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Convergence-order analysis for differential-inequalities-based bounds and relaxations of the solutions of ODEs

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Abstract For the performance of global optimization algorithms, the rate of convergence of convex relaxations to the objective and constraint functions is critical. We extend results from Bompadre and Mitsos (*J. Glob. Optim.* 52(1): 1–28, 2012) to characterize the convergence rate of parametric bounds and relaxations of the solutions of ordinary differential equations (ODEs). Such bounds and relaxations are used for global dynamic optimization and are computed using auxiliary ODE systems that use interval arithmetic and McCormick relaxations. Two ODE relaxation methods (Scott, Chachuat, and Barton (*Optim. Control Appl. and Meth.* 34(2), 145–163, 2013); Scott and Barton (*J. Glob. Optim.* 57:143–176, 2013)) are shown to give second-order convergence, yet they can behave very differently from each other in practice. As time progresses, the prefactor in the convergence-order bound tends to grow much more slowly for one of these methods, and can even decrease over time, yielding global optimization procedures that require significantly less computation time.

Keywords deterministic global optimization · convergence-order analysis · nonconvex optimization · dynamic optimization

Mathematics Subject Classification (2010) 34A40 · 49M20 · 49M37 · 65L05 · 65L20 · 90C26

1 Introduction

Dynamic optimization or *optimal control* problems seek to minimize an objective function that depends on the solution of an ordinary differential equation (ODE) or differential-algebraic equation (DAE) system. There are numerous applications such as minimizing

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the cost of a chemical process containing a plug-flow reactor, batch reactor, or product changeovers [23, 27, 39]; optimizing the steering, braking, and acceleration of an autonomous vehicle to conserve fuel or minimize time to a destination while obeying safety constraints [22, 29, 38]; or identifying the best-fit parameters for a dynamic model [59]. Many methods have been developed for local dynamic optimization, but for some applications such as safety analysis or rejecting a model that fails to accurately predict system behavior [59], a certificate of global optimality is essential. For some dynamic optimization problems, such as those involving chemical reactions, suboptimal local optima can be very numerous [28, 40, 59], rendering local optimization techniques ineffective.

This article provides an analysis of the convergence order of methods for solving dynamic optimization problems to global optimality. We address dynamic models containing ODEs only. Local dynamic optimization with DAEs embedded is also possible [6, 23, 65], as is rigorous deterministic global optimization with DAEs embedded [47, 50, 52, 53], but both are outside the scope of this article.

Global optimization techniques can be broadly divided into stochastic and deterministic methods. Several stochastic global dynamic optimization techniques have been proposed, such as [2, 31, 40], but they cannot rigorously guarantee global optimality and we do not consider them further. Deterministic global dynamic optimization techniques rely on methods of generating pointwise-in-time lower and upper bounds on the parametric solution of the ODEs on successively refined subsets of the decision space. Some techniques also generate convex relaxations of the parametric solution. For non-dynamic global optimization problems it has been observed that convex relaxations, rather than interval bounds alone, can significantly improve the performance of global optimization methods due to their higher convergence order and the enhanced ability to apply domain reduction techniques. The present contribution shows that these advantages extend to the dynamic optimization methods studied.

Historically, two major approaches have been proposed for generating the necessary bounds and relaxations for deterministic global dynamic optimization. The first is based on Taylor models [18, 24–26, 41–43]. A convergence-order analysis for bounds and relaxations generated by these methods was recently published [5]. The second major approach uses auxiliary ODE systems that, when solved, provide the required bounds and relaxations [7, 15, 48, 49, 51, 54, 57, 58, 62–64]. Now, the line between methods based on Taylor models and auxiliary ODEs has been blurred, with methods that combine the two, such as [8, 66]. There are also methods that propagate other types of convex sets instead of intervals. For example, ellipsoids guaranteed to enclose the solutions of ODEs [17, 19].

The auxiliary-ODE approach uses interval arithmetic [32–34] and generalized McCormick relaxations [30, 55] to obtain global information on the variation of functions of interest on a desired domain with low computational cost. Villanueva et al. [66] recently provided a unifying framework for auxiliary-ODE-based bounding methods. In the present contribution, we develop convergence-order bounds for this auxiliary ODE approach.

Convergence order in various senses is often a key measure of the performance of numerical algorithms. In this article, by *convergence order* we mean the rate at which bounds or relaxations of a function (such as a state variable, objective function, or constraint function) approach the (possibly nonconvex) function being relaxed as the size of the domain is reduced. Convergence order in this sense has long been studied for interval analysis [1, 32, 33, 46] and has recently been formalized for McCormick-based convex relaxations [4, 21, 36]. Recently, Villanueva et al. [66] showed that differential inequalities [14, 49, 57] can be used to generate first-order-convergent bounds on the solutions of ODEs.

Table 1.1 Scaling of number of boxes in a branch-and-bound algorithm (with branch-and-bound absolute tolerance ε_{BB}) differs depending on which regime dominates. For most problems, the true scaling tends to behave between these extreme cases. Order refers to the order of Hausdorff convergence in P of the bounding method, n is problem dimension, and τ is the convergence order prefactor.

