evolution of many of the same observables.

The most obvious difference between the two frameworks is that the evolution variable for the GFFs is the \( \overline{\text{MS}} \) renormalization scale \( \mu \), whereas the generating functional evolution is in terms of \( t \), the integral over the collinear divergence in the matrix element as defined by Eq. (4.13). This gap can be partially bridged by making a change of variables using Eq. (4.20) to rewrite the GFA equations as an expansion in \( \alpha_s \) instead of \( t \). However, the direction of the evolution, and therefore the initial conditions required, also differs between the two frameworks. The GFF evolution formally works in both directions, but in practice is extremely unstable when evolving from high scale to low scale (see App. A.4). Since the scale for the GFF evolution is \( \mu = p_T R \), evolving to higher scale means evolving to a larger radius. This means that the GFF evolution requires boundary conditions at small \( R \), specifically an initial condition for each hadron in the jet. On the other hand, it is clear from Eq. (4.13) that the generating functional evolution variable \( t \) increases with decreasing \( R \). Thus the generating functional initial conditions are at large \( R \); for \( R = R_{\text{jet}} \), the momentum fraction carried by the parton initiating the jet is unity.

The generating functionals are purely perturbative objects which do not include hadronization information. The GFFs include hadronization information, which is
obtained by fitting to experiments (or parton showers). For comparison to the generating functional, in the following sections this information is not included, so that only perturbative objects are being compared. As explained in Sec. 4.2.1, this merely amounts to a change in the boundary condition for the perturbative evolution.

A less obvious difference in the formalisms is the way in which the definition of an observable is implemented. In the GFF approach, there is a different GFF for each collinear-unsafe observable, and the definition of this observable is included explicitly in the evolution equation through the recursion relation \( \hat{x}(z, x_1, x_2) \). In the GFA, \( Q(x, t) \) and \( G(x, t) \) only describe the momentum fraction carried by a quark or gluon at some value of \( t \). The observable is not relevant for the generating functional evolution. Instead, it is used to define the region of phase space over which the final partonic configuration obtained from the generating functional evolution is integrated.

In Eq. (4.3) and Eq. (4.4), there is an integral over the arguments of the GFFs, \( x_1 \) and \( x_2 \), as well as the momentum fraction \( z \). By contrast, Eq. (4.14) and Eq. (4.15) have an integral only over \( z \). One of these extra integrals is accounted for by the \( \delta \)-function enforcing the recursion relation at each splitting. In the generating functional evolution, this constraint is always the same, that is the momentum fractions must add to one, so it is more convenient to integrate out the \( \delta \)-function. The other extra integral in the GFF evolution comes from the freedom to choose arbitrary boundary conditions for each hadron species, whereas the generating functional boundary condition is always one. This difference in form makes it impossible to rewrite the evolution equations in exactly the same form.

The quantities which can be compared directly are moments of the distributions of observables which are calculable in both frameworks. In the GFF formalism, the \( n \)-th moment of the order \( \alpha_s^k \) distribution for parton \( i \) is defined by

\[
\bar{F}_i^{(k)}(n, \mu) = \int dx \ x^n F_i^{(k)}(x, \mu). \tag{4.26}
\]

The generating functionals do not themselves directly parametrize an observable distribution, but must first be integrated over the appropriate region of phase space.
This requires the relations

\[
\int dx\, x^n q(xz) = \int dx\, x^n g(xz) = z^n, \tag{4.27}
\]

\[
\int dx\, x^n g(xz) g(x(1-z)) = \int dx\, x^n q(xz) q(x(1-z)) \tag{4.28}
\]

\[= \int dx\, x^n g(xz) q(x(1-z)) = (z + (1-z))^n = 1.\]

For an arbitrary observable \(\mathcal{O}\), measured on a jet initiated by a fragmenting parton \(i\), we will denote the \(n\)-th moment of the distribution of \(\mathcal{O}\) at order \(\alpha_s^k\), calculated using the GFA, by \(\langle x^n \rangle_i^{(k)}\). We can then calculate

\[
\langle x^n \rangle_i^{(k)} = \int \left( \prod_{m=1}^k dz_m \right) \mathcal{O}^n(\{z_m\}) PS_i^{(k)}(\{z_m\}), \tag{4.29}
\]

where the phase-space at scale \(t\), \(PS_i^{(k)}(z)\) is just the order \(\alpha_s^k\) generating functional, \(PS_Q^{(k)}(\{z_m\}) = Q^{(k)}(\{z_m\})\) and \(PS_G^{(k)}(\{z_m\}) = G^{(k)}(\{z_m\})\). Of course if all moments of the distribution are known, a transformation back to \(x\) space recovers the exact distribution, and an arbitrarily accurate approximation can be achieved with a finite number of moments. This provides an exact comparison between concrete predictions of the two techniques.

### 4.2.4 N-th Moment for Weighted Energy Fractions

We first compare the GFF and GFA expressions for general moments of the distributions of weighted energy fractions, defined in Eq. (4.2). Note that neither framework has analytic control for \(\kappa \leq 0\), where the observable is not soft safe. We will explain the comparison for quark jets for concreteness. The calculation is exactly the same for gluon jets with the proper replacements of the splitting functions.\(^3\) In the generating functional approach, the moments can be derived starting with Eqns. (3.12a-f)

\(^3\)The only subtlety is that for gluon evolution, there is a mixing between terms proportional to \(T_F\) coming from the running coupling and from the \(p_{gg}\) splitting functions. Comparison between GFF expressions in terms of \(\mu\) and GFA expressions in \(\theta/R_0\) only agree after accounting for terms proportional to \(T_F\) from both sources.
in [138]. From this, one can straightforwardly express Eq. (4.29) up to $O(\alpha_s^2)$ as

\[
\langle \hat{a}^n \rangle_q = 1 + \frac{\alpha_s}{2\pi} \ln \frac{R_0^2}{\theta^2} \int dz p_{qq}(z) \left[ (z^k + (1 - z)^k)^n - 1 \right] \\
+ \frac{1}{2} \left( \frac{\alpha_s}{2\pi} \right)^2 \ln^2 \frac{R_0^2}{\theta^2} \int dz dz' \left\{ p_{qq}(z) p_{qq}(z') \left[ ((1 - z)^k + z^k(1 - z')^k + z^k z'^k)^n - ((1 - z')^k + z'^k) + (1 - z)^k z'^k)^n + 1 \right] \\
+ p_{qq}(z) p_{gg}(z') \left[ (z^k + (1 - z)^k(1 - z')^k + z^k (1 - z')^k)^n - (z^k + (1 - z)^k)^n \right] \\
+ p_{qq}(z) p_{gg}(z') \left[ (z^k + (1 - z)^k(1 - z')^k + (1 - z)^k z'^k)^n - ((1 - z)^k + z'^k)^n \right] \\
+ \frac{\beta_0}{4} \left( \frac{\alpha_s}{2\pi} \right)^2 \ln^2 \frac{R_0^2}{\theta^2} \int dz p_{qq}(z) \left[ (z^k + (1 - z)^k)^n - 1 \right].
\] (4.30)

The last terms comes from the conversion between an expansion in $t$ and $\alpha_s$:

\[
t = \frac{\alpha_s}{2\pi} \ln \frac{R_0^2}{\theta^2} + \left( \frac{\alpha_s}{2\pi} \right)^2 \ln^2 \frac{R_0^2}{\theta^2} + O(\alpha_s^3), \quad \beta_0 = \frac{11C_A - 4T_R n_f}{3}. \quad (4.31)
\]

Now consider the GFF formalism. We start by writing the terms of the expansion Eq. (4.10) explicitly. Using the weighted-energy-fraction recursion relation, Eq. (4.5), and considering as before the partonic initial condition $F_i^{(0)}(x, 0) = \delta(1 - x)$, we obtain the quark fragmentation function

\[
F_q^{(1)} = \ln \left( \frac{\mu^2}{\Lambda^2} \right) \int dz dx_1 dx_2 P_{q\rightarrow qg}(z) F_q^{(0)}(x_1) F_g^{(0)}(x_2) \delta(x - \hat{x}(z, x_1, x_2)),
\]

\[
= \ln \left( \frac{\mu^2}{\Lambda^2} \right) \int dz P_{q\rightarrow qg}(z) \delta(x - \hat{x}(z, 1, 1)). \quad (4.32)
\]

At order $\alpha_s^2$, after integrating the $\ln \frac{\mu^2}{\mu}$ term, we obtain

\[
F_q^{(2)} = \frac{1}{2} \ln^2 \left( \frac{\mu^2}{\Lambda^2} \right) \int dx_1 dx_2 dz \left[ P_{q\rightarrow qg}(z) F_q^{(1)}(x_1) \delta(1 - x_2) \delta(x - \hat{x}(z, x_1, x_2)) \\
+ P_{q\rightarrow qg}(z) F_q^{(1)}(x_2) \delta(1 - x_1) \delta(x - \hat{x}(z, x_1, x_2)) \right].
\]
which can be reduced to

\[ F^{(2)}_q = \frac{1}{2} \ln^2(\frac{\mu^2}{\Lambda^2}) \int dz dz' [P_{q \to qg}(z)P_{q \to qg}(z') \delta(x - \hat{x}(z, \hat{x}(z', 1, 1), 1)) \]
\[ + P_{q \to qg}(z) \frac{1}{2} P_{g \to qg}(z') \delta(x - \hat{x}(z, 1, \hat{x}(z', 1, 1))) \]
\[ + P_{q \to qg}(z) \eta_f P_{g \to qq}(z') \delta(x - \hat{x}(z, 1, \hat{x}(z', 1, 1))) \] (4.33)

It is straightforward to see how these expressions can be recursively solved to yet higher orders in \( \alpha_s \).

Let us now insert the recursion relation Eq. (4.5). We can then compute the \( n \)-th moment of \( F_q \) from Eq. (4.26), obtaining up to order \( \alpha_s^2 \)

\[ \bar{F}^{(2)}_q(n, \mu) = 1 + \frac{\alpha_s(\mu)}{2\pi} \ln^2(\frac{\mu^2}{\Lambda^2}) \int dz P_{q \to qg}(z) \left( z^k + (1 - z)^k \right)^n \]
\[ + \frac{1}{2} \left( \frac{\alpha_s(\mu)}{2\pi} \right)^2 \ln^2(\frac{\mu^2}{\Lambda^2}) \int dz dz' [P_{q \to qg}(z)P_{q \to qg}(z') \times \]
\[ \times \left( z^k z'^k + z^k (1 - z')^k + (1 - z)^k \right)^n \]
\[ + P_{q \to qg}(z) \frac{1}{2} P_{g \to qg}(z') \left( z^k + (1 - z)^k z'^k + (1 - z)^k (1 - z')^k \right)^n \]
\[ + P_{q \to qg}(z) \eta_f P_{g \to qq}(z') \left( z^k + (1 - z)^k z'^k + (1 - z)^k (1 - z')^k \right)^n \]
\[ + \frac{\beta_0}{4} \left( \frac{\alpha_s(\mu)}{2\pi} \right)^2 \ln^2(\frac{\mu^2}{\Lambda^2}) \int dz P_{qq}(z) \left[ (z^k + (1 - z)^k)^n \right] \] (4.34)

The terms proportional to \( \beta_0 \) came from the running of \( \alpha_s \) from the initial scale \( \Lambda \) to the final scale \( \mu \),

\[ \alpha_s(\mu) = \alpha_s(\Lambda) - \frac{\alpha_s(\Lambda)^2}{4\pi} \beta_0 \ln(\mu^2/\Lambda^2) + \mathcal{O}(\alpha_s^3) \]
\[ \implies \alpha_s(\Lambda) = \alpha_s(\mu) + \frac{\alpha_s(\Lambda)^2}{4\pi} \beta_0 \ln(\mu^2/\Lambda^2) + \mathcal{O}(\alpha_s^3) \] (4.35)

The expression Eq. (4.34) is identical to the corresponding one for the GFA, Eq. (4.30) with the replacement \( \mu/\Lambda \to R_0/\theta \), and trading the plus function regulated splitting functions \( P_{ij} \) for the real ones, \( p_{ij} \), explicitly separating the virtual term. Recall that the GFF and GFA evolution equations run in opposite directions, hence the inverted
evolution variables.

4.2.5 Hardest-Particle Energy Fraction

In this subsection, we consider the observable $x_{\text{hard}}$, the momentum fraction carried by the hardest parton in a jet. This is a simple observable which is inclusive enough that its distribution, $f_i(x_{\text{hard}})$, can be computed in the GFA without first transforming to moment space, and therefore is a useful probe of the GFA/GFF connection.\(^4\) In order to see that this is an inclusive observable, we can write it as the limit of a weighted energy fraction measured on all particles as [158],

$$x_{\text{hard}} = \lim_{k \to \infty} \left[ \sum_{i \in \text{jet}} z_i^k \right]^{1/k}. \quad (4.36)$$

For a jet consisting of two partons, the observable $x$ is defined as

$$\hat{x}(z, x_1, x_2) = \max(z x_1, (1 - z) x_2), \quad (4.37)$$

which is the recursive form of the observable used in the GFF evolution, Eqs. (4.3) and (4.4). As before we expand $F_i$ in powers of $\alpha_s$ according to Eq. (4.10), but now instead of solving iteratively for the generating functional using Eq. (4.19), we solve at the distribution level. Thus we can expand $f_i(x_{\text{hard}})$ in powers of $t$ and compare distributions in $x_{\text{hard}}$ space.

$$f_i(x_{\text{hard}}) = \delta(1 - x_{\text{hard}}) + t f_i^{(1)}(x_{\text{hard}}) + \frac{1}{2} t^2 f_i^{(2)}(x_{\text{hard}}) + \ldots \quad (4.38)$$

