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Using Large Language Models for Evolutionary Search

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Citation: OREILLY, UNA-MAY and Hemberg, Erik. 2024. "Using Large Language Models for Evolutionary Search."

As Published: <https://doi.org/10.1145/3638530.3648432>


Publisher: ACM|Genetic and Evolutionary Computation Conference

Persistent URL: <https://hdl.handle.net/1721.1/156670>


Version: Final published version: final published article, as it appeared in a journal, conference proceedings, or other formally published context

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Using Large Language Models for Evolutionary Search




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GECCO 24 Companion, July 14–18, 2024, Melbourne, VIC, Australia
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ACM ISBN 979-8-4007-0495-6/24/07.
<https://doi.org/10.1145/3638530.3648432>



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Instructor: Una-May O'Reilly



- Leader: AnyScale Learning For All Group, MIT CSAIL
- Experience solving real world, complex problems requiring AI/machine learning where evolutionary computation is a core capability
- Applications include
 - Cybersecurity
 - Waveform data mining – medical applications
 - Behavioral data mining – MOOC
 - Circuits, network coding
 - Sparse matrix data mapping on parallel architectures
 - Finance
 - Flavor design
 - Wind energy
 - Turbine layout
 - Resource assessment
- Focus on innovation in genetic programming
 - Coevolution
 - Improving its competence
 - Program synthesis
 - Large Language Models

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Instructor: Erik Hemberg


- Research Scientist: AnyScale Learning For All Group, MIT CSAIL
- Experience solving complex problems requiring AI and machine learning with evolutionary computation as a core capability, Bronze HUMIE 2018
- Applications include
 - Cybersecurity
 - Behavioral data mining – MOOC
 - Pylon design
 - Network controllers
 - Tax avoidance
- Focus on innovation and implementation in genetic programming
 - Grammatical representation
 - Coevolution
 - Estimation of Distribution
 - Large Language Models

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Agenda

1. Evolutionary Algorithm
2. Large Language Model
3. EA + LLM use case
 1. Genetic Programming
 1. Tutorial_GP demo
 2. Genetic Programming +Large Language Model
 1. Tutorial_LLM-GP demo
4. EA + LLM Discussion
5. Reference Material



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Evolving Solutions with a Large Language Model

- A Large Language Model works in the input-output space of natural language.
 - It is often a pre-trained transformer model with complex patterns of statistical associations within a massive training text.
- Evolutionary Algorithms (EA) operate on a population of candidate solutions.
 - A basic EA is set up with its operators.
 - Before execution of a run, it is provided with
 - a solution representation
 - a fitness function.
 - Genetic Programming is an evolutionary algorithm, one that evolves code.
- Objectives of this tutorial are
 - describe how an algorithm, with the general algorithmic structure of an EA and evolutionary operators, can use an LLM to evolve solutions in the form of code
 - provide an implementation and demonstration of a simple LLM GP variant.
 - to demystify the approach and provide a hands-on starting point for exploration

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Neo-Darwinian Evolution

- Survival and thriving in the environment
- Offspring quantity - based on survival of the fittest
- Offspring variation: genetic crossover and mutation
- Population-based adaptation over generations
- Genotype-phenotype duality
- Complex and non-deterministic

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Evolutionary Algorithm

$$\max_{x \in \mathcal{X}} f(x)$$

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Problem Domains where EAs are Used

- Where there is need for complex solutions
 - evolution is a process that gives rise to complexity
 - a continually evolving, adapting process, potentially with changing environment from which emerges modularity, hierarchy, complex behavior and complex system relationships
- Combinatorial optimization
 - NP-complete and/or poorly scaling solutions via LP or convex optimization
 - unyielding to approximations (SQP, GEO-P)
 - E.g. TSP, graph coloring, bin-packing, flows
 - for: logistics, planning, scheduling, networks, bio gene knockouts
 - Typified by discrete variables
 - Solved by Genetic Algorithm (GA)
- Continuous Optimization
 - non-differentiable, discontinuous, multi-modal, large scale objective functions "black box"
 - applications: engineering, mechanical, material, physics
 - Typified by continuous variables
 - Solved by Evolutionary Strategy (ES)
- Program Search
 - program as s/w system component, design, strategy, model
 - common: system identification aka symbolic regression, modeling
 - Symbolic regression is a form of supervised machine learning
 - GP offers some unsupervised ML techniques as well
 - Clustering