Order	Boxes Uniformly Distributed [45]	Boxes Near Minima Dominate [67]	
		τ not necessarily small	τ sufficiently small
1	$\propto \left(\frac{\tau}{\varepsilon_{BB}}\right)^n$	$\propto \left(\frac{\tau}{\sqrt{\varepsilon_{BB}}}\right)^n$	cases from 1 box (2^0) up to $\propto 2^{17}$ shown for arbitrary n depending on the size of τ
2	$\propto \left(\frac{\tau}{\varepsilon_{BB}}\right)^{\frac{n}{2}}$	$\propto \tau^{\frac{n}{2}}$	
3	$\propto \left(\frac{\tau}{\varepsilon_{BB}}\right)^{-\frac{n}{3}}$	$\propto \left(\tau^{\frac{1}{3}} \varepsilon_{BB}^{\frac{1}{6}}\right)^n$	

The number of nodes explored by a branch-and-bound algorithm depends strongly on the convergence order [10] as well as the convergence-order prefactor [67]. Several estimates for the scaling relationship have been published. Schöbel et al. [45, Theorem 2] present an upper bound on the number of boxes considered in a branch-and-bound algorithm as a sum of the boxes considered in each level of the tree, assuming that the search space is divided into 2^n times as many congruent boxes at each successive level of the tree, for an n -dimensional search space. They assume that the convergence-order bound (Definition 2.14) for the relaxations for the objective function holds with equality. They make very weak hypotheses, neglecting even the curvature of the objective function, arriving at an upper bound that is broadly applicable but potentially very conservative. At the other extreme, one can assume that boxes cluster in the vicinity of the global minima, and that those boxes dominate the total number of boxes, as in Du and Kearfott [10]. This “clustering” analysis gives the following scaling estimate: (i) the number of nodes visited by a branch-and-bound algorithm always scales exponentially with problem size, (ii) for first-order-convergent bounding methods, the base of the exponentiation scales as $\frac{1}{\sqrt{\varepsilon_{BB}}}$, where ε_{BB} is the branch-and-bound absolute tolerance, (iii) for second-order bounding methods, the number of nodes in the clustering region is constant with respect to ε_{BB} , and (iv) for third-order bounding methods, the number of nodes in the clustering region actually decreases with tightening ε_{BB} . However, it is widely believed that third-order-convergent methods are NP-hard [37], so second-order methods are the most attractive in practice. Wechsung et al [67, Theorem 1] confirmed that with a convergence order of 2, the number of boxes is insensitive to ε_{BB} , but elucidated the importance of convergence-order prefactor. They showed that using a bounding method with convergence order of 2, the exponential scaling of the number of boxes with problem dimension can be prevented by a sufficiently small convergence-order prefactor. Some illustrative cases for two of the analyses are presented in Table 1.1.

In this article, we analyze the convergence order and prefactor of the differential-inequalities-based ODE bounding method developed in [14] and the ODE relaxation method developed in [54] and subsequently improved in [51]. The developments are organized as follows. In Section 2, we give some necessary definitions and lemmas, including three notions of convergence order. In Section 3, we state the problem of finding convergence-order bounds on the bounds and relaxations of the solutions of ODEs. In Section 4, we recall results from [66] which show that the method of [14] produces bounds on the solutions of parametric ODEs that converge at least first-order as the parameter space is refined (Theorem 4.8). Next we use the logarithmic norm [9, 60] to show that, under appropriate conditions, the bounds can ac-

tually become tighter as time increases—the convergence-order prefactor can decrease over time and asymptotically approach a fixed value as time tends to infinity (Theorem 4.12). In Section 5, we show that the methods described in [51, 54] produce relaxations of the parametric solutions of ODEs with second-order convergence as the parameter space is refined (Theorems 5.19 and 5.21). We next use the logarithmic norm to show that for the improved relaxation method in [51], the convergence-order prefactor can decrease as time progresses and asymptotically approach a fixed value (Theorem 5.25). Relaxations constructed using the improved relaxation method [51] have much more favorable dependence on time than relaxations constructed using the older relaxation method [54]. For the improved method, the prefactor can decrease over time, whereas for the older method, the prefactor can never decrease once a certain level of conservatism has been introduced. In Section 6 we give an overall numerical comparison between the two relaxation methods and discuss one numerical example in detail. Concluding remarks are given in Section 7.

2 Preliminaries

2.1 Gronwall-Bellman inequalities and the logarithmic norm

The convergence results in §4–5 rely on the Gronwall-Bellman inequality and a generalization stated in Lemma 2.2 below.

Lemma 2.1 (Gronwall-Bellman inequality [20, Lemma A.1]). *Let $I \subset \mathbb{R}$. If $x : I \rightarrow \mathbb{R}$, $\lambda : I \rightarrow \mathbb{R}$, and $\mu : I \rightarrow \mathbb{R}$ are continuous functions, μ is nonnegative, and x satisfies*

$$x(t) \leq \lambda(t) + \int_{t_0}^t \mu(s)x(s)ds, \quad \forall t \in I,$$

then

$$x(t) \leq \lambda(t) + \int_{t_0}^t \lambda(s)\mu(s) \exp \left[\int_s^t \mu(\tau)d\tau \right] ds, \quad \forall t \in I.$$

If λ and $\mu \geq 0$ are constants, then $x(t) \leq \lambda \exp[\mu(t - t_0)]$, $\forall t \in I$.

The following result is similar to Lemma 2.1 but allows μ to be a negative constant.

Lemma 2.2. *Let $\lambda_0, \lambda_1 \in \mathbb{R}_+$, $\mu \in \mathbb{R}$, and $I \equiv [t_0, t_f]$. Let $x : I \rightarrow \mathbb{R}$ be continuous. If*

$$x(t) \leq \lambda_0 + \lambda_1(t - t_0) + \int_{t_0}^t \mu x(s)ds, \quad \forall t \in I, \quad (2.1)$$

then

$$\begin{cases} x(t) \leq \left(\lambda_0 + \frac{\lambda_1}{\mu} \right) \exp(\mu(t - t_0)) - \frac{\lambda_1}{\mu} & \text{if } \mu \neq 0, \\ x(t) \leq \lambda_0 + \lambda_1(t - t_0) & \text{if } \mu = 0, \end{cases} \quad \forall t \in I.$$

Proof. See Appendix A. □

In §4–5, we make use of the *logarithmic norm* [9, 60] to derive tight bounds on the convergence behavior of bounds and relaxations for the solutions of ODEs.

Definition 2.3. Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $p \in \{1, 2, \infty\}$. The *logarithmic norm* of $\mathbf{A}$ is

$$\mu_p(\mathbf{A}) \equiv \lim_{h \rightarrow 0^+} \frac{\|\mathbf{I} + h\mathbf{A}\|_p - 1}{h},$$

where $\|\cdot\|_p$ is the induced p -norm.