\(^4\)This distribution was denoted by $f_{\text{hardest}}(x)$ by the authors of Ref. [138], who used the GFA to perform an all-orders computation.
Computing these expansions to lowest nontrivial order by iteratively solving the evolution equations produces

\[
f_q^{(1)}(x_{\text{hard}}) = \int dz \, p_{qq}(z) \left[ \delta(x_{\text{hard}} - \max(z, 1 - z)) - \delta(x_{\text{hard}} - 1) \right], \tag{4.39}
\]

\[
f_g^{(1)}(x_{\text{hard}}) = \int dz \, (p_{qq}(z) + p_{gg}(z)) \left[ \delta(x_{\text{hard}} - \max(z, 1 - z)) - \delta(x_{\text{hard}} - 1) \right], \tag{4.40}
\]

\[
\mathcal{F}_q^{(1)}(x_{\text{hard}}) = \ln \left( \frac{\mu^2}{\Lambda^2} \right) \int dz \, p_{qq}(z) \left[ \delta(x_{\text{hard}} - \max(z, 1 - z)) - \delta(x_{\text{hard}} - 1) \right], \tag{4.41}
\]

\[
\mathcal{F}_g^{(1)}(x_{\text{hard}}) = \ln \left( \frac{\mu^2}{\Lambda^2} \right) \int dz \, (p_{gg}(z) + p_{qq}(z)) \left[ \delta(x_{\text{hard}} - \max(z, 1 - z)) - \delta(x_{\text{hard}} - 1) \right]. \tag{4.42}
\]

We continue the expansion to second nontrivial order, now only showing results for quark distributions. The gluon distributions are identical with the appropriate replacements of splitting functions.

\[
f_q^{(2)}(x_{\text{hard}}) = \int dz \, dz' \left[ p_{qq}(z) p_{qq}(z') \mathcal{P}^{\text{GFA},2a}(z, z', x_{\text{hard}}) + p_{qq}(z) p_{gg}(z') \mathcal{P}^{\text{GFA},2b}(z, z', x_{\text{hard}}) + p_{qq}(z) p_{qg}(z') \mathcal{P}^{\text{GFA},2b}(z, z', x_{\text{hard}}) \right], \tag{4.43}
\]

\[
\mathcal{F}_q^{(2)}(x_{\text{hard}}) = \int dz \, dz' \left[ \mathcal{P}_{q\rightarrow qg}(z) \mathcal{P}_{q\rightarrow qg}(z') \mathcal{P}^{\text{GFF},2a}(z, z', x_{\text{hard}}) + \mathcal{P}_{q\rightarrow qg}(z) \mathcal{P}_{g\rightarrow gg}(z') \mathcal{P}^{\text{GFF},2b}(z, z', x_{\text{hard}}) + \mathcal{P}_{q\rightarrow qg}(z) \mathcal{P}_{g\rightarrow qg}(z') \mathcal{P}^{\text{GFF},2b}(z, z', x_{\text{hard}}) \right]. \tag{4.44}
\]
The differing phase space factors in the integrals come from the choice of using real or standard splitting functions, and are given explicitly by

\[
PS^{GFA,2a}(x, z, z') = \Theta(z - \frac{1}{1+x^2})\Theta(z' - \frac{1}{2})\delta(zz' - x) - \Theta(z - \frac{1}{2})\delta(z - x)
- \Theta(z' - \frac{1}{2})\delta(z' - x) + \Theta(\frac{1}{1+z^2} - z)\Theta(\frac{1}{2-z'} - z)\delta(1 - z - x)
+ \Theta(\frac{1}{2} - z')\Theta(z - \frac{1}{2-z'})\delta((1 - z')z - x) - \Theta(\frac{1}{2} - z)\delta(1 - z - x)
- \Theta(\frac{1}{2} - z')\delta(1 - z' - x) + \delta(1 - x),
\]

\[
PS^{GFF,2a}(x, z, z') = \Theta(z' - \frac{1}{2})\Theta(\frac{z'}{1+z'} - z)\delta(x - z' (1 - z))
+ \Theta(z' - \frac{1}{2})\Theta(z - \frac{z'}{1+z'})\delta(x - z)
+ \Theta(\frac{1}{2} - z')\Theta(\frac{1-z'}{2-z'} - z)\delta(x - (1 - z')(1 - z))
+ \Theta(\frac{1}{2} - z')\Theta(z - \frac{1-z'}{2-z'})\delta(x - z),
\]

(4.46)

\[
PS^{GFA,2b}(x, z, z') = \Theta(z - \frac{z'}{1+z'})\Theta(z - \frac{1-z'}{2-z})\delta(z - x) - \Theta(z - \frac{1}{2})\delta(z - x)
+ \Theta(\frac{z'}{1+z'} - z)\Theta(z' - \frac{1}{2})\delta((1 - z)z' - x)
+ \Theta(\frac{1-z'}{2-z'} - z)\Theta(\frac{1}{2} - z')\delta((1 - z)(1 - z') - x)
- \Theta(\frac{1}{2} - z)\delta(1 - z - x),
\]

\[
PS^{GFF,2b}(x, z, z') = \Theta(z' - \frac{1}{2})\Theta(z - \frac{1}{1+z'})\delta(x - zz')
+ \Theta(z' - \frac{1}{2})\Theta\left(\frac{1+z}{1+z'} - z\right)\delta(x - (1 - z))
+ \Theta(\frac{1}{2} - z')\Theta\left(z - \frac{1}{2-z'}\right)\delta(x - z(1 - z'))
+ \Theta(\frac{1}{2} - z')\Theta\left(\frac{1-z'}{2-z'} - z\right)\delta(x - (1 - z)).
\]

(4.47)

Rewriting Eq. (4.43) in terms of the \(P_{ijk}\) splitting functions, or Eq. (4.44) using the real splitting functions \(p_{ij}\), these equations are identical. One can also still compare numerical values in moment space, for example,

\[
t(f_q)^{(2)} = \frac{\alpha_s}{2\pi} \ln^2(R_0^2/\theta^2) \left[ 0.812941C_F^2 - 0.233594C_AC_F - 0.0355182n_f T_F C_F \right],
\]

(4.48)
\[
\frac{\alpha_s}{2\pi} \hat{F}^{(2)}_q(1, \mu) = \frac{\alpha_s}{2\pi} \ln^2(\mu^2) \left[ 0.812941 C_F^2 - 0.233594 C_A C_F - 0.0355182 n_f T_F C_F \right].
\]

4.3 Energy drop with Recursive Soft Drop

In this section, we aim to study the fraction of the ungroomed jet energy retained after recursive soft drop (RSD) grooming, an observable that is IRC safe only for \( \beta > 0 \). The generating functional approach allows for reliable leading-logarithmic calculations in this regime. After reviewing the RSD algorithm, we first discuss the \( \beta > 0 \) IRC-safe case in the GFA formalism. We then discuss the unsafe case with \( \beta = 0 \) in both the GFA and GFF approaches, making explicit comparisons up to \( \mathcal{O}(\alpha_s^2) \).

4.3.1 Review of Recursive Soft Drop

Let us first review the RSD algorithm, a recent generalization of the modified mass-drop tagger and soft-drop algorithms [140, 139, 254] which implements multiple levels of grooming. The algorithm starts from a jet \( j \) which has been reclustered using a C/A algorithm, and proceeds with the following steps:

1. Split \( j \) into two subjets \( j_1 \) and \( j_2 \) by undoing the last clustering step.

2. If the subjets pass the soft-drop condition

\[
z_{12} > z_{\text{cut}} \left( \frac{\Delta R_{12}}{R_0} \right)^\beta, \quad z_{12} \equiv \frac{\min(p_{t,1}, p_{t,2})}{p_{t,1} + p_{t,2}},
\]

then we keep both branches, otherwise the softer subjet is removed. \( \Delta R_{12} \) is the rapidity-azimuth separation between the subjet axes, and \( R_0 \) is the jet radius parameter from the C/A reclustering.

3. Redefine \( j \) to be the subjet whose two constituents have widest separation \( \Delta R \) among the remaining branches.
4. Iterate this process until condition (4.50) has been satisfied $N$ times, or until we have recursed through the full C/A tree.

In the limit that $N \to \infty$, all soft and wide-angle radiation is removed from the jet. In this limit, RSD grooming produces jets with the interesting property of having zero jet area, such that naive area-based subtraction methods are not suitable after grooming.

### 4.3.2 Generating Functionals for Jet Grooming

We can easily modify the generating functional evolution equations, Eqs. (4.14) and (4.15), for an initial quark or gluon fragmenting into a jet groomed with RSD.\(^5\) For jets reclustered with a C/A algorithm, because the evolution is angular ordered, this is simply obtained by separating out splittings where the soft-drop condition in Eq. (4.50) is not satisfied, and removing the softer parton from the subsequent evolution. The modified evolution equations one obtains are then given by

$$\frac{dQ(x,t)}{dt} = \int dz p_{qq}(z)\left[Q(zx,t)G((1-z)x,t)\Theta_{SD}(z,t)
+ Q(zx,t)(1 - \Theta_{SD}(z,t))\Theta(z - \frac{1}{2})
+ G((1-z)x,t)(1 - \Theta_{SD}(z,t))\Theta(\frac{1}{2} - z - Q(x,t))\right].$$

\(^5\)Alternately, in practice we could apply RSD to the full partonic configuration obtained from the ungroomed generating functional calculation, but for numerical simplicity and obtaining analytic expressions, this approach is more useful.
\[
\frac{dG(x,t)}{dt} = \int dz \, p_{gg}(z) \left[ G(zx,t)G((1-z)x,t)\Theta_{SD}(z,t) \\
+ G(zx,t)(1-\Theta_{SD}(z,t))\Theta(z - \frac{1}{2}) \\
+ G((1-z)x,t)(1-\Theta_{SD}(z,t))\Theta(\frac{1}{2} - z) - G(x,t) \right] \\
+ \int dz \, p_{qg}(z) \left[ Q(zx,t)Q((1-z)x,t)\Theta_{SD}(z,t) \\
+ Q(zx,t)(1-\Theta_{SD}(z,t))\Theta(z - \frac{1}{2}) \\
+ Q((1-z)x,t)(1-\Theta_{SD}(z,t))\Theta(\frac{1}{2} - z) - G(x,t) \right],
\]

(4.52)

where we defined the soft-drop condition

\[
\Theta_{SD}(z,t) = \begin{cases} 
1 & \text{if } \min(z,1-z) > z_{\text{cut}}\left(\frac{\theta(t)}{R_0}\right)^\beta \\
0 & \text{otherwise}
\end{cases}.
\]

(4.53)

Recasting these evolution equations as integral equations, we obtain

\[
Q(x,t) = \Delta_q(t)Q(x,0) + \int_0^t dt' \Delta_q(t-t') \int_\epsilon^{1-\epsilon} dz \, p_{qq}(z) \times \\
\times \left[ Q(zx,t')G((1-z)x,t')\Theta_{SD}(z,t) \\
+ (1-\Theta_{SD}(z,t'))(Q(zx,t')\Theta(z - \frac{1}{2}) + G((1-z)x,t')\Theta(\frac{1}{2} - z)) \right],
\]

(4.54)

\[
G(x,t) = \Delta_g(t)G(x,0) \\
+ \int_0^t dt' \Delta_g(t-t') \int_\epsilon^{1-\epsilon} dz \left\{ p_{gg}(z) \left[ G(zx,t')G((1-z)x,t')\Theta_{SD}(z,t') \\
+ (1-\Theta_{SD}(z,t'))(G(zx,t')\Theta(z - \frac{1}{2}) + G((1-z)x,t')\Theta(\frac{1}{2} - z)) \\
+ p_{qg}(z) \left[ Q(zx,t)Q((1-z)x,t')\Theta_{SD}(z,t') \\
+ (1-\Theta_{SD}(z,t'))(Q(zx,t)\Theta(z - \frac{1}{2}) + Q((1-z)x,t')\Theta(\frac{1}{2} - z)) \right] \right\}.
\]

(4.55)

The Sudakov form factors are unchanged by the RSD grooming, and are still given by Eq. (4.24). Note that we can also obtain results for finite \( N \) RSD straightforwardly.
from these integral equations. As the scale $t$ is evolved, one simply needs to count the number of passed SD conditions, and revert to a full evolution after $N$ iterations.\footnote{In order to apply finite $N$ RSD at the level of the differential evolution equations, Eqs. (4.51) and (4.52), one would have to keep track of the evolution of a set of generating functionals $Q_i$ and $G_i$ for $0 \leq i \leq N$, which evolve according to Eqs. (4.51) and (4.52), and another pair $Q_{>N}$ and $G_{>N}$, which evolve according to Eqs. (4.14) and (4.15).} It is straightforward to obtain the modified versions of the fixed-order expansions and all-orders expressions for the generating functionals including RSD.

With the generating functionals defined in Eqs. (4.54) and (4.55), we can now define the groomed fragmentation functions $f_{j/i}^{SD}(x, t)$ which determine the probability distribution of the momentum fraction $z$ for a parton with flavour $j$ in a groomed jet initiated by a parton $i$,

$$f_{j/i}^{SD}(x, t) = \frac{\delta F_i(1, t)}{\delta j(z)} \bigg|_{vq(x)=g(x)=1},$$

(4.56)

where $F_i$ is the quark or gluon generating functional, i.e. $F_q(x, t) = Q(x, t)$ and $F_g(x, t) = G(x, t)$. For convenience, we also define the groomed jet fragmentation function summed over all final-state flavours, $f_{\text{jet}/i}^{SD}(x, t) = \sum_j f_{j/i}^{SD}(x, t)$.

We can now use this formalism to calculate the energy drop $\Delta E$ of a groomed jet. By solving Eqs. (4.54) and (4.55) numerically, we can resum collinear logarithms in $\Delta E$. This is shown in Fig. 4-1, where we considered jets with energy $E = 2$ TeV. For the numerical evolution, we take a cutoff scale $t = 1$,\footnote{This corresponds to a shower evolution where emissions are resolved down to an angle $\theta(t, Q) \sim 5 \cdot 10^{-5}$ (see also Fig. 1 of [138]).} evolving from $t = 0$, and verified that the results do not depend on the cutoff scale. We look separately at the energy drop for quark jets (Fig. 4-1a) and gluon jets (Fig. 4-1b), and display results obtained both in the generating functional approach (bottom), and corresponding values derived from parton shower generators (top). For the latter, we use the $qq \rightarrow qq$ and $gg \rightarrow gg$ processes in PYTHIA 8.223 [305], where the jets are clustered with the anti-$k_t$ algorithm and radius $R = 1$, taking jets with $p_T > 2$ TeV and $|y| < 3$. 