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EA Individual Examples

Problem	Gene	Genome	Phenotype	Fitness Function
TSP	110	sequence of cities	tour	tour length
Function optimization	3.21	variables \mathbf{x} of function	$f(\mathbf{x})$	$lmin-f(\mathbf{x})$
Graph k-coloring	Permutation element	sequence for greedy coloring	coloring	# of colors
Investment strategy	rule	agent rule set	trading strategy	portfolio change
Regress data	Executable sub-expression	Executable expression	model	Model error on training set (L1, L2)

Evolutionary Computation and Evolutionary Algorithms

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Overview: Large Language Models

- An LLM, with a chatbot or Natural Language API, typically works in the space of natural language.
 - Large is $> 10^8$ parameters (θ)
- The LLM is often a pre-trained transformer model with complex patterns of statistical associations from massive training texts.
 - When the training and task is code, it is called a code model
- Pre-training back-propagates errors arising from predictions that complete text sequences.
- Reinforcement Learning with Human Feedback sets up prompt-response capability.
- The LLM is then further fine-tuned on specific data.
 - The LLM performs approximate retrieval of these patterns to respond to input sequences.

Rewrite 1 + 2 + x

Text \rightarrow LLM θ \rightarrow Text

3 + x

Inference

1 + 2 + x

Text \rightarrow LLM θ \rightarrow Text

1 - 2 + x

Error

Training

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EA Relevant LLM components

- Prompt formulation
- Context window
- Tokenization
- Encoding
- Generation
- Guardrails

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Overview: Regression

Inputs

$x_1^4 \ x_1^3 \ x_1^2 \ x_1^1$

$x_2^4 \ x_2^3 \ x_2^2 \ x_2^1$

$x_3^4 \ x_3^3 \ x_3^2 \ x_3^1$

System

$f(x)$

Output

$y^4 \ y^3 \ y^2 \ y^1$

Also Known As:

- Explanatory variables
- Independent variables
- Manipulated variables
- Control variables
- Decision variables
- Features

- Response variable
- Dependent variable
- Label

GOAL: FIND $f(x)$ THAT GENERATES y

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Regression

- Regress a relationship between a set of explanatory variables and a response variable
- Linear regression:
 - Assume linear model: $y=ax+b$
 - Optimize parameters (a,b) so data best fits model
- Logistic regression for classification
 - Maps linear model into sigmoid family

$$F(x) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$$

- Symbolic regression does NOT assume a model
 - Not parameter search
 - Model is intrinsic in GP solutions

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Genetic Programming Parse Trees

Inorder: 2+3
Preorder: + 2 3
Post-order: 2 3 +

Inorder: (2-3) + (a max best)
Preorder: (+ (-2 3) (max a best))
Post-order: (2 3 -) (a best max) +

Invariant to parse order:

- Preorder (node, left-child, right-child)
- Post-order (left-child, right-child, node)
- Inorder (left, node, right)

GP Evolves Executable Expressions

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A Lisp GP system

A Lisp GP system is a large set of functions which are interpreted by evaluating the entry function

- Some are definitions of primitives you write!
 - (defun protectedDivide ...)
- Rest is software logic for evolutionary algorithms

A GP system has functions that are self-defined (by compilation or interpretation) for use as primitives and logic that handles

- Population initialization, mutation, selection, breeding, replacement, *fitness evaluation*

GP expressions are first class objects in LISP so the GP software logic can manipulate them as data/variables as well as have the interpreter read and evaluate them

GP Evolves Executable Expressions

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How to Evaluate an Expression in GP