Note that the logarithmic norm is not truly a norm because it can be negative.

Proposition 2.4. The logarithmic ∞ -norm satisfies:

$$\mu_\infty(\mathbf{A}) = \max_{i=1, \dots, n} \left(a_{ii} + \sum_{k \neq i} |a_{ik}| \right).$$

Proof. See [9, §1.2] or [13, Theorem I.10.5]. $\square$

The formula above is equivalent to the regular matrix ∞ -norm except that $|\cdot|$ is not applied for the diagonal terms.

2.2 Interval analysis and inclusion functions

Definition 2.5 (Interval). For $\mathbf{p}^L, \mathbf{p}^U \in \mathbb{R}^{n_p}$ with $\mathbf{p}^L \leq \mathbf{p}^U$, define the interval $[\mathbf{p}^L, \mathbf{p}^U]$ as the compact, connected set $\{\mathbf{p} \in \mathbb{R}^{n_p} : \mathbf{p}^L \leq \mathbf{p} \leq \mathbf{p}^U\}$. We will also write $P = [\mathbf{p}^L, \mathbf{p}^U] = [p_1^L, p_1^U] \times \dots \times [p_{n_p}^L, p_{n_p}^U]$. We will sometimes use a single real vector to denote a singleton interval, as in $\mathbf{p} \equiv [\mathbf{p}, \mathbf{p}]$. The set of all interval subsets of $D \subset \mathbb{R}^{n_p}$ is denoted $\mathbb{I}D$. In particular, $\mathbb{I}\mathbb{R}^{n_p}$ is the set of all interval subsets of $\mathbb{R}^{n_p}$.

Definition 2.6 (Diameter of a set). The *diameter* of a set $P \subset \mathbb{R}^{n_p}$ is given by

$$w(P) = \sup_{\mathbf{p}_1, \mathbf{p}_2 \in P} \|\mathbf{p}_1 - \mathbf{p}_2\|_\infty.$$

Furthermore, let $w_V(P) \in \mathbb{R}^{n_p}$ be the vector with i th component $\sup_{\mathbf{p}_1, \mathbf{p}_2 \in P} |p_{1,i} - p_{2,i}|$.

Definition 2.7 (Hausdorff metric). For $X, Y \subset \mathbb{R}^n$ compact and nonempty, the Hausdorff metric is given by

$$d_H(X, Y) \equiv \max \left\{ \sup_{\mathbf{x} \in X} \inf_{\mathbf{y} \in Y} \|\mathbf{x} - \mathbf{y}\|_\infty, \sup_{\mathbf{y} \in Y} \inf_{\mathbf{x} \in X} \|\mathbf{x} - \mathbf{y}\|_\infty \right\}.$$

Proposition 2.8 (Hausdorff metric for intervals). Let $X = [\mathbf{x}^L, \mathbf{x}^U]$ and $Y = [\mathbf{y}^L, \mathbf{y}^U]$ be two intervals in $\mathbb{I}\mathbb{R}^n$. Then the Hausdorff metric $d_H(X, Y)$ is equivalent to

$$d_H(X, Y) = \max_{i \in \{1, \dots, n\}} \max \left\{ |x_i^L - y_i^L|, |x_i^U - y_i^U| \right\} = \max_{i \in \{1, \dots, n\}} d_H(X_i, Y_i).$$

Definition 2.9 (Interval hull). For any nonempty, bounded set $P \subset \mathbb{R}^{n_p}$, the *interval hull* of P is denoted by $\square P$ and is the smallest interval containing P :

$$\square P \equiv [\inf\{p_1 : \mathbf{p} \in P\}, \sup\{p_1 : \mathbf{p} \in P\}] \times \dots \times [\inf\{p_{n_p} : \mathbf{p} \in P\}, \sup\{p_{n_p} : \mathbf{p} \in P\}].$$

Definition 2.10 (Image and inclusion function). Let $P \subset \mathbb{R}^{n_p}$ and $\mathbf{f} : P \rightarrow \mathbb{R}^n$. The *image* of $\hat{P} \subset P$ under $\mathbf{f}$ is $\mathbf{f}(\hat{P}) \equiv \{\mathbf{f}(\mathbf{p}) : \mathbf{p} \in \hat{P}\}$. Moreover, an interval function $F : \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^n$ is an *inclusion function* for $\mathbf{f}$ on $\mathbb{I}P$ if

$$\mathbf{f}(\hat{P}) \subset F(\hat{P}), \quad \forall \hat{P} \in \mathbb{I}P.$$

Finally, F is *inclusion monotonic* if $F(\hat{P}) \subset F(\hat{Q})$ for all $\hat{P}, \hat{Q} \in \mathbb{I}P$ satisfying $\hat{P} \subset \hat{Q}$.

A specific inclusion function called the natural interval extension can be efficiently computed if $\mathbf{f}$ is a *factorable function* [32, 34]. A function is factorable if it can be decomposed into a finite sequence of binary arithmetic operations $\{+, -, \div, \times\}$ and compositions with standard univariate functions, such as x^n , e^x , $\sin(x)$, etc. This includes essentially every function that can be written explicitly in computer code.

2.3 Convex relaxations and schemes of estimators

Definition 2.11. Let $P \subset \mathbb{R}^{n_p}$ be convex and let $\mathbf{f} : P \rightarrow \mathbb{R}^n$. Functions $\mathbf{f}^{cv}, \mathbf{f}^{cc} : P \rightarrow \mathbb{R}^n$ are called *convex and concave relaxations of $\mathbf{f}$ on P* , respectively, if $\mathbf{f}^{cv}$ is convex on P , $\mathbf{f}^{cc}$ is concave on P , and $\mathbf{f}^{cv}(\mathbf{p}) \leq \mathbf{f}(\mathbf{p}) \leq \mathbf{f}^{cc}(\mathbf{p}), \forall \mathbf{p} \in P$.