\footnote{This corresponds to a shower evolution where emissions are resolved down to an angle $\theta(t, Q) \sim 5 \cdot 10^{-5}$ (see also Fig. 1 of [138]).}
In the $\beta = 0$ limit, the $\Theta_{SD}(z) = \Theta(\min(z, 1 - z) - z_{\text{cut}})$ function only depends on $z$, since there is no angular dependence in Eq. (4.50). We can then straightforwardly derive explicit expressions for the first two terms of the generating functional expansions given in Eq. (4.19). At order $t$ we obtain

\begin{align*}
Q_1(x) = \int dz p_{qq}(z) &\left[ q(x)g(x(1 - z))\Theta(\min(z, 1 - z) - z_{\text{cut}}) + q(xz)\Theta(z_{\text{cut}} - z) \\
&\quad + g(x(1 - z))\Theta(z_{\text{cut}} - (1 - z)) - g(x) \right], \tag{4.57}
\end{align*}
\[
G_1(x) = \int dz p_{gg}(z) [g(xz)g(x(1-z))\Theta(\min(z, 1-z) - z_{\text{cut}}) + g(xz)\Theta(z_{\text{cut}} - z) \\
+ g(x(1-z))\Theta(z_{\text{cut}} - (1-z)) - g(x)] \\
+ \int dz p_{qq}(z) [q(xz)q(x(1-z))\Theta(\min(z, 1-z) - z_{\text{cut}}) + q(xz)\Theta(z_{\text{cut}} - z) \\
+ q(x(1-z))\Theta(z_{\text{cut}} - (1-z)) - g(x)].
\]

Eqs. (4.51) and (4.52) and these \( \mathcal{O}(\alpha_s) \) expressions derived from them have unregulated collinear singularities in this limit, such that results diverge as the cutoff angle \( \theta(t) \) is taken to the limiting value \( \theta(t = \infty) \). Nevertheless, one can still evaluate observables in the \( \beta = 0 \) limit by taking a finite cutoff. For observables that are not IRC or Sudakov safe, such as the \( \beta = 0 \) RSD energy drop, results will then depend on the specific cutoff scale.

### 4.3.4 GFFs for Jet Grooming

In the case of RSD-groomed observables, the GFF formalism is valid for \( \beta = 0 \), precisely where the GFA loses analytic control. The collinear singularities arising at \( \beta = 0 \) are regulated by non-perturbative effects, allowing for a description of the evolution between different scales of the energy-drop distribution in the \( \beta = 0 \) limit. Recursive soft drop can be implemented as part of the observable recursion relation \( \hat{x} \). For the energy drop from RSD, this recursion relation is

\[
\hat{x}(z, x_1, x_2) = \begin{cases} 
  zx_1 + (1-z)x_2 & \text{if } \min(z, 1-z) > z_{\text{cut}} \\
  (1-z)x_2 & \text{if } z < z_{\text{cut}} \\
  zx_1 & \text{if } 1-z < z_{\text{cut}}
\end{cases}
\]
which allows us to write the evolution equation as

\[
\frac{d}{d\mu} \mathcal{F}_i(x, \mu) = \frac{1}{2} \sum_{jk} \int dz \, d\alpha_{\mu}(\mu) \frac{d}{d\mu} p_{i \to jk}(z) \mathcal{F}_j(x_1) \mathcal{F}_k(x_2) \delta(x - \hat{x}(z, x_1, x_2)) \\
= \frac{1}{2} \sum_{jk} \int dz \, \alpha_{\mu}(\mu) p_{i \to jk}(z) \left[ \int d\alpha_{\mu}(\mu) \mathcal{F}_j(x_1) \mathcal{F}_k(x_2) \times \\
\delta(x - z x_1 - (1 - z)x_2) \Theta_{\text{SD}}(z) \\
+ \int d\alpha_{\mu}(\mu) \delta(x - (1 - z)x_2) \Theta(z_{\text{cut}} - z) \\
+ \int d\alpha_{\mu}(\mu) \delta(x - z x_1) \Theta(z_{\text{cut}} - (1 - z)) \right].
\]

(4.60)

Plotted in Fig. 4-2 are distributions of \( x = \Delta E/E \) for (a) quark jets and (b) gluon jets, in PYTHIA 2.230 at scale \( \mu = 100 \) GeV, \( \mu = 3 \) TeV, and the result of using the 100 GeV distribution as an initial conditions for Eq. (4.60). The parton shower curves are samples of anti-\( k_T \) jets with \( R = 1 \), groomed with RSD parameters \( z_{\text{cut}} = 0.05 \), \( \beta = 0 \), and \( N = \infty \). We see that the leading-order evolution from Eq. (4.60) undershoots the change in the first moment as compared to the evolution in PYTHIA, especially for quark jets.

### 4.3.5 Fixed-Order Comparison for RSD with \( \beta = 0 \)

In order to make an explicit comparison between the groomed energy fraction in the GFF and GFA frameworks, we again use the expansions in Eqs. (4.10) and (4.19), this time in the evolution equations for the groomed energy fraction, Eqs. (4.51), (4.52), and (4.60). Written in terms of the real splitting functions \( p_{ji} \), the analytic distributions obtained from the GFF approach at \( \mathcal{O}(\alpha_s) \) are

\[
\frac{\alpha_s}{2\pi} \mathcal{F}_q^{(1)}(x, \mu) = \frac{\alpha_s}{2\pi} \ln \left( \frac{\mu^2}{\Lambda^2} \right) \int dz \, p_{qq}(z) \left[ \delta(x - z - (1 - z)) \Theta(\min(z, 1 - z) - z_{\text{cut}}) \\
+ \delta(x - (1 - z)) \Theta(z_{\text{cut}} - z) + \delta(x - z) \Theta(z_{\text{cut}} - (1 - z)) \right].
\]

(4.61)
Figure 4-2: Evolution comparison between PYTHIA 8.230 and Eqs. (4.3) and (4.4) for (a) initial quarks and (b) initial gluons.

\[
\frac{\alpha_s}{2\pi} F_g^{(1)}(x, \mu) = \frac{\alpha_s}{2\pi} \ln \left( \frac{\mu^2}{\Lambda^2} \right) \int dz \left( p_{gg}(z) + p_{qg}(z) \right) \left[ \delta(x - z - (1 - z)) \Theta(\min(z, 1 - z) - z_{cut}) + \delta(x - (1 - z)) \Theta(z_{cut} - z) + \delta(x - z) \Theta(z_{cut} - (1 - z)) - \delta(1 - x) \right].
\]

\[
\left(4.62\right)
\]

Now we transform to moment space, for the final result

\[
\frac{\alpha_s}{2\pi} F_q^{(1)}(n, \mu) = \frac{\alpha_s}{2\pi} \ln \left( \frac{\mu^2}{\Lambda^2} \right) \int dz p_{qg}(z) \left[ \Theta(\min(z, 1 - z) - z_{cut}) + (1 - z)^n \Theta(z_{cut} - z) + z^n \Theta(z_{cut} - (1 - z)) - 1 \right],
\]

\[
\left(4.63\right)
\]

\[
\frac{\alpha_s}{2\pi} F_g^{(1)}(n, \mu) = \frac{\alpha_s}{2\pi} \ln \left( \frac{\mu^2}{\Lambda^2} \right) \int dz \left( p_{gg}(z) + p_{qg}(z) \right) \left[ \Theta(\min(z, 1 - z) - z_{cut}) + (1 - z)^n \Theta(z_{cut} - (1 - z)) - z^n \Theta(z_{cut} - (1 - z)) - 1 \right].
\]

\[
\left(4.64\right)
\]

We obtain the same expression for \( \langle x^n \rangle_i \) from the GFA by using the leading-order term in the expansion of the evolution variable \( t \), Eq. (4.20), and taking the
$n$-th moment of Eq. (4.57) and Eq. (4.58), with the replacement

$$\frac{\alpha_s}{2\pi} \ln \left( \frac{\mu^2}{\Lambda^2} \right) \to t.$$  \hspace{1cm} (4.65)

It is straightforward to continue this calculation to higher orders in $\alpha_s$ and $t$, but we do not include explicit expressions here as the grooming causes the complexity of the phase-space integrals to increase rapidly. In addition, at sub-leading order, terms due to the running coupling begin to contribute, as we saw in Sec. 4.2.4.

### 4.4 Conclusions

In this chapter, we have compared two frameworks for performing perturbative QCD calculations, the generalized fragmentation function formalism and the generating functional approach. The GFF method incorporates non-perturbative information by fitting to empirical distributions extracted from data, while the generating functionals are purely perturbative objects. However, the GFFs obey a perturbative evolution equation that is a non-linear version of the DGLAP equations. The evolution of the generating functionals in the angular scale $t$ is a very similar non-linear equation. Iterative solutions of these equations can be used to obtain moments of observable distributions which can be compared directly between the two formalisms. We made this comparison for two simple observables: the weighted energy fractions defined in Eq. (4.2) and the energy fraction carried by the hardest parton in a jet. The recently developed recursive soft-drop groomer is a generalization of the soft-drop algorithm which produces jets with decreased sensitivity to non-perturbative effects and the unusual property of having zero catchment area. For values of the grooming parameter $\beta > 0$, the fraction of the jet's energy which remains after RSD grooming is an IRC-safe observable. We apply the GFA to perform an all-orders calculation of the distributions of the groomed energy fraction. For $\beta = 0$, this observable becomes IRC unsafe, and the GFA calculation diverges. This collinear singularity can be regulated by the GFF formalism. We compare leading-order distributions of the groomed energy fraction.
fraction between the GFA and GFF frameworks. Understanding the connections between these two frameworks, and the differences in their applications, will hopefully be of value to theorists trying to choose the most helpful tool to investigate a particular problem.
Chapter 5

Conclusions

In this thesis, I have developed the formalism of generalized fragmentation functions and considered many applications with direct relevance to high-energy physics at the LHC. GFFs extend the calculational power of ordinary fragmentation functions to enable perturbative calculations of jet substructure observables measured on a subset of the jet particles labeled by arbitrary quantum numbers (aside from momentum). I derived a non-linear evolution equation for the GFFs corresponding to a group of collinear-unsafe jet observables, the weighted energy fractions, some of which have already been measured at the LHC. I extended this evolution equation to construct a new class of non-associative jet observables, with structure that parallels the parton-showering process. As an application of these non-associative observables, I studied their application for quark/gluon discrimination, and found that, in the context of parton-shower event generators, certain examples were competitive with or stronger than benchmark quark/gluon discriminants used by LHC experiments.

High resolution measurements of jet mass are a key experimental target, which are of direct importance to both precision measurements and new physics searches. Improved angular resolution is achievable at experiments by leveraging the fine granularity of the charged-particle tracking detectors. With this motivation in mind, I explored generalized track-assisted mass (GTAM) as an observable closely related to jet mass which requires directional information only from charged particles. I used the GFF formalism, specifically track functions, to calculate GTAM distributions at
next-to-leading logarithmic order and matched them to fixed-order distributions at \( \mathcal{O}(\alpha_s) \). I also showed that this observable can be calculated for jets groomed with soft-drop.

As a formal connection to other tools for describing QCD, I performed an in-depth study of the connections between the GFF formalism and the related generating functional approach. This comparison clarified the relationship between these two calculational tools, and demonstrated their agreement for example observables which are calculable in both frameworks.

The utility of this new set of tools can be exploited to make many new comparisons between theory and experiment. I hope that GFFs will find numerous applications probing the structure of high-energy quantum chromodynamics.
Appendix A

Generalized Fragmentation Function
Formalism

A.1 Generalized Fragmentation in Inclusive Jet Production

In this appendix, we explicitly verify Eq. (2.17) at $\mathcal{O}(\alpha_s)$. We first calculate the left-hand side of this equation for the measurement of the fractal variable $x$ together with the fraction of the center-of-mass energy carried by the jet, $z_J \equiv 2E_{\text{jet}}/E_{\text{cm}}$. Assuming that $R$ is not so large that all final-state partons get clustered into one jet, we get

$$\frac{1}{\sigma^{(0)}} \frac{d\sigma}{dz_J dx} = \frac{1}{\sigma^{(0)}} \int dy_1 dy_2 \frac{d\sigma}{dy_1 dy_2} \left\{ \sum_{i<j} \theta(R - \phi_{ij}) \left( \delta(z_J - y_k) \mathcal{F}_k^{(0)}(x, \mu) \right. \right.$$  

$$+ \left. \delta(z_J - y_i - y_j) \int dx_1 dx_2 \mathcal{F}_i^{(0)}(x_1, \mu) \mathcal{F}_j^{(0)}(x_2, \mu) \delta \left[ x - \hat{x} \left( \frac{y_i}{y_i + y_j}, x_1, x_2 \right) \right] \right.$$  

$$+ \theta(\phi_{12} - R) \theta(\phi_{13} - R) \theta(\phi_{23} - R) \sum_i \delta(z_J - y_i) \mathcal{F}_i^{(0)}(x, \mu) \right\}. \quad (A.1)$$

Here, $i, j = 1, 2, 3$ and $y_i$ is the parton momentum fraction normalized such that $y_1 + y_2 + y_3 = 2$. In the following calculations, we identify parton 1 with the quark, 2 with the antiquark, and 3 with the gluon. The angle $\phi_{ij}$ between partons $i$ and $j$ is
given by

$$\phi_{ij} = \arccos \left[ 1 - \frac{2(1 - y_k)}{y_i y_j} \right], \quad (A.2)$$

and $k$ denotes the parton different from $i$ and $j$. Although the angle $\phi_{ij}$ becomes ambiguous when $y_i$ or $y_j$ is zero, IR safety ensures that the measurement is not. The term in Eq. (A.1) with $\phi_{ij} < R$ describes the situation where partons $i$ and $j$ are clustered in a jet but parton $k$ is in a separate jet. The final term, where all $\phi_{ij} > R$, corresponds to the situation where all partons are in separate jets. Each of the three partons has a leading-order GFF attached to it. The squared matrix element that enters in Eq. (A.1) is given up to $\mathcal{O}(\alpha_s)$ by

$$\frac{1}{\sigma^{(0)}} \frac{d\sigma}{dy_1 dy_2} = \delta(1-y_1)\delta(1-y_2) + \frac{\alpha_s C_F}{2\pi} \left\{ \frac{\theta(1-y_3)(y_1^2 + y_2^2)}{2(1-y_1)+1(1-y_2)} \right\}
\begin{aligned}
&+ \left( \frac{\pi^2}{2} - 4 \right) \delta(1-y_1)\delta(1-y_2) + \delta(1-y_2) \left[ \frac{P_{q\rightarrow g}(y_1)}{C_F} \left( -\frac{1}{\epsilon_{IR}} + \ln \frac{y_1 E_{cm}^2}{\mu^2} \right) \right] \\
&+ (1+y_1^2) \left( \frac{\ln(1-y_1)}{1-y_1} \right) + 1-y_1 \left( y_1 \leftrightarrow y_2 \right) \right\}, \quad (A.3)
\end{aligned}
$$

where

$$P_{q\rightarrow g}(y) = C_F \left( \frac{1+y^2}{1-y} \right). \quad (A.4)$$

Let us now focus on the right-hand side of Eq. (2.17). In our case, the coefficients $C_i$ are the standard ones for inclusive fragmentation in $e^+e^-$ collisions [135, 173, 48] since the only kinematic variable appearing on the left-hand side of Eq. (A.1) is the jet energy fraction $z_J$:

$$C_q(z, E_{cm}, \mu) = \delta(1-z) + \frac{\alpha_s}{2\pi} \left\{ P_{q\rightarrow g}(z) \ln \frac{E_{cm}^2}{\mu^2} + C_F \left[ (1+z^2) \left( \frac{\ln(1-z)}{1-z} \right) + \right. \right. \\
\begin{aligned}
&+ 2 \ln \frac{1-z}{1-z} \right) - \frac{3}{2(1-z)} + \delta(1-z) \left( \frac{2\pi^2}{3} - \frac{9}{2} \right) - \frac{3}{2} + \frac{5}{2} \} \right\}, \\
C_g(z, E_{cm}, \mu) = \frac{\alpha_s}{2\pi} P_{q\rightarrow g}(1-z) \left( \ln \frac{E_{cm}^2}{\mu^2} + \ln(1-z) + 2 \ln z \right). \quad (A.5)
\end{aligned}$$