- interpreter beneath your code
 - Lisp example
- interpreter within your code
 - typical,
 - examples: tutorial_gp.py
- compile then execute on your OS

```

def evaluate(self, node: List[Any], case: List[float]) -> float:
    """
    Evaluate a node recursively. The node's symbol string is evaluated.
    """
    symbol = node[0]
    symbol = symbol.strip()

    # Identify the node symbol
    if symbol == "+":
        # Add the values of the node's children
        return self.evaluate(node[1], case) + self.evaluate(node[2], case)
    elif symbol == "-":
        # Subtract the values of the node's children
        return self.evaluate(node[1], case) - self.evaluate(node[2], case)
    elif symbol == "*":
        # Multiply the values of the node's children
        return self.evaluate(node[1], case) * self.evaluate(node[2], case)
    elif symbol == "/":
        # Divide the values of the node's children. The low values of the
        # denominator returns the numerator
        numerator = self.evaluate(node[1], case)
        denominator = self.evaluate(node[2], case)
        if abs(denominator) < 0.00001:
            denominator = 1
        return numerator / denominator

    elif symbol.startswith("$"):
        # Get the variable value
        return case[int(symbol[1])]
    else:
        # The symbol is a constant
        return float(symbol)
    
```

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How to Manipulate and Vary Expressions as Data

- For Crossover and Mutation
 - offspring can be different size and structure than parents
 - syntactic correctness
 - randomness in replication and variation
- GP solution
 - reference the parse tree
 - Crossover - swap subtrees between trees of parents
 - Mutation: insert, substitute or delete from a parse tree (PT)

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GP Preparatory Steps

Assume we have a GP system with internal expression evaluator.

- Decide upon functions and terminals
 - Terminals bind to decision variables in problem
 - Combinatorial expression space defines the search space
- Set up the fitness function
 - Translation of problem goal to GP goal
 - Minimization of error between desired and evolved expression when executed
 - Maximization of a problem-based score
 - Construct test cases for program (input examples, desired output)
- Decide upon run parameters
 - Population size is most important
 - GP is robust to many other parameter choices
- Determine a halt criteria and result to be returned
 - Maximum number of fitness evaluations
 - Time
 - Minimum acceptable error
 - Good enough solution (satisficing)

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Top Level GP Algorithm

```

Begin
  pop = random programs from a set of operators and operands
  repeat
    execute each program in pop with each set of inputs
    measure each program's fitness
    repeat
      select 2 parents
      copy 2 offspring from parents
      crossover
      mutate
      add to new-pop
    until pop-size
  pop = new-pop
  until max-generation
  or
  adequate program found
End
    
```

Annotations:

- Grow or Full
- Ramped-half-half
- Max-init-tree-height
- Tournament selection
- Fitness proportional selection
- Tournament size
- Mutation probs
- Sub-tree substitution
- Permute
- Edit
- Sub-tree crossover
- Prob to crossover
- Prepare input data
- Designate solution
- Define error between actual and expected
- Max-tree-height
- Leaf node bias

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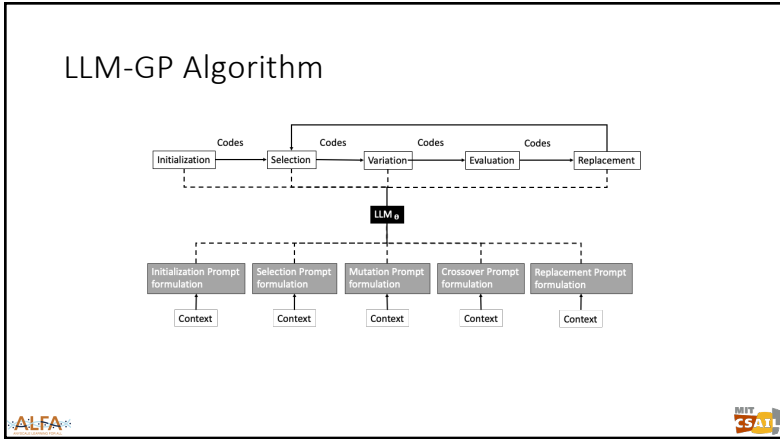
Tutorial_GP: Simple Symbolic Regression

- Given a set of independent decision variables and corresponding values for a dependent variable
 - Test problem:
 - $f(x) = (x_0 + x_1) + (x_1 + x_1)$
 - Want: a model that predicts the dependent variable
 - Domain of X_0 and X_1 [-5.0, 5.0]
 - Choose the 4 operands (terminals)
 - $x_0, x_1, 1.0, 0$
 - Choose the 4 operators (functions)
 - $+, -, *, /$ (protected)
 - protected divide: if denominator=0, return numerator
 - Fitness function: sum of mean squared error between y_i and expression's return values
 - Prepare 121 randomized points for testing
 - Out of sample training/testing ratio is 70:30, random selection of points as training or test
- Usually: designer provides a model, and a regression (ordinary least squares, Fourier series) determines coefficients
 - With genetic programming, the model (structure) and the coefficients can be learned