When $P \subset \mathbb{R}^{n_p}$ is an interval and $\mathbf{f}$ is factorable, convex and concave relaxations can be computed automatically and efficiently using, e.g., McCormick's relaxation procedure [30]. To express the dependence of such relaxations on P , which is necessary for analyzing their convergence, Bompadre and Mitsos defined *schemes of estimators* as follows [4].

Definition 2.12 (Scheme of estimators). Let $P \subset \mathbb{R}^{n_p}$ and let $\mathbf{f} : P \rightarrow \mathbb{R}^n$. A pair of functions $(\mathbf{f}^{cv}, \mathbf{f}^{cc}) : \mathbb{I}P \times P \rightarrow \mathbb{R}^n \times \mathbb{R}^n$ is called a *scheme of estimators* for $\mathbf{f}$ in P if, for each $\hat{P} \in \mathbb{I}P$, $\mathbf{f}^{cv}(\hat{P}, \cdot)$ and $\mathbf{f}^{cc}(\hat{P}, \cdot)$ are convex and concave relaxations of $\mathbf{f}$ on $\hat{P}$, respectively. A scheme of estimators is called *continuous* if $\mathbf{f}^{cv}(\hat{P}, \cdot)$ and $\mathbf{f}^{cc}(\hat{P}, \cdot)$ are continuous on $\hat{P}$ for all $\hat{P} \in \mathbb{I}P$. Finally, define the shorthand $F^C \equiv [\mathbf{f}^{cv}, \mathbf{f}^{cc}]$.

Definition 2.13 (Inclusion function associated with a scheme of estimators). Let $\mathbf{f} : P \subset \mathbb{R}^{n_p} \rightarrow \mathbb{R}^n$ and let $F^C : \mathbb{I}P \times P \rightarrow \mathbb{I}\mathbb{R}^n$ be a scheme of estimators for $\mathbf{f}$ in P . The *inclusion function associated to F^C* is the function $H_{\mathbf{f}} : \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^n$ defined by

$$H_{\mathbf{f}}(\hat{P}) \equiv \left[\inf_{\mathbf{p} \in \hat{P}} f_1^{cv}(\hat{P}, \mathbf{p}), \sup_{\mathbf{p} \in \hat{P}} f_1^{cc}(\hat{P}, \mathbf{p}) \right] \times \cdots \times \left[\inf_{\mathbf{p} \in \hat{P}} f_n^{cv}(\hat{P}, \mathbf{p}), \sup_{\mathbf{p} \in \hat{P}} f_n^{cc}(\hat{P}, \mathbf{p}) \right].$$

2.4 Convergence of inclusion functions and schemes of estimators

In this section, we define several notions of convergence for inclusion functions and schemes of estimators.

Definition 2.14 (Hausdorff convergence). Let $P \subset \mathbb{R}^{n_p}$ be bounded, let $\mathbf{f} : P \rightarrow \mathbb{R}^n$, and let $F : \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^n$ be an inclusion function for $\mathbf{f}$ on $\mathbb{I}P$. F has *Hausdorff convergence in P of order β with prefactor τ* if there exist constants $\tau, \beta > 0$ such that

$$d_H(\square \mathbf{f}(\hat{P}), F(\hat{P})) \leq \tau w(\hat{P})^\beta, \quad \forall \hat{P} \in \mathbb{I}P. \quad (2.2)$$

Let $I \subset \mathbb{R}$, $\mathbf{g} : I \times P \rightarrow \mathbb{R}^n$, and let $G(t, \cdot)$ be an inclusion function for $\mathbf{g}(t, \cdot)$ on $\mathbb{I}P$ for every $t \in I$. G has Hausdorff convergence in P of order β with prefactor τ uniformly on I if there exist constants $\tau, \beta > 0$ such that

$$d_H(\square \mathbf{g}(t, \hat{P}), G(t, \hat{P})) \leq \tau w(\hat{P})^\beta, \quad \forall (t, \hat{P}) \in I \times \mathbb{I}P.$$

We now define a stronger notion of convergence for interval functions that holds for many types of inclusion functions and implies Hausdorff convergence.

Definition 2.15 (Convergence in diameter). Let $P \subset \mathbb{R}^{n_p}$ be bounded. An interval function $F : \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^n$ converges in diameter in P with order β and prefactor τ if there exist constants $\tau, \beta > 0$ such that

$$w(F(\hat{P})) \leq \tau w(\hat{P})^\beta, \quad \forall \hat{P} \in \mathbb{I}P. \quad (2.3)$$

Moreover, with $I \subset \mathbb{R}$, the interval function $G : I \times \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^n$ converges in diameter in P with order β and prefactor τ uniformly on I if there exist constants $\tau, \beta > 0$ such that

$$w(G(t, \hat{P})) \leq \tau w(\hat{P})^\beta, \quad \forall (t, \hat{P}) \in I \times \mathbb{I}P.$$

Lemma 2.16. Let $I \subset \mathbb{R}$, $\mathbf{g} : I \times P \rightarrow \mathbb{R}^n$, and let $G(t, \cdot)$ be an inclusion function for $\mathbf{g}(t, \cdot)$ on $\mathbb{I}P$ for every $t \in I$. If G converges in diameter in P with order β uniformly on I , then G has Hausdorff convergence in P of order β uniformly on I . The converse holds for $\beta = 1$ if $\mathbf{g}$ is Lipschitz continuous on $I \times P$.