The coefficients $\mathcal{J}_{q\rightarrow gg}^{(1)}$ and $\mathcal{J}_{q\rightarrow gq}^{(1)}$ for an $e^+e^-$ $k_T$-like jet algorithm were calculated

176
using the \( \overline{\text{MS}} \) scheme in Ref. [328],

\[
\mathcal{J}^{(1)}_{q\rightarrow qg}(z, E_{\text{jet}} R, \mu) = \frac{\alpha_s}{2\pi} \left\{ 2C_F L^2 \delta(1-z) + \left[ 2P_{q\rightarrow qg}(z) - 3C_F \delta(1-z) \right] \right\} L
\]

\[
+ C_F \left[ 4z \left( \frac{\ln(1-z)}{1-z} \right) + 2(1-z) \ln(1-z) \right.
\]

\[
+ 2 \left( \frac{1+z^2}{1-z} \right) \ln z + 1 - z - \frac{\pi^2}{12} \delta(1-z) \right\},
\]

\[
\mathcal{J}^{(1)}_{q\rightarrow qg}(z, E_{\text{jet}} R, \mu) = \mathcal{J}^{(1)}_{q\rightarrow qg}(1-z, E_{\text{jet}} R, \mu), \tag{A.6}
\]

while \( \mathcal{J}^{(1)}_{q\rightarrow q} \) and \( \mathcal{J}^{(1)}_{q\rightarrow g} \) are given by the finite terms of Eq. (2.34) and Eq. (2.35) in Ref. [229]

\[
\mathcal{J}^{(1)}_{q\rightarrow q}(z, E_{\text{jet}} R, \mu) = \frac{\alpha_s}{2\pi} \left\{ C_F \delta(1-z) \left( -2L^2 + 3L + \frac{\pi^2}{12} \right) \right.
\]

\[
- 2LP_{q\rightarrow qg}(z) - 2C_F(1+z^2) \left( \frac{\ln(1-z)}{1-z} \right) + C_F(1-z) \right\},
\]

\[
\mathcal{J}^{(1)}_{q\rightarrow g}(z, E_{\text{jet}} R, \mu) = \mathcal{J}^{(1)}_{q\rightarrow q}(1-z, \frac{1-z}{z} E_{\text{jet}} R, \mu), \tag{A.7}
\]

where

\[
L \equiv \ln \left( \frac{E_{\text{jet}} R}{\mu} \right). \tag{A.8}
\]

The coefficients for anti-quarks are identical. Note that the relation between \( \mathcal{J}^{(1)}_{q\rightarrow q} \) and \( \mathcal{J}^{(1)}_{q\rightarrow g} \) is not simply \( z \leftrightarrow 1-z \), because the jet energy \( E_{\text{jet}} \) rather than the energy of the initiating parton is held fixed. Since \( \mathcal{J}^{(1)}_{q\rightarrow q} \) and \( \mathcal{J}^{(1)}_{q\rightarrow qg} \) describe the same splitting in complementary regions of phase space (in-jet versus out-of-jet), their sum vanishes in dimensional regularization,

\[
\mathcal{J}^{(1)}_{q\rightarrow qg}(z, E_{\text{jet}} R, \mu) + \mathcal{J}^{(1)}_{q\rightarrow q}(z, z E_{\text{jet}} R, \mu) = 0. \tag{A.9}
\]

The final ingredient we need is the renormalized one-loop expression for the GFF (see
Eq. (2.20),

\[ \mathcal{F}_i(x) = \mathcal{F}_i^{(0)}(x) - \frac{1}{2\epsilon_{\text{IR}}} \sum_{j,k} \int dz \frac{\alpha_s(\mu)}{2\pi} P_{i\to jk}(z) \times \int dx_1 \, dx_2 \mathcal{F}_j^{(0)}(x_1, \mu) \mathcal{F}_k^{(0)}(x_2, \mu) \delta[x - \hat{x}(z, x_1, x_2)]. \]  

Let us first verify the cancellation of IR divergences between left- and right-hand sides in Eq. (2.17). On the latter, these solely come from \( C_q^{(0)}(z_j, E_{\text{cm}}, \mu) \mathcal{F}_q^{(1)}(x, \mu) + \mathcal{F}_q^{(1)}(x, \mu) \). On the left-hand side, we find

\[
\frac{1}{\sigma^{(0)}} \frac{d\sigma}{dz_j \, dx} \bigg|_{\text{IR div}} = \int dy_1 \, dy_2 \frac{\alpha_s}{2\pi} \left[ \frac{1}{\epsilon_{\text{IR}}} \delta(1 - y_1) P_{q\to qg}(y_2) \right] \delta(z_j - 1) \left[ \mathcal{F}_q^{(0)}(x, \mu) \right. \\
+ \left. \int dx_1 \, dx_2 \mathcal{F}_q^{(0)}(x_1, \mu) \mathcal{F}_q^{(0)}(x_2, \mu) \delta \left[x - \hat{x}(y_2, x_1, x_2)\right] \right] + (q \leftrightarrow \bar{q}) \\
= \delta(z_j - 1) [\mathcal{F}_q^{(1)}(x, \mu) + \mathcal{F}_q^{(1)}(x, \mu)],
\]

which demonstrate the cancellation of the IR divergences. Note that the term on the first line of Eq. (A.11) proportional to \( \mathcal{F}_q^{(0)} \) does not contribute here because it is \( y_2 \)-independent and

\[
\int dy_2 \, P_{q\to qg}(y_2) = 0. \]

To verify that also the finite terms match in Eq. (2.17), we expand the angular constraint in the small \( R \) limit as

\[
\theta(R - \phi_{ij}) \approx \theta \left( \frac{R^2}{4} - \frac{1 - y_k}{y_i y_j} \right),
\]

which implies \( y_k \approx 1 \) and \( y_j \approx 1 - y_i \). We first consider the \( \theta(R - \phi_{13}) \) term in
Eq. (A.1), which gives

\[
\frac{1}{\sigma^{(0)}} \frac{d\sigma}{dz_J dx} \bigg|_{13} = \alpha_s C_F \frac{\alpha}{2\pi} \int dy_1 dy_2 \left\{ \frac{1 + y_1^2}{(1 - y_1)_+} \frac{1}{(1 - y_2)_+} + (\pi^2 - 8)\delta(1 - y_1)\delta(1 - y_2) \\
+ \delta(1 - y_2) \left[ \frac{P_{q \to gq}(y_1)}{C_F} \ln \frac{y_1 E_{cm}^2}{\mu^2} + (1 + y_1^2) \left( \frac{\ln(1 - y_1)}{1 - y_1} \right)_+ + 1 - y_1 \right] \right\} \\
\times \theta\left( \frac{R^2}{4} - \frac{1 - y_2}{y_1 (1 - y_1)} \right) \left[ \delta(z_J - 1)F_q^{(0)}(x, \mu) \\
+ \delta(z_J - 1) \int dx_1 dx_2 F_q^{(0)}(x_1, \mu) F_g^{(0)}(x_2, \mu) \delta(x - \hat{x}(y_1, x_1, x_2)) \right] \\
= \frac{\alpha_s}{2\pi} \int dz \left\{ P_{q \to gq}(z) \ln \frac{z^2 E_{jet}^2 R^2}{\mu^2} + C_F \left[ 2(1 + z^2) \left( \frac{\ln(1 - z)}{1 - z} \right)_+ \\
+ 1 - z + (\ldots)\delta(1 - z) \right] \right\} \left[ \delta(z_J - 1)F_q^{(0)}(x, \mu) \\
+ \delta(z_J - 1) \int dx_1 dx_2 F_q^{(0)}(x_1, \mu) F_g^{(0)}(x_2, \mu) \delta(x - \hat{x}(z, x_1, x_2)) \right] \\
= \delta(1 - z_J) \int dz dx_1 dx_2 \mathcal{J}^{(1)}_{q \to gq}(z, E_{jet} R, \mu) \mathcal{F}_q(x_1, \mu) F_g(x_2, \mu) \\
\times \delta[x - \hat{x}(z, x_1, x_2)] + (\ldots)_{13}. \tag{A.14}
\]

As the integral over $y_2$ yields a $\ln(1 - y_1)$, the resulting $\ln(1 - y_1)/(1 - y)_+$ is not properly regularized, leaving the coefficient of $\delta(1 - z)$ undetermined. As we will see, however, this ambiguity cancels exactly against the one arising from $\mathcal{J}^{(1)}_{q \to gq}$, due to Eq. (A.9). The $\theta(R - \phi_{23})$ term gives the corresponding contribution with quark and anti-quark interchanged, whereas the $\theta(R - \phi_{12})$ term is $\mathcal{O}(R^2)$ suppressed due to the $e^+e^- \to q\bar{q}g$ squared matrix element.

For the last contribution in Eq. (A.1), we rewrite

\[
\theta(\phi_{12} - R) \theta(\phi_{13} - R) \theta(\phi_{23} - R) = 1 - \theta(R - \phi_{12}) - \theta(R - \phi_{13}) - \theta(R - \phi_{23}). \tag{A.15}
\]

where the first term in the sum corresponds to the calculation of the matching coefficients for inclusive fragmentation, thus yielding the $C_i(z_J, E_{cm}, \mu)\mathcal{F}_i(x, \mu)$ contribution on the right-hand side of Eq. (2.17). For the remaining terms, we can follow the
same strategy as in Eq. (A.14). For example, the \(-\theta(R - \phi_{13})\) term gives

\[
\left. \frac{1}{\sigma^{(0)}} \frac{d\sigma}{dz_J dx} \right|_{-13} = -\frac{\alpha_s C_F}{2\pi} \int dy_1 dy_2 \left\{ \frac{1 + y_1^2}{(1 - y_1)_+} \frac{1}{(1 - y_2)_+} + (\pi^2 - 8)\delta(1 - y_1)\delta(1 - y_2) + \delta(1 - y_2) \left[ \frac{P_{q\to qg}(y_1)}{C_F} \ln \frac{y_1 E_{cm}^2}{\mu^2} + (1 + y_1^2) \left( \frac{\ln(1 - y_1)}{1 - y_1} + 1 - y_1 \right) \right] \right. \\
\times \theta \left( \frac{R^2}{4} - \frac{1 - y_2}{y_1 (1 - y_1)} \right) \left[ \delta(z_J - y_1) F_{q}^{(0)}(x, \mu) + \delta(z_J - y_1) F_{g}^{(0)}(x, \mu) \right] \\
+ \delta(z_J - 1) F_{q}^{(0)}(x, \mu) + \delta(z_J - 1 - y_1) F_{g}^{(0)}(x, \mu) \right\}
\]

\[
= -\frac{\alpha_s}{2\pi} \int dz \left\{ P_{q\to qg}(z) \ln \frac{z^2 E_{cm}^2}{4\mu^2} + C_F \left[ 2(1 + z^2) \left( \frac{\ln(1 - z)}{1 - z} \right) + 1 - z + (\ldots)\delta(1 - z) \right] \right\} \left[ \delta(z_J - z) F_{q}^{(0)}(x, \mu) + \delta(z_J - z) F_{g}^{(0)}(x, \mu) \right] \\
+ \delta(z_J - 1) F_{q}^{(0)}(x, \mu) + \delta(z_J - 1 + z) F_{g}^{(0)}(x, \mu) \right\}
\]

\[
= J_{q\to qg}^{(1)}(z_J, E_{\text{jet}} R, \mu) F_{q}(x, \mu) + J_{q\to qg}^{(1)}(z_J, E_{\text{jet}} R, \mu) F_{g}(x, \mu) - (\ldots)_{13}.
\]

(A.16)

The similarity with the calculation in Eq. (A.14) and the relationship between \(J_{q\to qg}^{(1)}\), \(J_{q\to g}^{(1)}\) in Eq. (A.7) together with Eq. (A.9) make this straightforward to verify. The \((\ldots)_{13}\) term cancels in the sum with Eq. (A.14). The \(-\theta(R - \phi_{23})\) term corresponds to the term with quark and anti-quark interchanged and the \(-\theta(R - \phi_{12})\) contribution is again suppressed by \(\mathcal{O}(R^2)\). This completes the check of Eq. (2.17) at \(\mathcal{O}(\alpha_s)\).

A.2 A Non-Fractal Example: Sums of Weighted Energy Fractions

While Eq. (2.1) is rather general, there are of course many collinear-unsafe observables that are not fractal jet observables. In this appendix, we give an explicit example of an observable that does not satisfy the requirements in Sec. 2.2.3.

180
Consider two weighted energy fractions

\[ x = \sum_{i \in \text{jet}} w_i z_i^\kappa, \quad y = \sum_{i \in \text{jet}} v_i z_i^\lambda, \]  

\[ t = x + y \]  

for particle weights \( w_i \) and \( v_i \), and energy exponents \( \kappa \) and \( \lambda \). Individually, \( x \) and \( y \) are described by the evolution equation in Eq. (2.18). On the other hand, their sum

\[ t = x + y \]  

is not a fractal jet observable, though it still can be described by a GFF.