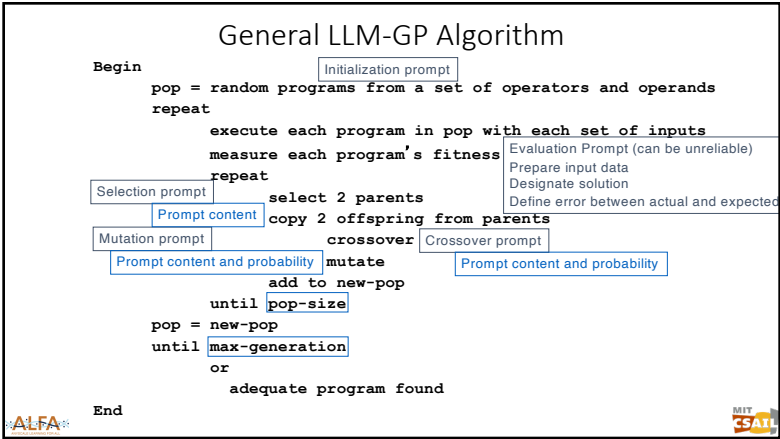
Examples

- GOTO: VS Code debugger
- Evaluation
- Mutation Operator

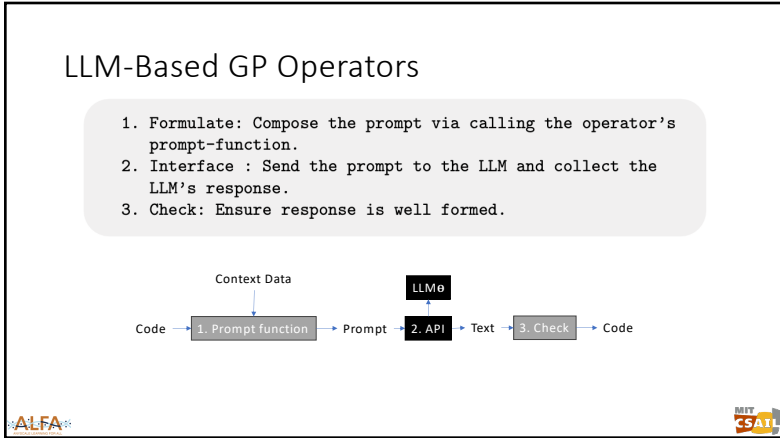
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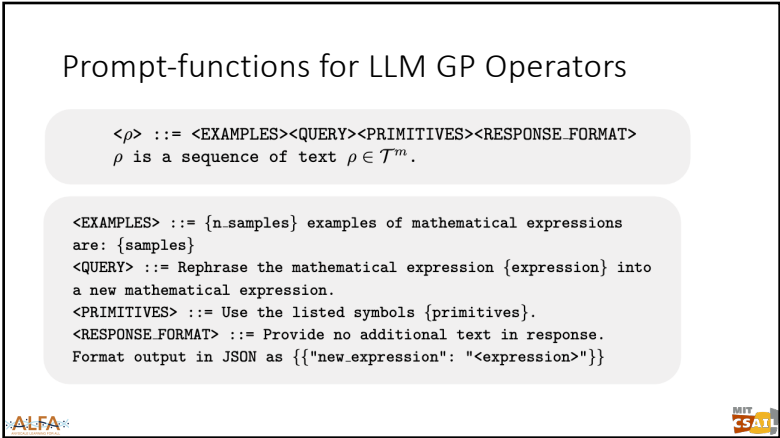
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Example of LLM-GP Mutation