Proof. Note that $d_H(Z', Z) \leq w(Z)$ for all $Z, Z' \in \mathbb{I}\mathbb{R}^n$ with $Z' \subset Z$. In particular, this implies $d_H(\square \mathbf{g}(t, \hat{P}), G(t, \hat{P})) \leq w(G(t, \hat{P}))$. Thus, convergence in diameter implies Hausdorff convergence. Conversely, using the Hausdorff convergence in P of order 1, Proposition 2.8, and $\square \mathbf{g}(t, \hat{P}) \subset G(t, \hat{P})$, we have

$$w(G(t, \hat{P})) \leq w(\square \mathbf{g}(t, \hat{P})) + 2\tau w(\hat{P}), \quad \forall (t, \hat{P}) \in I \times \mathbb{I}P.$$

Letting L be a Lipschitz constant for $\mathbf{g}$ on $I \times P$, Lemma 1 in [4] gives $w(\square \mathbf{g}(t, \hat{P})) \leq Lw(\hat{P})$, and hence $w(G(t, \hat{P})) \leq (L + 2\tau)w(\hat{P})$, $\forall (t, \hat{P}) \in I \times \mathbb{I}P$. $\square$

The following lemma shows that both forms of convergence above are implied by Lipschitz continuity of the inclusion function, provided that $w(G(t, [\mathbf{p}, \mathbf{p}])) = 0$.

Lemma 2.17. Let $I \subset \mathbb{R}$ and $P \subset \mathbb{R}^{n_p}$. Let $G : I \times \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^n$ be an inclusion function. If $w(G(t, [\mathbf{p}, \mathbf{p}])) = 0$, $\forall (t, \mathbf{p}) \in I \times P$, and $\exists L \in \mathbb{R}_+$ satisfying

$$d_H(G(t, P_1), G(t, P_2)) \leq Ld_H(P_1, P_2), \quad \forall (t, P_1, P_2) \in I \times \mathbb{I}P \times \mathbb{I}P, \quad (2.4)$$

then G converges in diameter in P with order 1 and prefactor $2L$ uniformly on I .

Proof. For any $(t, \hat{P}) \in I \times \mathbb{I}P$ and any $\mathbf{p} \in \hat{P}$, the Lipschitz condition implies that $d_H(G(t, \hat{P}), G(t, [\mathbf{p}, \mathbf{p}])) \leq Ld_H(\hat{P}, [\mathbf{p}, \mathbf{p}]) \leq Lw(\hat{P})$. It follows from Proposition 2.8 and $G(t, [\mathbf{p}, \mathbf{p}]) \subset G(t, \hat{P})$ that

$$w(G(t, \hat{P})) \leq w(G(t, [\mathbf{p}, \mathbf{p}])) + 2Lw(\hat{P}) = 2Lw(\hat{P}),$$

for all $(t, \hat{P}) \in I \times \mathbb{I}P$. $\square$

We now define a notion of convergence for schemes of estimators based on [4].

Definition 2.18 (Pointwise convergence order and prefactor). Let $P \subset \mathbb{R}^{n_p}$ be bounded. Let $\mathbf{f} : P \subset \mathbb{R}^{n_p} \rightarrow \mathbb{R}^n$ and let $F^C : \mathbb{I}P \times P \rightarrow \mathbb{I}\mathbb{R}^n$ be a scheme of estimators for $\mathbf{f}$ in P . F has *pointwise convergence in P of order γ with prefactor τ* if there exist constants $\tau, \gamma > 0$ such that

$$\sup_{\mathbf{p} \in \hat{P}} w\left(F^C(\hat{P}, \mathbf{p})\right) \leq \tau w(\hat{P})^\gamma, \quad \forall \hat{P} \in \mathbb{I}P.$$

Let $I \subset \mathbb{R}$, $\mathbf{g} : I \times P \rightarrow \mathbb{R}^n$, and let $G^C(t, \cdot, \cdot)$ be a scheme of estimators for $\mathbf{g}(t, \cdot)$ in P for every $t \in I$. G^C has *pointwise convergence in P of order γ with prefactor τ uniformly on I* if there exist constants $\tau, \gamma > 0$ such that

$$\sup_{\mathbf{p} \in \hat{P}} w\left(G^C(t, \hat{P}, \mathbf{p})\right) \leq \tau w(\hat{P})^\gamma, \quad \forall (t, \hat{P}) \in I \times \mathbb{I}P.$$

The reader can verify that pointwise convergence in the sense of Definition 2.18 and pointwise convergence in the sense of [4] are equivalent to within a factor of two.

In the definitions above, the order and prefactor may depend on the host set P , but not on $\hat{P}$. Also, note that these definitions do not require the convergence order to be the highest possible (e.g., if F has second-order Hausdorff convergence, then it also has first-order Hausdorff convergence). In addition to establishing theoretical convergence-order bounds, which can be weak, we will also discuss what we call the *empirical convergence behavior* in the context of our numerical examples, by which we mean the γ value consistent with a computed plot of the Hausdorff distance $d_H(\square \mathbf{f}(\hat{P}), F(\hat{P}))$ versus $w(\hat{P})$ for a particular sequence as $w(\hat{P})$ is decreased to zero. This sheds light on how different methods can perform in practice, with different regimes as the host set is partitioned. For example, valid bounds can exist with convergence orders both 1 and 2. An example is shown in Figure 2.1.

3 Problem statement

Let $I = [t_0, t_f] \subset \mathbb{R}$ be a time horizon of interest, $D \subset \mathbb{R}^{n_x}$ an open and connected set, $P \subset \mathbb{R}^{n_p}$ a set of possible parameter values, $\mathbf{f} : I \times D \times P \rightarrow \mathbb{R}^{n_x}$ a locally Lipschitz continuous vector field, and $\mathbf{x}_0 : P \rightarrow D$ a locally Lipschitz continuous initial condition function. Consider the following initial value problem (IVP) in ODEs:

$$\begin{aligned} \dot{\mathbf{x}}(t, \mathbf{p}) &= \mathbf{f}(t, \mathbf{x}(t, \mathbf{p}), \mathbf{p}), \quad \forall t \in (t_0, t_f], \\ \mathbf{x}(t_0, \mathbf{p}) &= \mathbf{x}_0(\mathbf{p}). \end{aligned} \tag{3.1}$$

We assume that a unique solution $\mathbf{x}(\cdot, \mathbf{p})$ exists on all of I for every $\mathbf{p} \in P$. State bounds and state relaxations for this solution are defined below.