To see this, consider the GFF for \( t \), \( \mathcal{F}_i(t) \), which can be written in terms of a joint GFF for \( x \) and \( y \) as

\[ \mathcal{F}_i(t) = \int dx \, dy \, \mathcal{F}_i(x, y) \, \delta[t - x - y]. \]  

The evolution equation for the joint GFF follows from the analysis in Eq. (2.20), leading to

\[ \frac{\mu}{d\mu} \mathcal{F}_i(x, y; \mu) = \frac{\alpha_s(\mu)}{2\pi} \sum_{j,k} \int dz \, dx_1 \, dx_2 \, dy_1 \, dy_2 \, P_{i\rightarrow jk}(z) \mathcal{F}_j(x_1, y_1; \mu) \mathcal{F}_k(x_2, y_2; \mu) \]

\[ \times \delta \left[ x - z^\kappa x_1 - (1 - z)^\kappa x_2 \right] \delta \left[ y - z^\lambda y_1 - (1 - z)^\lambda y_2 \right]. \]  

\[ (A.20) \]

Plugging Eq. (A.20) into Eq. (A.19), we can insert a factor of

\[ 1 \equiv \int dt_1 \, dt_2 \, \delta[t_1 - x_1 - y_1] \delta[t_2 - x_2 - y_2] \]  

\[ (A.21) \]
to perform the integrals over \(y_1\) and \(y_2\). The resulting equation is

\[
\mu \frac{d}{d\mu} \mathcal{F}_i(t; \mu) = \frac{\alpha_s(\mu)}{2\pi} \sum_{j,k} \int dz \, dt_1 \, dt_2 \, dx_1 \, dx_2 \, P_{i \rightarrow jk}(z) \mathcal{F}_j(x_1, t_1 - x_1) \mathcal{F}_k(x_2, t_2 - x_2) \\
\times \delta \left[ t - z^\lambda t_1 - (1 - z)^\lambda t_2 - (z^\kappa - z^\lambda) x_1 - ((1 - z)^\kappa - (1 - z)^\lambda) x_2 \right].
\] (A.22)

As written, this is a valid GFF evolution equation, but the GFF for \(t\) explicitly involves the joint GFF for \(x\) and \(y\), so we do not get an evolution equation of the form of Eq. (2.18).

If and only if \(\kappa = \lambda\), can we cancel the \(x_1\) and \(x_2\) terms inside of the \(\delta\) function in Eq. (A.22). In that case, we can rewrite the joint probabilities as probability densities for the sums \(t_1 = x_1 + y_1\) and \(t_2 = x_2 + y_2\), so that the evolution equation is of the desired fractal form. Of course, \(\kappa = \lambda\) just corresponds to a regular weighted energy fraction with weights \(w_i + v_i\), so this is not a new fractal observable.

A.3 Software Implementation

The software to perform the RG evolution in this chapter is available from the authors upon request. In this chapter, we discuss some of the specifics of its implementation. A public version of the code is planned for a release some time in the future.

A.3.1 Running Coupling

Because we only perform leading-order evolution, the running of \(\alpha_s\) is strictly speaking only required at leading-logarithmic accuracy. In our implementation, though, the running of the strong coupling is included using the \(\beta\) function at \(\mathcal{O}(\alpha_s^3)\),

\[
\mu \frac{d\alpha_s(\mu)}{d\mu} = -2\alpha_s \left( \beta_0 \left( \frac{\alpha_s}{4\pi} \right) + \beta_1 \left( \frac{\alpha_s}{4\pi} \right)^2 \right),
\] (A.23)

\[
\beta_0 = \frac{11}{3} C_A - \frac{4}{3} T_F n_f, \quad \beta_1 = \frac{34}{3} C_A^2 - \frac{20}{3} C_A T_F n_f - 4 C_F T_F n_f.
\] (A.24)
The running coupling at the scale $\mu$ is given by solving Eq. (A.23) iteratively to order $\mathcal{O}(\alpha_s^3)$,

$$\alpha_s(\mu) = \frac{4\pi}{\beta_0} \left( \frac{1}{L} - \frac{\beta_1}{\beta_0^2 L^2} \ln L \right),$$

(A.25)

where $L = \ln \frac{\mu^2}{\Lambda_{\text{QCD}}}$. Using the PDG value $\alpha_s(M_Z) = 0.1181$ gives the boundary condition $\Lambda_{\text{QCD}} = 0.2275$ GeV. The group theory factors for QCD are $C_F = \frac{4}{3}$, $T_F = \frac{1}{2}$, and $C_A = 3$. For applications to the LHC running at 13 TeV, the number of quark flavors is $n_f = 5$.

### A.3.2 Discretization

The evolution equation in Eq. (2.18) can be solved by binning the values of the GFFs in the $x$ variable. If the GFF domain is partitioned into $N$ bins, Eq. (2.18) becomes a set of $(2n_f + 1)N$ coupled ordinary differential equations. The evolution equation for the binned GFF for bin $n$, $\tilde{F}_i(n, \mu)$, is given by\(^1\)

$$\frac{d}{d\ln \mu} \tilde{F}_i(n, \mu) = \frac{d}{d\ln \mu} \int_{x(n-1)/N}^{x/n/N} dx \mathcal{F}_i(x, \mu)$$

\begin{align*}
&= \frac{N}{2} \sum_{j,k} \int_{x(n-1)/N}^{x/n/N} dx \sum_{n_1,n_2} \int_{x(n_1-1)/N}^{x(n_1)/N} dx_1 \int_{x(n_2-1)/N}^{x(n_2)/N} dx_2 \int_0^1 dz P_{i\rightarrow jk}(z) \\
&\quad \times \mathcal{F}_j(x_1, \mu) \mathcal{F}_k(x_2, \mu) \delta \left[ x - \hat{x}(z, x_1, x_2) \right] \\
&= \frac{N}{2} \sum_{j,k} \int_{x(n-1)/N}^{x/n/N} dx \sum_{n_1,n_2} \int_0^1 dz P_{i\rightarrow jk}(z) \tilde{F}_j(n_1, \mu) \tilde{F}_k(n_2, \mu) \\
&\quad \times \delta \left[ x - \hat{x}(z, x_{n_1}, x_{n_2}) \right],
\end{align*}

(A.26)

where $x_{n_1}$ and $x_{n_2}$ are the positions of the midpoints of the $n_1$-th and $n_2$-th bins. Note that Eq. (A.26) is written in terms of $\ln \mu$ instead of $\mu$, since this is how the evolution was implemented numerically to make the step size and numerical errors more consistent. In principle, the $\delta$ function could be used to carry out the $z$ integral exactly. In practice, it is easier to discretize the $z$ integral and use the $\delta$ function to\(^1\)This equation is written for $N$ equal-width bins for simplicity of notation. The generalization to unequal bins is straightforward, and the software implementation is set up to handle variable bin widths if desired.

183
choose the $x$-bin corresponding to each triplet $(z, x_1, x_2)$. This is because inverting $\hat{x}$ to solve for $z$ analytically for general $x_1$ and $x_2$ is not possible. Doing so in advance separately for each value of $x$, $x_1$ and $x_2$ can be prohibitively memory intensive for large numbers of bins.

The splitting functions are approximated by the analytic value of their integral over the width of the bin. For our analysis, we need the following splitting functions:

\[
P_{q\to qg}(z) = P_{q\to qg}(1 - z) = C_F \left( \frac{1 + (1 - z)^2}{z_+} + \frac{3}{2} \delta(z) \right),
\]

\[
P_{g\to qg}(z) = T_F \left( z^2 + (1 - z)^2 \right),
\]

\[
P_{g\to gg}(z) = 2C_A \left( \frac{1 - z}{z_+} + \frac{z}{(1 - z)_+} + z(1 - z) \right) + \frac{\beta_0}{2} (\delta[1 - z] + \delta[z]),
\]

where $P_{q\to qg}(z)$ is the splitting function for a quark radiating a gluon with momentum fraction $z$, the integration constant for integrals of the plus distributions are fixed by

\[
\int_0^1 \frac{dz}{z_+} = 0, \quad \int_0^1 \frac{dz}{(1 - z)_+} = 0,
\]

and $\beta_0$ is given in Eq. (A.24). When performing the integration, terms with a plus-function regulator must be handled correctly for the endpoint bins. If the regulated functions have the following primitives

\[
\frac{dF(z)}{dz} = \frac{f(z)}{z}, \quad \frac{dG(z)}{dz} = \frac{g(z)}{1 - z},
\]

then their integrals over the $n$-th bin are implemented by

\[
\int_{z - \Delta z}^{z + \Delta z} dz' \frac{f(z')}{z'_+} = \begin{cases} F(z + 0.5 \Delta z) - F(z - 0.5 \Delta z) & n \neq 0, \\ F(z + 0.5 \Delta z) & n = 0, \end{cases}
\]

\[
\int_{z - \Delta z}^{z + \Delta z} dz' \frac{g(z')}{(1 - z')_+} = \begin{cases} G(z + 0.5 \Delta z) - G(z - 0.5 \Delta z) & n \neq n_{\text{final}}, \\ G(z - 0.5 \Delta z) & n = n_{\text{final}}. \end{cases}
\]
Figure A-1: Sensitivity of the evolution from $\mu = 100$ GeV to 4 TeV on the choice of fine bin width. Shown are the (left) gluon GFF and (right) quark-singlet GFF for the weighted energy fraction with $\kappa = 0.5$. The curves labeled $\Delta n_X$ are the difference between the result using $n_{\text{fine}} = X$ and the result using $n_{\text{fine}} = 1000$. For the default value of $n_{\text{fine}} = 100$ used in this chapter, the results are indistinguishable by eye.

In our implementation, the integration range $z \in [0, 1]$ is divided into $n_{\text{rough}}$ bins, and the first and last bin are then further subdivided by a factor of $n_{\text{fine}}$. The user can specify these two parameters. For the results presented in this chapter, the values used were $n_{\text{rough}} = 1000$ and $n_{\text{fine}} = 100$. The finer division of the endpoint bins is necessary to accurately capture the singular behavior of the splitting functions near $z = 0$ and $z = 1$. For many GFFs, this is not necessary, but consider the weighted energy fractions, whose recursion relation satisfies

$$\hat{x}(z, x_1, x_2) = z^\kappa x_1 + (1 - z)^\kappa x_2 \implies \frac{\partial \hat{x}}{\partial z} = \kappa(z^{\kappa-1}x_1 - (1 - z)^{\kappa-1}x_2).$$  \hspace{0.5cm} (A.31)

For $\kappa < 1$, there are poles in the derivative of $\hat{x}$ at $z = 0$ and $z = 1$, resulting in a noticeable dependence on $n_{\text{fine}}$. This is shown in Fig. A-1 for the case of $\kappa = 0.5$, with all particle weights one. Once we increase $n_{\text{fine}} = 100 \rightarrow 1000$, the maximum change in the value of the evolved GFFs in a single $x$-bin is less than 0.06%.
A.3.3 Runge-Kutta Algorithm

After the discretization in Eq. (A.26), the RG evolution is performed with an embedded fifth-order Runge-Kutta method adapted from Ref. [293]. This method requires six evaluations of the right side of Eq. (2.18), which on the kth step can be combined to give a fifth-order estimate $y_{k+1}$ of the desired function after a step of size $h_k$. These computations can be recombined with different coefficients to give a fourth-order Runge-Kutta estimate $y_k^*$. The difference between these two methods then gives an estimate of the local truncation error. The error estimated this way applies to the fourth-order value $y_k^*$, but we take the (more accurate) fifth-order value. This ensures that our solution is actually slightly more accurate than our indications. Estimating the error on this fifth-order solution would require calculating a still-higher order step.

Once a step $h_k$ is taken, with an error $\mathcal{E}_k$, we would like to choose an appropriate trial value for our next step. This fourth-order error estimate scales as $\mathcal{O}(h^5)$, so we choose the next step, $h_{k+1}$, to be

$$h_{k+1} = \begin{cases} \frac{S h_k |\mathcal{E}_{k+1}/\mathcal{E}_k|^{0.25} \mathcal{E}_{k+1} > \mathcal{E}_k}{S h_k |\mathcal{E}_{k+1}/\mathcal{E}_k|^{0.20} \mathcal{E}_{k+1} < \mathcal{E}_n}. \end{cases}$$  \hspace{1cm} (A.32)

Here, $\mathcal{E}_{k+1}$ is the projected error in the $(k+1)$th step, and $S$ is a safety factor taken to be 0.9. This formula allows the step size to grow if the error is much smaller than our tolerance. If the error is larger than the tolerance, the step fails, and is retried with a smaller step.

It is important that the algorithm be able to dynamically change step size in order to evolve a solution efficiently while keeping errors within desired limits. At low scales, the strong coupling grows large, and the solution changes rapidly. Numerical precision therefore requires small step sizes in this region. At high scales, asymptotic freedom ensures that the solutions change slowly, so much larger step sizes result in the same level of accuracy. This procedure requires a prescription for the maximal acceptable error. For a system of $M \equiv (2n_f + 1)n$ coupled ODEs, there is a separate $\mathcal{E}_k^m$ for
each $m \in M$. The step is considered a failure unless every equation is within its error tolerance. The error $\mathcal{E}_k^m$ for the $m$th equation on the $k$th step is required to satisfy

$$
\left| \frac{\mathcal{E}_k^m}{|y_k^m| + |h_k(dy_k^m/d\ln\mu)| + 10^{-6}} \right| < \varepsilon. \tag{A.33}
$$

The value $\varepsilon$ is an overall upper limit which was set to $10^{-9}$ for the GFF evolution. The last numerical term in the denominator is required to avoid artificially large errors when the domain of the GFFs input into the program exceeds the actual support of the GFF. As an additional constraint, our algorithm sets a maximum step size of $d\ln\mu \leq 0.4$. Note that the same step size is used for every equation in the system.
Figure A-2: Downward evolution from $\mu = 4$ TeV to $\mu = 100$ GeV of the (left column) gluon GFF and (right column) quark-singlet GFF with (top row) $\kappa = 0.5$ and (bottom row) $\kappa = 2.0$. The envelopes of the evolved distributions are constructed as in Sec. 2.4.2 by varying the jet radius $R$ and the choice of parton shower, which highlight the numerical instability of downward evolution.
A.4 Numerical Stability

All of the RG results in this chapter are based on the numerical solution of Eq. (2.18) for upwards evolution in the scale $\mu$. The reason is because downward evolution is numerically unstable, in the sense that small irregularities in the initial conditions amplify into large fluctuations, especially for the gluon GFFs. This behavior is illustrated in Fig. A-2, where gluon and quark-singlet GFFs are evolved downward from 4 TeV to 100 GeV.