2 examples of mathematical expressions are: $[(x0 + x1) + (x0 - x1) + 1]$, $[x0 + x1 + (1 - 0)]$
 Suppress the mathematical expression $(x0 + x1) + (1 - 0)$ into a new mathematical expression. Use the listed symbols $['+', '-', '*', '^', 'sin', 'cos', 'exp', 'log']$.
 Provide no additional text in response. Format output in JSON as `{"new_expression": "new expression"}`

```
def format_response_rephrase_mutation(self, response: str, expression: str) -> str:
    try:
        phenotype = json.loads(response)["new_expression"]
    except (json.decoder.JSONDecodeError, KeyError, TypeError) as e:
        phenotype = expression
        logging.error(f"({e}) when formatting response for rephrase_mutation for {response}")
    return phenotype

RESPONSE: {"new_expression": "(x0 * x1) + 1"}
INDIVIDUAL (PHENOTYPE): (x0 * x1) + 1
```

```
def form_prompt_rephrase_mutation(self, expression: str, samples: Optional[List[Any]] = None) -> str:
    if samples is not None:
        n_samples = min(10, len(samples), self.n_batches)
        // Randomly sample examples to provide context for the LLM
        sample_input = random.sample(list(samples.keys()), n_samples)
    else:
        sample_input = ""
        n_sample = 0
    prompt = self.REPHRASE_MUTATION_PROMPT_FEW_SHOT.format(
        expression=expression,
        constraints=self.constraints,
        samples=sample_input,
        n_sample=n_sample,
    )
    return prompt
```

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LLM-GP Preparatory Steps

Assume we have an LLM-GP system with internal expression evaluator.

- Decide upon functions and terminals
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 - Construct test cases for program (input examples, desired output)
- Decide upon run parameters
 - Population size is most important
 - GP is robust to many other parameter choices
- Determine a halt criteria and result to be returned
 - Maximum number of fitness evaluations
 - Time
 - Minimum acceptable error
 - Good enough solution (satisficing)

SPECIFY:

- the programming language that will express the candidate solutions plus problem-dependent hand-written primitives and any primitives built-in to the programming language to be used.
- the prompt-functions of all operators implemented using an LLM.
- the hyper-parameters for controlling the run, including the termination criterion, i.e. Run Hyper-Parameters

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LLM-GP considerations

LLM Training: Effort, and Resources

LLM Inference: Bias, Effort and Resources

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Implementation: Error handling and logging

```
def format_response_individual_generation(self, response: str) -> str:
    try:
        phenotype = json.loads(response)["expression"]
    except TypeError:
        phenotype = self.DEFAULT_PHENOTYPE
        logging.error(f"({e}) when formatting response for individual generation for {response}")
    return phenotype

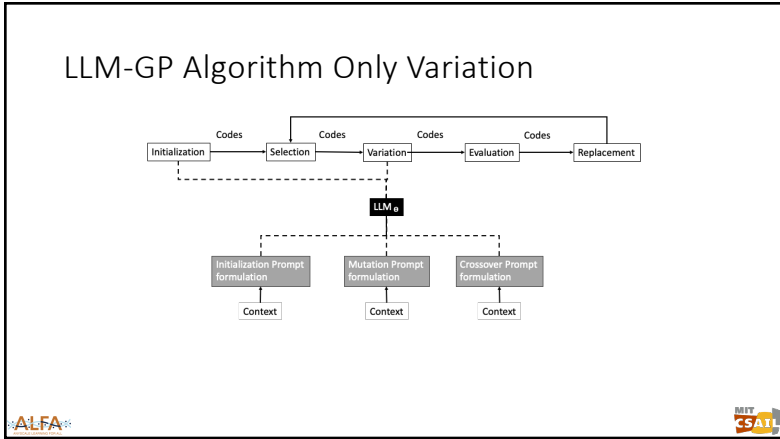
class GPT4Interface:
    def __init__(self):
        self.client = OpenAI(api_key=os.environ.get("OPENAI_API_KEY"), base_url="https://api.openai.com/v1")
        self.prompt_text_logger = self

    def predict_text(self, prompt: str, temp: float = 0.7):
        response = self.client.chat.completions.create(
            model="gpt-4",
            messages=[{"role": "user", "content": prompt}],
            temperature=temp,
            max_tokens=1024,
            n=1,
            stream=False,
        )
        return response.choices[0].message.content

    def predict_text_log(self, prompt: str, temp: float = 0.7):
        response = self.client.chat.completions.create(
            model="gpt-4",
            messages=[{"role": "user", "content": prompt}],
            temperature=temp,
            max_tokens=1024,
            n=1,
            stream=False,
        )
        content = response.choices[0].message.content
        self.prompt_text_logger.log(prompt, content)
        return content

def mutation(self, individual: Individual, fitness_function: FitnessFunction, llm_interface: GPT4Interface, generation_history: List[Tuple[str, str]], mutation_probability: float, samples: Optional[List[Any]] = None) -> List[Individual]:
    new_individual = Individual(individual.genome)
    new_individual.phenotype = individual.phenotype
    if random.random() < mutation_probability:
        prompt = fitness_function.form_prompt_rephrase_mutation(individual.phenotype, samples)
        response = llm_interface.predict_text_log(prompt, temp=1)
        response["operation"] = "mutation"
        generation_history.append(response)
        phenotype = fitness_function.format_response_rephrase_mutation(response["content"], individual.phenotype)
        new_individual.phenotype = phenotype
    return new_individual
```