Definition 3.1 (State bounds). Two functions $\mathbf{x}^L, \mathbf{x}^U : I \times \mathbb{I}P \rightarrow \mathbb{R}^{n_x}$ are *state bounds* if

$$\mathbf{x}^L(t, \hat{P}) \leq \mathbf{x}(t, \mathbf{p}) \leq \mathbf{x}^U(t, \hat{P}), \quad \forall (t, \mathbf{p}) \in I \times \hat{P}, \quad \forall \hat{P} \in \mathbb{I}P.$$

Moreover, let $X^B : I \times \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^{n_x}$ denote the corresponding inclusion function, defined by $X^B(t, \hat{P}) \equiv [\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})]$.

Fig. 2.1 Empirical convergence behavior for a hypothetical inclusion function satisfying both first- and second-order Hausdorff convergence. In this way, convergence of a given order does not preclude convergence of higher order. On larger sets, the first-order bound is stronger than the second-order bound. On smaller sets, the second-order bound is stronger.

Definition 3.2 (State relaxations). Two functions $\mathbf{x}^{cv}, \mathbf{x}^{cc} : I \times \mathbb{I}P \times P \rightarrow \mathbb{R}^{n_x}$ are *state relaxations* if, for each $t \in I$ and $\hat{P} \in \mathbb{I}P$, $\mathbf{x}^{cv}(t, \hat{P}, \cdot)$ and $\mathbf{x}^{cc}(t, \hat{P}, \cdot)$ are convex and concave relaxations of $\mathbf{x}(t, \cdot)$ on $\hat{P}$, respectively. Moreover, let $X^C : I \times \mathbb{I}P \times P \rightarrow \mathbb{I}\mathbb{R}^{n_x}$ denote the corresponding scheme of estimators, defined by $X^C(t, \hat{P}, \mathbf{p}) \equiv [\mathbf{x}^{cv}(t, \hat{P}, \mathbf{p}), \mathbf{x}^{cc}(t, \hat{P}, \mathbf{p})]$.

Our objective is to establish bounds on the convergence orders and prefactors of state bounds and state relaxations for (3.1) computed by the auxiliary ODE approach outlined in §1 [7, 48, 49, 51, 54, 57, 58].

4 Convergence of state bounds

In this section, we study the convergence behavior of state bounds for (3.1) computed using the auxiliary ODE approach first introduced by Harrison in [14]. Harrison’s method is based on Müller’s comparison theorem [35] and provides the basis for a number of improved methods of this type [8, 15, 16, 48, 49, 56, 57]. Müller provided the mathematical proof underlying the method, but Harrison proposed its application to practical bounding problems by numerically integrating an auxiliary system, so we choose to refer to it as Harrison’s method. Harrison’s method has already been shown to have first-order convergence in diam-

eter, and hence first-order Hausdorff convergence, as a special case of Corollary 1 in [66]. Here, we extend this result by establishing a tighter bound on the convergence prefactor using the logarithmic norm, and analyzing the dependence of this bound on time. We also compare Harrison’s method to a weaker method that also enjoys first-order convergence in diameter, but is known to produce much weaker bounds in practice. This method, which we call the *naïve method*, is obtained by removing a key constraint used in Harrison’s method. We show that Harrison’s method permits the width of the state bounds to decrease over time, and we provide sufficient conditions for this to occur. In contrast, such a decrease is impossible for the naïve method.

4.1 Methods for generating state relaxations

To define Harrison’s method, let $X_0 : \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^{n_x}$ and $F : \mathbb{I}I \times \mathbb{I}D \times \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^{n_x}$ denote inclusion functions for $\mathbf{x}_0$ and $\mathbf{f}$ in (3.1), respectively. Moreover, denote $X_0(P') = [\mathbf{x}_0^L(P'), \mathbf{x}_0^U(P')]$ and $F(I', X', P') = [\mathbf{f}^L(I', X', P'), \mathbf{f}^U(I', X', P')]$ for all $(I', X', P') \in \mathbb{I}I \times \mathbb{I}D \times \mathbb{I}P$.

We make the following assumption throughout the rest of the paper.

- Assumption 4.1.** 1. F and X_0 are locally Lipschitz continuous with respect to the Hausdorff metric on $\mathbb{I}I \times \mathbb{I}D \times \mathbb{I}P$ and $\mathbb{I}P$, respectively.
 2. F and X_0 have convergence in diameter of order 1 in any compact subset of $I \times D \times P$ and P , respectively.
 3. F and X_0 are inclusion monotonic on their domains.

Remark 4.2. By Theorem 2.5.12 in [47], the Lipschitz condition in Assumption 4.1 is equivalent to the assumption that the functions $(\mathbf{p}^L, \mathbf{p}^U) \mapsto \mathbf{x}_0^L([\mathbf{p}^L, \mathbf{p}^U])$ and $(\mathbf{p}^L, \mathbf{p}^U) \mapsto \mathbf{x}_0^U([\mathbf{p}^L, \mathbf{p}^U])$ are locally Lipschitz continuous on $\{\mathbf{p}^L, \mathbf{p}^U \in P : \mathbf{p}^L \leq \mathbf{p}^U\}$ in the conventional, real-valued sense, and similarly for $\mathbf{f}^L$ and $\mathbf{f}^U$. Moreover, for any compact $P' \subset P$, compactness of the set $\{\mathbf{p}^L, \mathbf{p}^U \in P' : \mathbf{p}^L \leq \mathbf{p}^U\}$ implies that $(\mathbf{p}^L, \mathbf{p}^U) \mapsto \mathbf{x}_0^L([\mathbf{p}^L, \mathbf{p}^U])$ and $(\mathbf{p}^L, \mathbf{p}^U) \mapsto \mathbf{x}_0^U([\mathbf{p}^L, \mathbf{p}^U])$ are Lipschitz there, and hence $\exists L \in \mathbb{R}^+$ such that

$$d_H(X_0(P_1), X_0(P_2)) \leq L d_H(P_1, P_2), \quad \forall (P_1, P_2) \in \mathbb{I}P' \times \mathbb{I}P'. \quad (4.1)$$

In other words, X_0 is Lipschitz continuous on $\mathbb{I}P'$ for any compact $P' \subset P$. Of course, the analogous statement holds for F . We use the assumption in this form in the proof of Theorem 4.14 below.