Heuristically, if evolution upwards in scale is analogous to convolution of the GFFs, evolution downwards is akin to deconvolution, a problem known to be ill-posed. To verify that the instability is inherent to the differential equation, and not merely a numerical artifact, we checked that the envelope shown in Fig. A-2 is not affected by choosing a smaller step size or more stringent error bound in the Runge-Kutta algorithm. To get a sensible result, one could use a numerical regularization method such as Tikhonov regularization [322], though we do not do so here. Note that in general, if the evolution in one direction is stable, such that small fluctuations get washed out, the evolution is expected to be unstable in the reverse direction.

A.5 Moment Space Details

In this appendix, we give details of the moment space analysis from Sec. 2.4.5, as well as perform similar analyses for the non-associative observables from Sec. 2.5. The moments of the GFFs are defined by

$$ \overline{F_i}(N, \mu) = \int dx \, x^N F_i(x, \mu), $$  \hfill (A.34)

where the zeroth moment is just the normalization,

$$ \overline{F_i}(0, \mu) = \int dx \, F_i(x, \mu) = 1. $$  \hfill (A.35)
This convention follows the standard nomenclature of probability theory. Applying $\int_{-\infty}^{+\infty} dx x^N$ to both sides of the evolution equation in Eq. (2.18) gives the moment space evolution equation,

$$\mu \frac{d}{d\mu} \mathcal{F}_i(N, \mu) = \frac{1}{2} \sum_{j,k} \int dz \, dx_1 \, dx_2 \left( \hat{x}(z, x_1, x_2) \right)^N \frac{\alpha_s(\mu)}{\pi} P_{i\to jk}(z) \mathcal{F}_j(x_1, \mu) \mathcal{F}_k(x_2, \mu).$$

(A.36)

In order to proceed further, we need the specific form of the recursion relation, $\hat{x}$. We now discuss the details for each of the sets of observables studied in this chapter.

### A.5.1 Weighted Energy Fractions

Inserting the weighted energy fraction recursion relation Eq. (2.25) into Eq. (A.36) leads to

$$\mu \frac{d}{d\mu} \mathcal{F}_i(N, \mu) = \frac{\alpha_s(\mu)}{2\pi} \sum_{j,k} \sum_{M=0}^{N} \binom{N}{M} \int_0^1 dz \, z^{\kappa(N-M)}(1-z)^{\kappa M} P_{i\to jk}(z)$$

$$\times \int dx_1 \, x_1^{N-M} \mathcal{F}_j(x_1, \mu) \int dx_2 \, x_2^M \mathcal{F}_k(x_2, \mu),$$

(A.37)

assuming that $N$ is integer and using the binomial theorem. As in Eq. (2.36), the moments of the splitting functions are defined as

$$\overline{P}_{i\to j,k}(N, M) = \int_0^1 dz \, z^N (1-z)^M P_{i\to j,k}(z),$$

(A.38)

with the convention that $\overline{P}_{i\to j,k}(N) \equiv \overline{P}_{i\to j,k}(N, 0)$. For any real $N > 0$, they can be expressed in terms of the digamma function $\psi_0(N)$ and the Euler-Mascheroni constant.
\[ \gamma_E, \]

\[ \overline{P}_{q\rightarrow qg}(N) = C_F \left( \frac{3}{2} + \frac{1}{N+1} + \frac{1}{N+2} - 2\gamma_E - 2\psi_0(N+3) \right), \]

\[ \overline{P}_{q\rightarrow gg}(N) = C_F \left( \frac{N^2 + 3N + 4}{N(N+1)(N+2)} \right), \]

\[ \overline{P}_{g\rightarrow qg}(N) = T_F \left( \frac{N^2 + 3N + 4}{(N+1)(N+2)(N+3)} \right), \]

\[ \overline{P}_{g\rightarrow gg}(N) = 2C_A \left( \frac{11}{12} + \frac{2(N^2 + 3N + 3)}{N(N+1)(N+2)(N+3)} - \gamma_E - \psi_0(N+2) \right) - \frac{2}{3} T_F n_f. \]  
(A.39)

Alternatively, one can use the harmonic number function, \( H_N = \gamma_E + \psi_0(N + 1) \). These expressions for all positive real numbers are necessary to evaluate the moment space evolution equation in Eq. (2.37) for non-integer \( \kappa \). Note that \( N \) is shifted up by one from the expression usually seen in the literature, because our convention for moments in Eq. (A.34) is shifted by one as well compared to Mellin moments.

### A.5.2 Node Products

We now insert the recursion relation for the node products from Eq. (2.42) into Eq. (A.36). This leads to evolution equations with additional terms compared to those for the weighted energy fractions. These terms have splitting kernels of the form

\[ \int_0^1 dz \left( 4z(1-z) \right)^a z^b (1-z)^c P_{i\rightarrow j,k}(z) \]  
(A.40)

for \( a > 0 \) and \( b, c \geq 0 \). These integrals are convergent, so no plus function regulators are required. They can also be performed analytically for general \( a, b, \) and \( c \).
Figure A-3: Moment space evolution of the node-product observables with (top row) \( \kappa = 1 \) and (bottom row) \( \kappa = 4 \) for the generalized-\( k - t \) clustering trees with (left column) \( p = -1 \), (middle column) \( p = 0 \), and (right column) \( p = 1 \). Shown are the first (solid curves) and second (dashed curves) moments of gluon (red) and quark-singlet (blue) GFFs. The first (second) moments extracted from the parton shower average at \( \mu = 4 \text{ TeV} \) are shown as points (diamonds).

Explicitly, the first moments of the quark-singlet and gluon GFFs evolve as

\[
\frac{d}{d\mu} \left( \frac{\mathcal{S}(1, \mu)}{\mathcal{F}_g(1, \mu)} \right) = \frac{\alpha_s(\mu)}{\pi} \left( \begin{array}{l}
\mathcal{P}_{\bar{q}q}(\kappa) \\
2n_f \mathcal{P}_{g\to q\bar{q}}(\kappa)
\end{array} \right) \left( \begin{array}{l}
\mathcal{S}(1, \mu) \\
\mathcal{P}_{gg}(\kappa)
\end{array} \right) + \frac{\alpha_s(\mu)}{\pi} \left( \begin{array}{l}
\mathcal{P}_{\bar{q}1} \left( \mathcal{F}_{\bar{q}1}^{\text{Node}}(\kappa) \right) \\
\mathcal{P}_{g1} \left( \mathcal{F}_{g1}^{\text{Node}}(\kappa) \right)
\end{array} \right).
\] (A.41)
The additional constant terms are defined as

\[
\begin{align*}
\overline{F}_{q_1}^{\text{Node}}(\kappa) &\equiv \frac{1}{2} \int_0^1 dz \left( P_{q\to qg}(z) + P_{q\to gg}(z) \right) (4z(1-z))^{\kappa/2}, \\
\overline{F}_{g_1}^{\text{Node}}(\kappa) &\equiv \frac{1}{2} \int_0^1 dz \left( 2n_f P_{g\to qg}(z) + P_{q\to gg}(z) \right) (4z(1-z))^{\kappa/2},
\end{align*}
\]

which can be evaluated in terms of \( \Gamma \) functions. The additional terms drop out of the equation for the first moments of the non-singlet GFFs, so these still evolve according to Eq. (2.38). The third term in Eq. (2.42) leads to several more terms in the evolution equations for higher moments.

In Fig. A-3, we plot the \( \mu \) evolution of the gluon and quark-singlet GFF moments for node products with \( \kappa = \{1,4\} \) and \( p = \{-1,0,1\} \). The first and second moments were computed at the scale \( \mu = 100 \text{ GeV} \) from the GFFs in Fig. 2-11, averaged over the different parton showers and \( R \) values (as described in Sec. 2.4.2). These average moments were evolved to the scale \( \mu = 10^7 \text{ GeV} \) using Eq. (A.41) and the corresponding second moment equation. For comparison, the first and second moments of the GFFs extracted from the parton shower average at the scale \( \mu = 4 \text{ TeV} \) are shown as dots and diamonds, respectively.

### A.5.3 Full-Tree Observables

For full-tree observables with recursion relation given in Eq. (2.45), the moment space evolution equations are of the same general form as for the weighted energy fractions,

\[
\mu \frac{d}{d\mu} \overline{F}_i(N, \mu) = \frac{\alpha_s(\mu)}{2\pi} \sum_{j,k} \sum_{M=0}^{N} \binom{N}{M} \overline{P}_{i\to j,k}(N, M) \overline{F}_j(N-M, \mu) \overline{F}_k(M, \mu),
\]

but with different splitting kernels,

\[
\overline{P}_{i\to j,k}^{\text{FT}}(N, M) \equiv \int_0^1 dz \, e^{Nz(1-z)} z^\kappa (N-M) (1-z)^\kappa M P_{i\to j,k}(z).
\]

To our knowledge, these integrals do not have a closed form solution for general values of the parameters \( \kappa \) and \( \xi \), but it is straightforward to evaluate them numerically. If
$M = 0$ or $M = N$, these integrals are sensitive to the plus-prescription in the splitting functions. Explicitly, for the first moment in the quark-singlet basis,

$$
\frac{d}{d\mu} \mathcal{S}(1, \mu) = \frac{\alpha_s(\mu)}{\pi} \left[ C_F \left( \frac{3}{2} + \int_0^1 dz \frac{e^{\xi z(1-z)z^2}(1 + z^2) - 2}{1 - z} \right) \mathcal{S}(1, \mu) \right. \\
+ C_F \int_0^1 dz \left( e^{\xi z(1-z)z^2} - 1 \right) \mathcal{F}_g(1, \mu) \right],
$$

$$
\frac{d}{d\mu} \mathcal{F}_g(1, \mu) = \frac{\alpha_s(\mu)}{\pi} \left[ 2n_f T_F \int_0^1 dz \left( e^{\xi z(1-z)z^2} - 1 \right) \mathcal{S}(1, \mu) \\
+ 2C_A \int_0^1 dz \left( e^{\xi z(1-z)z^2} - 1 \right) \mathcal{F}_g(1, \mu) \right].
$$

In Fig. A-4, we show the evolution of the first two moments of the GFFs for $\kappa = 2$, $\xi = \{-2, 2\}$, and $p = \{-1, 0, 1\}$. In this case, the evolution agrees well with the value extracted from the parton shower average at $\mu = 4$ TeV.
Figure A-4: The same as Fig. A-3, except now for the full-tree observables with $\kappa = 2$ measured on charged particles, with (top row) $\xi = -2$ and (bottom row) $\xi = 2$. 
Appendix B

Details of Generalized Track-Assisted Mass Calculation

B.1 Pure Quark and Gluon Ensembles

The analysis of GTAM in Sec. 3.2 was carried out using $pp \rightarrow$ dijet events generated with VINCIA 2.2.2. It is conceivable that the flavor content of the jet could change the best-fit parameters and the degree of the correspondence between jet mass and GTAM. To investigate this possibility, we repeated the analysis using ensembles of purely quark-initiated and purely gluon-initiated jets, as labeled by the VINCIA hard process.

The best-fit GTAM parameters $(\kappa_{\text{best}}, \lambda_{\text{best}})$ turn out to be rather insensitive to the species of parton initiating the jet. As shown in Fig. B-1, the best-fit values $(\kappa_{\text{best}}, \lambda_{\text{best}})$ were found to be $(0.55, 0.48)$ for gluons and $(0.57,0.48)$ for quarks, as compared to $(0.54,0.50)$ for a mixture of quark and gluon jets. GTAM is a closer match to jet mass by about a factor of two (as measured by $\Delta$) for gluon jets than for quark jets. This is to be expected, since the variance of the gluon track function is smaller than that of the quark track function ($\Delta T_g = 0.15$ and $\Delta T_q = 0.2$), so the track fraction reweighting factors with exponent $\lambda$ will smear the GTAM distribution less for gluons than for quarks. This also matches the conclusion from the analytic approximations in Sec. 3.3.2 where gluon jets produced a more complete cancellation.
Figure B-1: Distribution of $\Delta(\kappa, \lambda)$ for the processes $pp \rightarrow gg$ (top) and $pp \rightarrow q\bar{q}$ (bottom), to be compared to Fig. 3-12. The full two-dimensional distributions are on the left, and slices of these distributions are shown on the right.
of track function effects on the resummed GTAM distribution.
B.2 Details of Resummed Calculation

In order to obtain a finite differential distribution for the observable \( \rho \equiv M^2/(E_{\text{calo}}R)^2 \) in the region \( \rho \ll 1 \), where the fixed-order perturbative expansion breaks down due to large logarithms of \( \rho \), it is necessary to calculate contributions proportional to \( \alpha_s^n \log^{2n-1}(\rho) \) (LL) to all orders in perturbation theory. Quantitative agreement with experimental data requires resummation of terms up to at least NLL order.

Running coupling effects are taken into account with the two-loop \( \beta \)-function. The appropriate scheme for the coupling in the resummed cumulative distribution Eq. (3.18) is the CMW scheme \([107]\), which is related to the \( \overline{\text{MS}} \) scheme by

\[
\alpha_s^{\text{CMW}} = \alpha_s^{\overline{\text{MS}}} \left( 1 + \left[ C_A \left( \frac{67}{18} - \frac{\pi^2}{6} \right) - \frac{5}{9} n_f \right] \frac{\alpha_s^{\overline{\text{MS}}}}{2\pi} \right). \tag{B.1}
\]

The scale at which \( \alpha_s \) is evaluated in Eqs. (3.17) and (3.19) is \( \mu = E_{\text{calo}}z\theta \) (\( p_{T,\text{jet}}z\theta \) for \( pp \) collisions), the transverse momentum of the radiated particle in the soft-collinear limit. This scale enters the non-perturbative regime for low enough values of \( \rho \). To handle this effect, we freeze the coupling at \( \alpha_s(1 \text{ GeV}) = 0.42 \), which is the result of using the two-loop \( \beta \)-function to run from \( \alpha_s(M_Z) = 0.1182 \). In the derivative of the radiator, all terms are one logarithmic order lower than in the radiator itself, so to this order we can evaluate the coupling in \( R' \) at the hard scale \( E_{\text{calo}}R \).