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Demonstration Setup

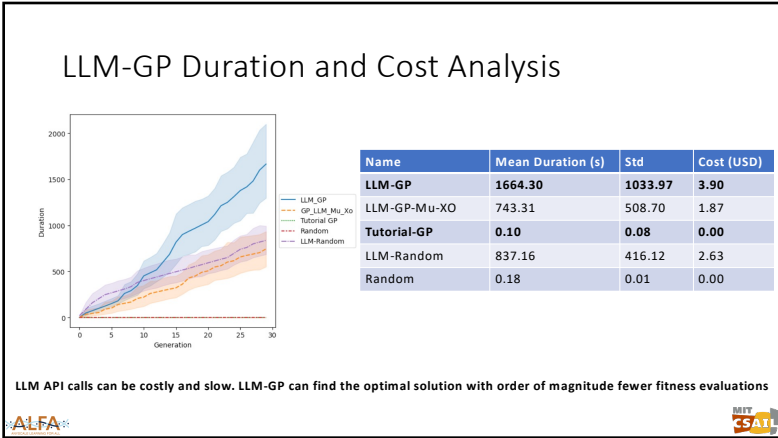
Resource	Description
Operating System	Ubuntu 22.04 LTS
RAM	64GB
CPU	Intel i7-8700K 3.70GHz
Budget	50 USD
Max Runtime	60000 Seconds
Fitness Evaluations	300
LLM version	Gpt-3.5-turbo-0613
Context window size	4096

Parameter	Tutorial GP	LLM-GP-MU-XO	LLM-GP
Trials		30	
Crossover Probability		0.8	
Mutation probability		0.2	
Population size		10	
Generations		30	
Primitives		+, *, x0,x1, 1, 0	
Solution		x02 + x12	
Exemplar splits		0.2 Hold-out, (0.7 Training, 0.3 Testing)	
Exemplars	121	10	
Few-shot exemplars	NA	2	
Mutation	Subtree	Prompt	
Crossover	Subtree	Prompt	
Initialization	Ramped Half-Half		
Max Depth	5	NA	
Selection	Tournament (size 2)	NA	
Replacement	Generational (Elite size 1)	NA	

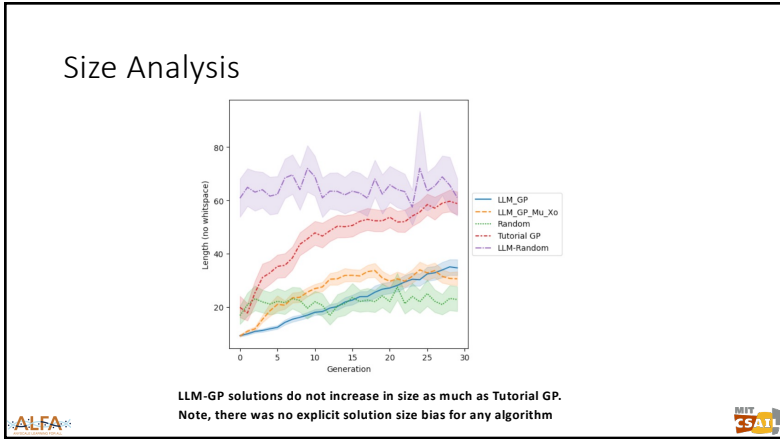
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- ### Tutorial_LLM-GP Demo
- Step Through
 - Run
 - Evaluation
 - Mutation
 - Logs