Remark 4.3. If $\mathbf{f}$ and $\mathbf{x}_0$ are factorable functions, then their natural interval extensions provide inclusion functions F and X_0 satisfying Assumption 4.1 under some mild technical conditions discussed in [47]. Conditions 1 and 3 are proven in Theorems 2.5.30 and 2.3.11 in [47], respectively, while Condition 2 follows from Condition 1 and Lemma 2.17 here.

Harrison’s method also requires the following interval functions.

Definition 4.4 ($\mathcal{B}_i^{L/U}$). Define the interval functions $\mathcal{B}_i^L, \mathcal{B}_i^U : \mathbb{I}\mathbb{R}^n \rightarrow \mathbb{I}\mathbb{R}^n$ by $\mathcal{B}_i^L([\mathbf{v}, \mathbf{w}]) \equiv \{\mathbf{z} \in [\mathbf{v}, \mathbf{w}] : z_i = v_i\}$ and $\mathcal{B}_i^U([\mathbf{v}, \mathbf{w}]) \equiv \{\mathbf{z} \in [\mathbf{v}, \mathbf{w}] : z_i = w_i\}$.

Definition 4.5 (Harrison’s method [14], as stated in [47], Equation (3.3)). *Harrison’s method* computes state bounds for (3.1) on $\hat{P} \in \mathbb{I}P$ as the solution of the following auxiliary ODEs

for $i = 1, \dots, n_x$, which we refer to as *Harrison's state bounding system*:

$$\begin{aligned}\dot{x}_i^L(t, \hat{P}) &= f_i^L([t, t], \mathcal{B}_i^L([\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})]), \hat{P}), \quad \forall t \in (t_0, t_f], \\ \dot{x}_i^U(t, \hat{P}) &= f_i^U([t, t], \mathcal{B}_i^U([\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})]), \hat{P}), \quad \forall t \in (t_0, t_f], \\ [x_i^L(t_0, \hat{P}), x_i^U(t_0, \hat{P})] &= X_{0,i}(\hat{P}).\end{aligned}$$

If a solution to Harrison's state bounding system exists, then it provides valid state bounds for (3.1) [47, §3.5.3]. Specifically, the initial conditions ensure that $\mathbf{x}^L(t)$ and $\mathbf{x}^U(t)$ bound the parametric solution of (3.1) at t_0 , while the ODEs maintain this property for $t > t_0$ by forcing each $x_i^L(t)$ and $x_i^U(t)$ to decrease and increase, respectively, faster than $x_i(t, \mathbf{p})$, $\forall \mathbf{p} \in \hat{P}$. The functions $\mathcal{B}_i^{L/U}$ are used because it is only necessary for $x_i^L(t)$ to decrease faster than the i^{th} component of trajectories $\mathbf{x}(t, \mathbf{p})$ that are already incident on the i^{th} lower bound (i.e., $x_i(t, \mathbf{p}) = x_i^L(t)$), and similarly for $x_i^U(t)$. In the analysis below, we show that this constraint is critically important to the behavior of Harrison's method. To do so, we compare Harrison's method to the naïve method obtained by omitting $\mathcal{B}_i^{L/U}$.

Definition 4.6 (Naïve method). The *naïve method* computes state bounds for (3.1) on $\hat{P} \in \mathbb{I}P$ as the solution of the following auxiliary ODEs for $i = 1, \dots, n_x$, which we refer to as the *naïve state bounding system*:

$$\begin{aligned}\dot{x}_i^L(t, \hat{P}) &= f_i^L([t, t], [\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})], \hat{P}), \quad \forall t \in (t_0, t_f], \\ \dot{x}_i^U(t, \hat{P}) &= f_i^U([t, t], [\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})], \hat{P}), \quad \forall t \in (t_0, t_f], \\ [x_i^L(t_0, \hat{P}), x_i^U(t_0, \hat{P})] &= X_{0,i}(\hat{P}).\end{aligned}$$

Theorem 4.7. Let $\mathbf{x}^L, \mathbf{x}^U : I \times \mathbb{I}P \rightarrow \mathbb{R}^{n_x}$ be a solution of either Harrison's state bounding system or the naïve state bounding system and let $X^B(t, \hat{P}) \equiv [\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})]$, $\forall (t, \hat{P}) \in I \times \mathbb{I}P$. For every $t \in I$, $X^B(t, \cdot)$ is an inclusion function for $\mathbf{x}(t, \cdot)$ on $\mathbb{I}P$.

Proof. This follows from Theorem 2 and Corollary 3 in [49]. $\square$

4.2 Convergence-order results

Theorem 4.8. Let $\mathbf{x}^L, \mathbf{x}^U : I \times \mathbb{I}P \rightarrow \mathbb{R}^{n_x}$ be a solution of either Harrison's state bounding system or the naïve state bounding system and let $X^B(t, \hat{P}) \equiv [\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})]$. Choose any $P' \in \mathbb{I}P$ and assume that $\cup_{t \in I, \hat{P} \in \mathbb{I}P'} X^B(t, \hat{P})$ is contained in a compact set $X' \subset D$. Then, X^B converges in diameter in P' with order at least 1, uniformly on I .