As described in Sec. 3.3.2, the running of the track function contributes only at NNLL order. Additionally, the first moment of the track functions is extremely scale insensitive, see Fig. 3-6b, with a fractional change of only 0.04% for gluon or quark-singlet (average over quark and anti-quark species) jets when evolved from 10 GeV to \( 10^6 \) GeV. The fractional change of the second moment is about 2% over this same scale evolution. The track functions are fixed at the hard scale \( \mu = E_{\text{calo}}R \) in the calculation of \( R \) and \( R' \). A higher-order calculation could include this effect using the nonlinear DGLAP-like evolution equation described in \([110, 158]\).

The radiators for quark and gluon jets also include the (real) reduced splitting
functions $P_q$ and $P_g$ respectively:

$$P_q(z) = P_{gq}(z) = C_F \left[ \frac{1 + (1 - z)^2}{z} \right], \quad \text{(B.2)}$$

$$P_g(z) = \frac{1}{2} P_{gg}(z) + n_f p_{qq}(z) = C_A \left[ \frac{2(1 - z)}{z} + z(1 - z) \right] + n_f T_F (z^2 + (1 - z)^2). \quad \text{(B.3)}$$

The splitting functions do not have a virtual part, and no plus function regularization is required, since the observable value $\rho$ cuts off the singularities in both the $z$ and $\theta$ integrals. The $z \leftrightarrow 1 - z$ symmetry in the $g \to gg$ splitting was exploited to write $p_{gg}$ in a form which is singular only at $z = 0$.

We give the full expressions needed for the cumulative track-assisted mass distributions, including soft-drop grooming with $\beta \geq 0$. Although they are already available in the literature [254], we give the equivalent expressions for ordinary jet mass and soft-drop groomed mass as well for comparison. In the fixed-coupling approximation (but without the endpoint approximations in Eq. (3.23)), the calorimeter and track radiators are given to NLL order by

$$R_{\text{calo}}(\rho) = \frac{\alpha_s C_i}{\pi} \left\{ \frac{1}{2} \ln^2 \left( \frac{1}{\rho} \right) + B_i \ln \left( \frac{1}{\rho} \right) \right\}, \quad \text{(B.4)}$$

$$R_{\text{TA}}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} \left\{ \frac{1}{2} \ln^2 \left( \frac{1}{\rho} \right) f^{g,0}(x_j \rho, 1) + \ln \left( \frac{1}{\rho} \right) \left[ f^{g,0}(x_j \rho, 1) (B_i - \ln(x_j)) \right. \right. \right.$$  

$$\left. + f^{g,1}(x_j \rho, 1) \right].$$

---

1 The cases $\beta > 0$ and $\beta = 0$ are distinct at NLL order because we are keeping finite $z_{\text{cut}}$ terms. For this reason, the $\beta \to 0$ limit of Eq. (B.5) does not recover Eq. (B.6). The ungroomed ($\beta = \infty$) case can be recovered from the $\beta > 0$ expression by taking either the $\beta \to \infty$ limit or the $z_{\text{cut}} \to 0$ limit. For $x_j \rho > 0$, this gives $f^{i,n}(y^*, 1) \to 0$ and $f^{i,n}(x, y') \to f^{i,n}(x, 1)$ for $z_{\text{cut}} = x_j \rho$. It is easy to see that for any $\rho > 0$, the ungroomed limits $z_{\text{cut}} \to 0$ or $\beta \to \infty$ commute with removing the tracking procedure by setting all track fractions to one and all track functions to $\delta(1 - x)$. 

201
(\beta > 0) :

\[
R_{\text{calo}}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} \left\{ \frac{1}{2} \ln^2 \left( \frac{1}{\rho} \right) \left[ \frac{\beta}{2 + \beta} \Theta(z_{\text{cut}} - \rho) + \Theta(\rho - z_{\text{cut}}) \right] + B_i \ln \left( \frac{1}{\rho} \right) + \frac{2}{2 + \beta} \Theta(z_{\text{cut}} - \rho) \ln \left( \frac{1}{\rho} \right) \ln \left( \frac{1}{z_{\text{cut}}} \right) \right\},
\]

\[
R_{\text{TA}}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} \left\{ \frac{1}{2} \ln^2 \left( \frac{1}{\rho} \right) \left[ \frac{\beta}{2 + \beta} f^{g,0} (y^*, 1) + f^{g,0} (x_j \rho, y^*) \right] + \ln \left( \frac{1}{\rho} \right) \left[ B_i f^{g,0} (x_j \rho, 1) - \ln(x_j) \left( \frac{\beta}{2 + \beta} f^{g,0} (y^*, 1) + f^{g,0} (x_j \rho, y^*) \right) + \frac{2}{2 + \beta} f^{g,0} (y^*, 1) \ln \left( \frac{1}{z_{\text{cut}}} \right) \right] \right\},
\]

(\beta = 0) :

\[
R_{\text{calo}}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} \left\{ \frac{1}{2} \ln^2 \left( \frac{1}{\rho} \right) + \ln \left( \frac{1}{\rho} \right) \right\},
\]

\[
R_{\text{TA}}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} \left\{ \frac{1}{2} \ln^2 \left( \frac{1}{\rho} \right) f^{g,0} (x_j \rho, y^*) + \ln \left( \frac{1}{\rho} \right) \left[ f^{g,0} (x_j \rho, y^*) \left( B_i - \ln(x_j) \right) + f^{g,1} (x_j \rho, y^*) + f^{g,0} (y^*, 1) \ln \left( \frac{1}{\rho} \right) \ln \left( \frac{1}{z_{\text{cut}}} \right) \right] \right\},
\]

where we have defined

\[
y^* = \min \left( \frac{x_j \rho}{z_{\text{cut}}}, 1 \right). \tag{B.7}
\]

The radiator derivatives appearing in the multiple-emissions prefactor are easily read off from the \( \ln^2 \frac{1}{\rho} \) terms, and can be expressed for \( \beta = \infty \) (ungroomed), \( \beta > 0 \), and \( \beta = 0 \) by

\[
R'_{\text{calo}}(\rho) = \frac{\alpha_s C_i}{\pi} \left[ \ln \left( \frac{1}{\rho} \right) \left( \frac{\beta}{2 + \beta} \Theta(z_{\text{cut}} - \rho) + \Theta(\rho - z_{\text{cut}}) \right) + \frac{2}{2 + \beta} \Theta(z_{\text{cut}} - \rho) \ln \left( \frac{1}{z_{\text{cut}}} \right) \right],
\]

\[
R'_{\text{TA}}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} \left[ \ln \left( \frac{1}{\rho} \right) \left( \frac{\beta}{2 + \beta} f^{g,0} (y^*, 1) + f^{g,0} (x_j \rho, y^*) \right) + \frac{2}{2 + \beta} f^{g,0} (y^*, 1) \ln \left( \frac{1}{z_{\text{cut}}} \right) \right]. \tag{B.8}
\]

The \( \ln z_{\text{cut}} \) term has been included in the multiple-emissions prefactor even though it is
formally beyond NLL order in $\rho$. Near $\rho \simeq z_{\text{cut}}$, the $\ln z_{\text{cut}}$ term is just as important as
the dominant log $\rho$ terms which are being resummed and cannot be neglected. Using
the radiators, Eqs. (B.5) and (B.6), and their derivatives, Eq. (B.8), in the general
expression for the cumulative distribution of a track-assisted observable, Eq. (3.18),
gives the fixed-coupling expressions for the cumulative distributions of track-assisted
mass for $\beta \geq 0$ values. To include the effects of the running coupling in our numerical
results, we integrate the radiator Eq. (3.46) instead of using Eqs. (B.5) and (B.6), but
we used Eq. (B.8) for the multiple-emissions prefactor. As mentioned in Sec. 3.3.5,
computing the GTAM distribution for parameters besides \( \kappa = 1 \) and \( \lambda = 0 \) simply
requires making the replacement $x_j \rightarrow x_j^{2\kappa-1} (x_j)^{2\lambda}$ in the appropriate radiator and
its derivative.

In the matching calculation in Sec. 3.3.4, we needed the $O(\alpha_s)$ piece of the fixed-order expansion of the differential NLL distribution. The coupling must be evaluated
in the $\overline{\text{MS}}$ scheme, not the CMW scheme, for the $O(\alpha_s)$ piece of the NLL distribution,
otherwise it cannot cancel the singular terms in the fixed-order distribution. For
completeness, we include these here:\footnote{The $\rho$-dependent endpoints do not contribute to this derivative. They are power suppressed, and therefore of the same order as other power-suppressed terms that were neglected in restricting to NLL order in the radiator. If terms of this order are to be included, they must all be computed for a consistent result.}

\begin{align}
(\beta = \infty) & : \quad \frac{1}{\sigma} \frac{d\sigma_{\text{NLL},a}}{d\rho} = \frac{\alpha_s C_i}{\pi} \int_0^1 dx_j T_j(x_j) \left\{ \frac{1}{\rho} \left[ f^{g,0}(x_j \rho, 1) \left( \ln \left( \frac{1}{\rho} \right) + B_i - \ln(x_j) \right) + f^{g,1}(x_j \rho, 1) \right] \right\}, \\
(\beta > 0) & : \quad \frac{1}{\sigma} \frac{d\sigma_{\text{NLL},a}}{d\rho} = \frac{\alpha_s C_i}{\pi} \int_0^1 dx_j T_j(x_j) \left\{ \frac{1}{\rho} \left[ f^{g,0}(x_j \rho, y^*) \left( \ln \left( \frac{1}{\rho} \right) + B_i - \ln(x_j) \right) \\
& \quad + f^{g,0}(y^*, 1) \left( \frac{\beta}{2 + \beta} \ln \left( \frac{1}{\rho} \right) - \ln(x_j) \right) + \frac{2}{2 + \beta} \ln \left( \frac{1}{z_{\text{cut}}} \right) + B_i \right] \\
& \quad + f^{g,1}(x_j \rho, y^*) + \frac{\beta}{2 + \beta} f^{g,1}(y^*, 1) \right\}, \\
(\beta = 0) & : \quad \frac{1}{\sigma} \frac{d\sigma_{\text{NLL},a}}{d\rho} = \frac{\alpha_s C_i}{\pi} \int_0^1 dx_j T_j(x_j) \left\{ \frac{1}{\rho} \left[ f^{g,0}(x_j \rho, y^*) \left( \ln \left( \frac{1}{\rho} \right) + B_i - \ln(x_j) \right) + f^{g,1}(x_j \rho, y^*) \right] \\
& \quad + f^{g,0}(y^*, 1) \left( B_i + \ln \left( \frac{1}{z_{\text{cut}}} \right) - \frac{1}{4} z_{\text{cut}}^2 + z_{\text{cut}} \right) \right\}.
\end{align}

B.3 Details of Fixed-Order Matching

B.3.1 Matrix Elements

When computing a collinear-unsafe observable such as track-assisted mass, the cancellation of IR singularities guaranteed by the KLN theorem for sufficiently inclusive observables does not take place. The key to the track function (and more broadly the GFF) formalism is that the collinear singularities in the parton-level matrix element are absorbed into the track functions. Canceling the collinear singularities in the $e^+e^- \to q\bar{q}g$ and $e^+e^- \to H \to ggg(q\bar{q}g)$ matrix elements, which appear at $\mathcal{O}(\alpha_s)$, requires computing the track functions at parton level also to $\mathcal{O}(\alpha_s)$. After this cancellation, the partonic cross section $\frac{d\sigma}{dy_1 dy_2}$ in Eq. (3.28) is replaced by a non-singular matching coefficient, which depends on the renormalization scheme used to calculate
the track functions. This procedure was demonstrated explicitly for quark track functions at $\mathcal{O}(\alpha_s)$ in Ref. [110]. For the process $e^+e^- \rightarrow q\bar{q}g$, the matching coefficient is just the part of the parton-level cross section not proportional to $\delta(1-y_1)$ or $\delta(1-y_2)$, the points in phase space where the collinear singularities appear,

$$\frac{d^2\hat{\sigma}}{dy_1dy_2} = \sigma_0 \frac{\alpha_s(\mu) C_F}{\pi} \Theta(y_1 + y_2 - 1)(y_1^2 + y_2^2) \left( \frac{1}{(1-y_1)(1-y_2)} \right),$$

(B.12)

Here $\sigma_0$ is the Born cross section and $y_i = 2E_i/Q$, with $Q = \sqrt{s}$ the center-of-mass energy of the collision.

Since we are computing the distribution of $\rho$ with a cutoff $\rho > 10^{-6}$, at LO we do not need to calculate virtual terms in the partonic cross sections in Eq. (3.28) and Eq. (3.49) or to compute the $\mathcal{O}(\alpha_s)$ gluon track function. We only need the squared, spin-summed matrix element for the process $e^+e^- \rightarrow H \rightarrow ggg(gq\bar{q})$. Since the Higgs couples to gluons through a quark loop, the lowest perturbative order at which this process can produce a non-zero jet mass is $\mathcal{O}(\alpha_s^2)$. In order to simplify the calculation, we work in the $m_t \rightarrow \infty$ limit, with an effective $Hgg$ coupling. The effective Lagrangian coupling the Higgs to gluons in this limit is [213, 147, 310]

$$\mathcal{L}_{\text{eff}} = \frac{\alpha_s A}{12\pi} G^A_{\mu\nu} G^{A,\mu\nu} \left( \frac{H}{v_{\text{EW}}} \right).$$

(B.13)

where $v_{\text{EW}}$ is the Higgs vacuum expectation value, $G^A_{\mu\nu}$ is the gluon field strength, and the $\mathcal{O}(\alpha_s^2)$ effective coupling constant $A = \frac{\alpha_s}{3\pi v_{\text{EW}}} \left( 1 + \frac{11\alpha_s}{3\pi} \right)$. The Feynman rules for the $Hgg$, $Hggg$, and $Hgggg$ vertices are proportional to the same tensors as the QCD gauge boson vertices. These are illustrated in Fig. B-2, where the relevant tensor structures are

\begin{align*}
T^{\mu\nu} &= g^{\mu\nu} p_1 \cdot p_2 - p_1^\mu p_2^\nu, \\
T^{\mu\nu\rho} &= (p_1 - p_2)^\rho g^{\mu\nu} + (p_2 - p_3)^\mu g^{\nu\rho} + (p_3 - p_1)^\nu g^{\mu\rho}, \\
T^{\mu\nu\rho\sigma}_{abcd} &= f^{abc} f^{d(e}(g^{\mu\rho} g^{\nu\sigma} - g^{\mu\sigma} g^{\nu\rho}) + f^{d(e} f^{f)(g^{\mu\rho} g^{\nu\sigma} - g^{\mu\sigma} g^{\nu\rho})} + f^{f(e} f^{d)(g^{\mu\rho} g^{\nu\sigma} - g^{\mu\sigma} g^{\nu\rho}).
\end{align*}

(B.14) (B.15) (B.16)

205
Figure B-2: Feynman rules for $Hgg$, $Hggg$, and $Hgggg$ couplings in the $m_t \to \infty$ EFT, where all momenta are taken to be ingoing.