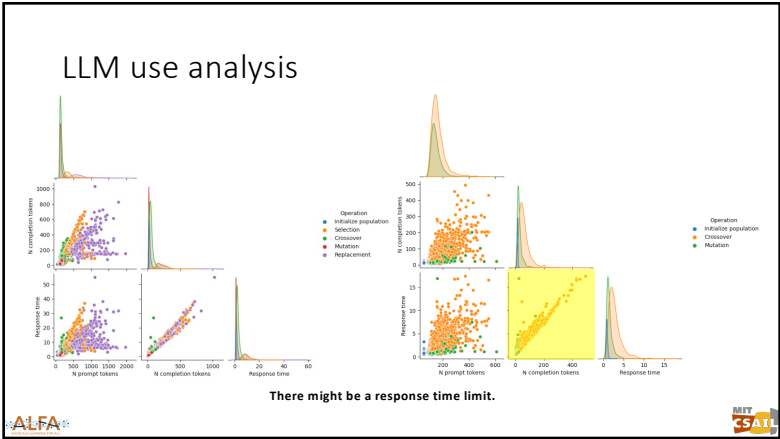
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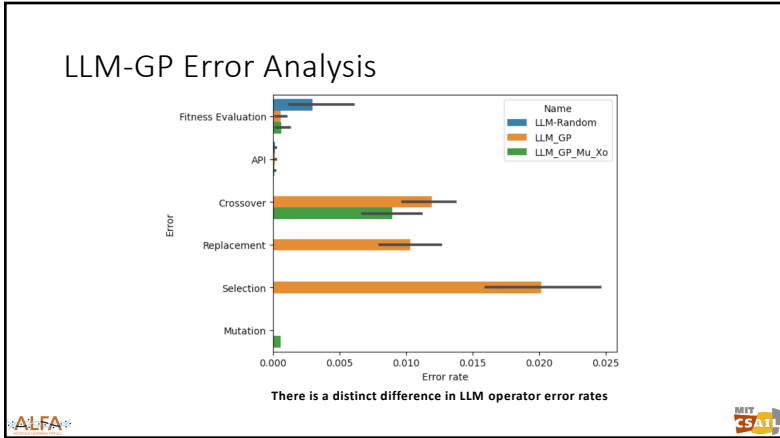
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- ### LLM-EA Example Domains
- Program synthesis
 - Code for Agent Controller
 - Boolean Parity
 - Symbolic Regression (Function Search)
 - Optimization Heuristics
 - Neural Architecture Search
 - Prompts
 - Data for LLM Tuning

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Example LLM Designs used for EA

LLM

- Temperature: Increase LLM variability for solution diversity
- Fine Tuning: Fine tune LLM on data generated during the evolutionary search

Prompt Engineering Techniques

- Zero shot: A predefined prompt
- Template: Prompt expanded with run-time information
- Few-shot: Examples of input and corresponding output
- Chaining: Sequence of LLM calls
- Summarization: Solutions are summarized and then provided as input
- Human Interaction: Human manipulates prompts and responses
- Optimization: External optimization of prompt



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Tutorial GP vs LLM-GP

Basis of Comparison	GP	LLM-GP
Computational environment referenced by the code-evolving system	Program execution environment	Program execution environment and LLM which is a generative pattern completion system using token sequence-based pattern-matching with built-in patterns
Run of a code-evolving system	A GP run executes procedural software where the code is data, the operators work on code structure, and the code is bespoke evaluated and assigned numerical fitness.	A LLM-GP run executes procedural software that, among other things, composes text-based NL prompts, sends them as inputs to an LLM, and collects responses.
Code as desired solution (genotype-phenotype duality)	Genotype/phenotype is a data structure with structural properties, e.g. tree, list, stack, and executability	Code is token sequence with code-snippet meaning, it has no structural properties, and it has implicit pattern-related properties related to the patterns, pattern-matching and bias within the LLM
Evolutionary Variation	Structural, blind to meaning	Not structural, opaque to user beyond prompt content. Internal to LLM it is based on built-in patterns and is a black box.
Evolutionary Selection/Replacement	Comparative, based on numeric ranking and fitness represented as a number	Comparative, prompt could include fitness, could task LLM to rank, could include other bases of comparison. Opaque to user beyond prompt content. Internal to LLM it is based on built-in patterns and is a black box.
Code evaluation	Uses bespoke execution environment (supporting the primitives) on top of a general-purpose program execution environment	Practical implementations will use a general-purpose program execution environment
Code Fitness	Numeric-based	Numeric or expressed with natural language