The diagrams contributing to the $e^+e^- \to H \to ggg(gqq)$ cross section are shown in Fig. B-3. Interference with the tree-level process $e^+e^- \to Z/\gamma^* \to gqq$ is chirally suppressed at high energy and can be neglected. We use the completeness relation for massless spin-one particles in the final state, with the fixed light-like vector $n^\mu = (1, 0, 0, 0)$ and $k_i \cdot n = E_i$ to project onto only the two physical polarizations,

$$\sum_\lambda \epsilon^\ast_\mu(k, \lambda)\epsilon_\nu(k, \lambda) = -g_{\mu\nu} + \frac{k_\mu n_\nu + k_\nu n_\mu}{k \cdot n} - \frac{k_\mu k_\nu}{(k \cdot n)^2}. \quad (B.17)$$

We rewrite the final-state momenta in terms of the energy fractions $y_i = 2E_i/\sqrt{s}$,

$$k_i \cdot n = \frac{1}{2} Qy_i,$$

$$k_i \cdot k_j = \frac{Q^2}{2}(1 - y_k), \quad (B.18)$$

$$2 = y_1 + y_2 + y_3.$$  

Using these variables, we write the squared, spin-summed matrix elements. First define

$$f(y_1, y_2) = 256\pi^2 \left(y_1^5 + y_1^4(3y_2 - 5) + y_1^3(5y_2^2 - 12y_2 + 10) + y_1^2(18y_2 - 10) - 15y_1^2y_2^2 - 14y_1y_2 + 6y_1 - 2 + 6y_2 + y_2^2(18y_1 - 10) + y_2^3(5y_1^2 - 12y_1 + 10) + y_2^4(3y_1 - 5) + y_2^5 \right). \quad (B.19)$$
Then the result for the $e^+e^- \rightarrow H \rightarrow ggg$ cross section is

$$\sum |M_1|^2 = \sigma_0 \alpha_s C_A \left( \frac{1 - y_1}{y_1^2(1 - y_2)(2 - y_1 - y_2)^2} \right) f(y_1, y_2),$$

$$\sum |M_3|^2 = \sigma_0 \alpha_s C_A \left( \frac{4(1 - y_1)(1 - y_2)}{y_1^2 y_2^2(2 - y_1 - y_2)^2} \right) f(y_1, y_2),$$

$$M_1 M_2^* = \sigma_0 \alpha_s C_A \left( \frac{1}{y_1 y_2(2 - y_1 - y_2)^2} \right) f(y_1, y_2),$$

$$M_1 M_3^* = -\sigma_0 \alpha_s C_A \left( \frac{2(1 - y_1)}{y_1^2 y_2(2 - y_1 - y_2)^2} \right) f(y_1, y_2),$$

and for the $e^+e^- \rightarrow H \rightarrow gq\bar{q}$ cross section,

$$\sum |M_4|^2 = 32\pi^2 \sigma_0 \left( \frac{(y_1 + y_2 - 1)^2 + (1 - y_1)^2}{1 - y_2} \right).$$

The remaining matrix elements can be obtained by exchanging $y_1 \leftrightarrow y_2$. 

207
B.3.2 Comparison of Matching Schemes

There are multiple possible schemes that could be used to match resummed and fixed-order cross sections [104, 106, 222, 181]. In Sec. 3.3.4, we chose the log-$R$ matching scheme defined by Eq. (3.29).

Another possible choice is a simple multiplicative matching scheme for the (normalized) differential distributions [272],

$$
\frac{1}{\sigma} \frac{d\sigma_{\text{NLL+LO}}^{\text{mult}}}{dp} = \left( \frac{1}{\sigma} \frac{d\sigma_{\text{NLL}}}{dp} \right) \left( \frac{1}{\sigma_0} \frac{d\sigma_{\text{LO}}}{dp} \right) \left( \frac{1}{\sigma} \frac{d\sigma_{\text{NLL},0}}{dp} \right)^{-1}. \quad (B.22)
$$

This scheme has the advantage that it automatically enforces that the $\rho$ distribution vanish as $\rho \to 0$ and above the LO kinematic limit Eq. (3.33), $\rho_{\text{max},\text{LO}} \approx 0.23$.

Another common matching scheme is the additive $R$ matching scheme for the cumulative distributions [104],

$$
\Sigma_{\text{NLL+LO}}^{\text{add}} = \Sigma_{\text{NLL}} + \Sigma_{\text{LO}} - \Sigma_{\text{NLL},0}. \quad (B.23)
$$

In order to get the kinematic endpoints correct, we must use the modified $R$ matching scheme. We first rewrite the resummed distribution in the form [104]

$$
\Sigma(\rho) = C(\alpha_s) \exp \left( L g_1 (\alpha_s L) + g_2 (\alpha_s L) + \alpha_s g_3 (\alpha_s L) + \ldots \right) + D(\rho, \alpha_s). \quad (B.24)
$$

Here $L = \log(1/\rho)$, $C(\alpha_s)$ is a perturbatively calculable $\rho$-independent coefficient, and the function $D(\rho, \alpha_s) \to 0$ as $\rho \to 0$. The function $g_1$ resums leading logarithms, $g_2$ resums next-to-leading logarithms, etc. These functions have the perturbative
expansions

\[ C(\alpha_s) = 1 + \sum_{n=1}^{\infty} C_n \left( \frac{\alpha_s}{2\pi} \right)^n, \quad (B.25) \]

\[ D(\rho, \alpha_s) = \sum_{n=1}^{\infty} \left( \frac{\alpha_s}{2\pi} \right)^n D_n(\rho), \quad (B.26) \]

\[ g_n(\alpha_s L) = \sum_{k=1}^{\infty} G_{k,k+2-n} \left( \frac{\alpha_s}{2\pi} \right)^k L^{k+2-n}. \quad (B.27) \]

In order to enforce the constraint that the matched cross section vanish at the upper kinematic boundary, in the \( R \) scheme we must again make the change of variables

\[ \frac{1}{\rho} \rightarrow \frac{1}{\rho} - \frac{1}{\rho_{\text{max,LO}}} + e^{-B_i}, \quad (B.28) \]

in addition to the replacements \[104\]

\[ G_{11} \rightarrow G_{11} \left( 1 - \frac{\rho}{\rho_{\text{max,LO}}} \right), \quad (B.29) \]

\[ \exp(Lg_1 + g_2 + \ldots) \rightarrow \exp(Lg_1 + g_2 + \ldots) \times \exp \left( -\frac{\rho}{\rho_{\text{max,LO}}} G_{11} \alpha_s \log \left( \frac{1}{\rho} \right) \right), \quad (B.30) \]

\[ D(\rho, \alpha_s) \rightarrow D(\rho, \alpha_s) + \left( 1 - \frac{\rho}{\rho_{\text{max,LO}}} G_{11} \alpha_s \log \left( \frac{1}{\rho} \right) \right). \quad (B.31) \]

The term \( G_{11} \) can be read off from Eq. (3.24),

\[ G_{11} = \frac{C_i}{\pi} \int_0^1 dx_j T_j(x_j) \left[ f^{g,0}(x_j,\rho,1)(B_i - \log(x_j)) + f^{g,1}(x_j,\rho,1) \right]. \quad (B.32) \]

Due to the \( \rho \) dependence in the lower endpoints of the track function logarithmic moments, this term technically includes power-suppressed terms beyond NLL order.

In Fig. B-4, we show results for the calorimeter and track-assisted mass at NLL+LO order computed using three different matching schemes: the log-\( R \) scheme, the multiplicative scheme, and the additive \( R \) scheme. The log-\( R \) scheme produces distribution with a pronounced bulge on the high-\( \rho \) side as compared to the other two schemes.
B.4 Alternative Soft-Drop Implementation

Since soft drop changes the jet mass spectrum by design, we argued in Sec. 3.4 that the appropriate distribution to compare with the soft-drop groomed GTAM distribution was the soft-drop groomed jet mass distribution. To get the closest match in these distributions, the factor of $p_{T,\text{calo}}$ in Eq. (3.5) should then be the total calorimeter $p_T$ of the soft-drop groomed jet. This is the reason why we applied soft drop before computing the track mass in Sec. 3.4, such that the charged particles removed by grooming are the same in $p_{T,\text{calo}}$ and $p_{T,\text{track}}$.

On the other hand, applying soft-drop grooming to the calorimeter jet introduces angular resolution issues for neutral particles in the soft-drop procedure. Thus, an alternate way to calculate GTAM with soft-drop grooming is to first recluster just the charged particles into a jet and then groom this charged-only jet. The advantage of this approach is that $M_{\text{track}}$ is calculated using only charged particles from begin-
ning to end, including the soft-drop declustering step. In this appendix, we describe analytic calculations for this alternative possibility.

At parton level, the soft-drop condition becomes

$$\frac{\min(x_1pT,1, x_2pT,2)}{x_1pT,1 + x_2pT,2} > z_{\text{cut}} \left( \frac{\Delta R_{12}}{R_0} \right)^\beta,$$

(B.33)

$$\frac{x_kz}{x_j(1-z) + x_kz} \approx \frac{x_kz}{x_j} > z_{\text{cut}} \left( \frac{\theta}{R} \right)^\beta.$$  

(Eq. B.34) follows from Eq. (B.33) in the soft-collinear limit for a splitting \( i \rightarrow jk \), where parton \( k \) carries a fraction \( z \ll \frac{1}{2} \) of parton \( i \)'s original momentum. For a NLL calculation, only the leading order in an expansion in \( z \) is required. This changes the grooming \( \Theta \)-function in the radiator, Eq. (3.46), to

$$\Theta \left( \frac{x_kz}{x_j} - z_{\text{cut}} \left( \frac{\theta}{R} \right)^\beta \right).$$

(B.35)

Using this \( \Theta \)-function in the radiator, we can derive the explicit form of the radiators for \( \beta > 0 \) and \( \beta = 0 \) in the fixed-coupling approximation. If \( \rho > z_{\text{cut}} \), soft-drop grooming is not active, and the result is the same as the ungroomed case. For \( \rho < z_{\text{cut}} \):

\( \beta > 0 \):

$$R_{\text{TA}}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} \left\{ \frac{1}{2} f^{g,0}(x^*, 1) \frac{\beta}{2 + \beta} \ln^2 \left( \frac{1}{\rho} \right) + \ln \left( \frac{1}{\rho} \right) f^{g,0}(x^*, 1) [B_i - \ln(x_j)] 
- \frac{2}{2 + \beta} \ln(z_{\text{cut}}) \right\} + \ln \left( \frac{1}{\rho} \right) f^{g,1}(x^*, 1) \right\},$$

(B.36)

\( \beta = 0 \):

$$R_{\text{TA}}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} \ln \left( \frac{1}{\rho} \right) \{ f^{g,0}(x_j z_{\text{cut}}, 1) [B_i - \ln(x_j) - \ln(z_{\text{cut}})] 
+ f^{g,1}(x_j z_{\text{cut}}, 1) + G_i(x_j z_{\text{cut}}) \}$$

(B.37)
where we define,

\[ x^* = x_j \rho^{\frac{\beta}{2+\beta}} \frac{2}{z_{\text{cut}}^{2+\beta}} \]  \hspace{1cm} (B.39)

\[ G_q(a) = -\frac{1}{2} \tilde{g}(a, 2) + \tilde{g}(a, 1), \]  \hspace{1cm} (B.40)

\[ G_g(a) = -\frac{3}{4} \tilde{g}(a, 3) + \frac{3}{5} \tilde{g}(a, 2) - \frac{3}{5} \tilde{g}(a, 1) - B_g \left[ \tilde{g}(a, 3) - \frac{3}{5} \tilde{g}(a, 2) + \frac{3}{5} \tilde{g}(a, 1) \right], \]  \hspace{1cm} (B.41)

\[ \tilde{g}(a, n) = a^n \int_0^1 dx x^{-n} T_g(x), \quad \lim_{a \to 0} \tilde{g}(a, n) = 0. \]  \hspace{1cm} (B.42)

Note that the quantity \( \tilde{g}(a, n) \) is well defined as \( a \to 0 \), so there is no divergence as \( x_j \rho \to 0 \). The radiator derivatives appearing in the multiple-emissions prefactor are

\[ (\beta > 0) : \quad R_{\text{T}A}^{\prime}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} f^{g,0}(x^*, 1) \frac{\beta}{2+\beta} \left[ \ln(\frac{1}{\rho}) - \frac{2}{\beta} \ln(z_{\text{cut}}) \right], \]  \hspace{1cm} (B.43)

\[ (\beta = 0) : \quad R_{\text{T}A}^{\prime}(\rho, x_j) = \frac{\alpha_s C_i}{\pi} \left[ - f^{g,0}(x_j z_{\text{cut}}, 1) \ln(z_{\text{cut}}) \right]. \]  \hspace{1cm} (B.44)

As in Sec. 3.4, the terms proportional to \( \ln z_{\text{cut}} \) are formally beyond NLL order, but they make an important numerical contribution in the region \( \rho \approx z_{\text{cut}} \).

NLL resummed distributions for this alternate soft drop implementation are plotted in Fig. B-5 for \( \rho_{\text{T}A} \) of groomed jets with \( z_{\text{cut}} = 0.1 \) and \( \beta = 0, 1, 5, \) and \( \infty \). It is clear that changing the order of grooming and restricting to charged particles has very little quantitative impact.
Figure B-5: Comparison between track-assisted mass with soft-drop grooming for (a) gluon jets and (b) down-quark jets. The solid curves were computed by first grooming the jet and then restricting to charged particles. The dotted lines were computed by reclustering only the charged particles and then grooming.
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224


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241


244