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Risks of LLM use for EA research

- An algorithm's success depends on prompts and an LLM's responses are sensitive to prompt composition.
 - LLMs currently lack many facets of general intelligence, while they can appear to understand prompts. This risks assuming understanding.
 - Rigorous experiments need to investigate the sensitivity of the algorithm's performance to prompt design.
- An LLMs display biases based on their architecture, training dataset and pre-training.
 - These biases are, to date, poorly characterized or understood.
 - E.g. tokens and position in prompt
- An LLM is probabilistic and generative.
 - Performance is not consistent across LLMs. Accurately predicting and reporting performance of a LLM-EA system might require more effort than an EA system, as will transferring systems and solutions.
- LLM training is difficult and unavailable to some LLM users and data sets for training are not well documented or shared
 - A researcher may not be able to ensure that the rote solution (and problem description) are within the LLM training data
- An LLM used via a model-provider's API has replicability dependency on model release preservation



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LLM-EA investigation motivations

- LLMs offer a new computational paradigm, one working around pattern memory and matching.
 - How does this complement algorithms (not only EAs) solely using a procedural abstraction?
- How do the mechanisms of a LLM relate to mechanisms within Natural systems?
- Could pattern completion competence be effectively like highly environmentally-sensitive, self-adapted variation operators in the natural world?
- Could LLM-EA variants uncover insights into LLM capabilities that lead to advances in LLM design or usage, or EA approaches?
- Could evolving code with an LLM lead to improved understanding of the correspondences between an LLM's capabilities and Nature's mechanisms?



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Conducting LLM-EA Investigations

- Reporting:**
- Report the preparatory steps clearly.
 - Report time and cost of prompting during a run.
 - Report any biases beyond pre-training.
 - Probe prompt sensitivity, if possible, also probe different LLMs.
 - Maintain independent leaderboards on a benchmark for each of the EA and LLM-EA approaches.
 - Report the model version along with its pre-training costs, its training data and its fine-tuning.
- Methods:**
- Check if the problem and solution are in the data set
 - Compare an LLM-based approach against other LLM-based approaches when using a community benchmark. Consider whether it makes sense to compare with EAs.
 - Make well-aligned comparisons (apples to apples, not apples to oranges).
 - EA costs are incurred on different bases from EA LLM. Fitness evaluations dominate running cost so comparison among EA variants can be number of fitness evaluations.
 - LLM-EAs rely on a pre-trained model. Costs related to prompt response time and tokens have no EA equivalent.
 - How much human intelligence has gone into solving the EA problem ahead of the LLM-EA run and how would this differ in the case of EA?
 - Is domain information (not evolutionary information) contained in a prompt?
- Integrity:**
- Be responsible with environmental cost. The budget devoted to investigation has the hidden expense of training an LLM.
 - Use the LLM ethically and keep usage aligned with human values.



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Research Questions for LLM-EA

- Applications:**
- How can LLM-EA integrate software engineering domain knowledge?
 - How can LLM-EA solve prompt composition or other LLM development and use challenges?
 - How can LLM-EA solve with different units of evolution, e.g. strings, images, multi-modal candidates?
- Algorithm Variants:**
- How can we probe LLM-EA to understand the limits of its literal coding competence and more pragmatic coding competences?
 - How can an LLM-EA algorithm integrate design explorations related to cooperation, modularity, reuse, or competition?
 - How can an LLM-EA algorithm model biology differently from EAs?
 - How can an LLM-EA intrinsically, or with guidance, support open-ended evolution?
 - What new variants hybridizing EA, LLM-EA and/or another search heuristic are possible and in what respects are they advantageous?
 - Is there a relevant multi-objective optimization and many-objective optimization approach with LLM-EA?
- Analysis Avenues:**
- How well does LLM-EA scale with population size and problem complexity?
 - What is a search space in LLM-EA and how can it be characterized with respect to problem difficulty?
 - To what extent does an LLM-based approach intrinsically address novelty or quality-diversity?
 - What is the most accurate computational complexity of LLM-EA?



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Reference Material

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