Proof. X_0 and F converge in diameter with order one in P' and $I \times X' \times P'$, respectively. Moreover, $\mathbf{f}$ is Lipschitz continuous on $I \times X' \times P'$ as well. Thus, both results follow as special cases of Corollary 1 in [66]. $\square$

Although Harrison's method and the naïve method have the same convergence order, the latter produces much weaker state bounds in practice. Notably, the width of the Harrison's state bounds sometimes decreases over time, while such a decrease is never observed with the naïve method. The following proposition gives sufficient conditions under which Harrison's bounds can become tighter with increasing time ($\frac{d}{dt} w(X_k^B(t, \hat{P})) < 0$ for some t in the time horizon), and shows that improvement is theoretically impossible for the naïve method. This result is central to the improved bound on the convergence prefactor for Harrison's method established in Theorem 4.12.

Proposition 4.9. Let $\mathbf{x}^L, \mathbf{x}^U : I \times \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^{n_x}$ be a solution of Harrison's state bounding system and let $X^B(t, \hat{P}) \equiv [\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})]$. Choose any $P' \in \mathbb{I}P$ and assume that $\cup_{t \in I, \hat{P} \in \mathbb{I}P'} X^B(t, \hat{P})$ is contained in a compact set $X' \subset D$. Let $L \in \mathbb{R}_+$ be a Lipschitz constant for $\mathbf{f}$ on $I \times X' \times P'$, and let $\tau_k \in \mathbb{R}_+$ be the prefactor for convergence of F_k in diameter on $I \times X' \times P'$ as per Assumption 4.1. If, for some $(t, k, \hat{P}) \in I \times \{1, \dots, n_x\} \times \mathbb{I}P'$, there exists $\alpha_k \in \mathbb{R}$ such that

$$\begin{aligned} f_k(t, \mathbf{z}^{(1)}, \mathbf{p}) - f_k(t, \mathbf{z}^{(2)}, \mathbf{p}) &\leq \alpha_k (z_k^{(1)} - z_k^{(2)}), \\ \forall (\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \mathbf{p}) &\in X^B(t, \hat{P}) \times X^B(t, \hat{P}) \times \hat{P} : z_j^{(1)} = z_j^{(2)}, \forall j \neq k \text{ and } z_k^{(1)} \geq z_k^{(2)}, \end{aligned} \quad (4.2)$$

then

$$\frac{d}{dt} w(X_k^B(t, \hat{P})) \leq \alpha_k w(X_k^B(t, \hat{P})) + (L + 2\tau_k) \max \left\{ \max_{i \neq k} w(X_i^B(t, \hat{P})), w(\hat{P}) \right\}. \quad (4.3)$$

If $\alpha_k < 0$, this bound can be negative. In contrast, for the naïve method, it is not possible to obtain $\frac{d}{dt} w(X_k^B(t, \hat{P})) < 0$.

Remark 4.10. The condition (4.2) holds trivially with $\alpha_k = L \geq 0$. However, it can be shown to hold with $\alpha_k < 0$ in a number of important cases. For example, it holds for linear systems $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$ with at least one diagonal element of $\mathbf{A}$ bounded above by $\alpha_k < 0$. It also holds when f_k is differentiable and $\frac{\partial f_k}{\partial x_k}(t, \mathbf{z}, \mathbf{p}) \leq \alpha_k < 0$, $\forall (\mathbf{z}, \mathbf{p}) \in X^B(t, \hat{P}) \times \hat{P}$. Specific examples where (4.2) holds with $\alpha_k < 0$ include mass-action chemical kinetic systems in which at least one species can be consumed by reaction, the (nonlinear) Lorenz equations with positive values of the parameters σ and β , the Duffing equation with positive damping, and the Lotka-Volterra model whenever $x_2 > 1$ or $x_1 < 1$. Strictly decreasing functions restricted to compact subsets of their domains also obey such a bound with $\alpha_k < 0$.

Proof. Choose any $(t, k, \hat{P}) \in I \times \{1, \dots, n_x\} \times \mathbb{I}P'$ and assume that (4.2) holds. For this proof only, define the following nomenclature:

1. $F_{k,L}(t, \hat{P}) \equiv F_k(t, \mathcal{B}_k^L(X^B(t, \hat{P})), \hat{P})$,
2. $F_{k,U}(t, \hat{P}) \equiv F_k(t, \mathcal{B}_k^U(X^B(t, \hat{P})), \hat{P})$,
3. $f_k^{*,L}(t, \hat{P}) \equiv \inf \{f_k(t, \mathbf{z}, \mathbf{p}) : \mathbf{z} \in \mathcal{B}_k^L(X^B(t, \hat{P})), \mathbf{p} \in \hat{P}\}$,
4. $f_k^{*,U}(t, \hat{P}) \equiv \sup \{f_k(t, \mathbf{z}, \mathbf{p}) : \mathbf{z} \in \mathcal{B}_k^U(X^B(t, \hat{P})), \mathbf{p} \in \hat{P}\}$.

Furthermore, noting that $F_{k,L}(t, \hat{P})$ and $F_{k,U}(t, \hat{P})$ are intervals, denote $F_{k,L}(t, \hat{P}) = [F_{k,L}^L(t, \hat{P}), F_{k,L}^U(t, \hat{P})]$, and $F_{k,U}(t, \hat{P}) = [F_{k,U}^L(t, \hat{P}), F_{k,U}^U(t, \hat{P})]$. By the definition of Harrison's state bounding system, $\frac{d}{dt} w(X_k^B(t, \hat{P})) = F_{k,U}^U(t, \hat{P}) - F_{k,L}^L(t, \hat{P})$. Next, observe that, since F_k is an inclusion function for f_k , we have $f_k^{*,L}(t, \hat{P}) \in F_{k,L}(t, \hat{P})$ and $f_k^{*,U}(t, \hat{P}) \in F_{k,U}(t, \hat{P})$, and it follows that

$$\begin{aligned} \frac{d}{dt} w(X_k^B(t, \hat{P})) &\leq \left(f_k^{*,U}(t, \hat{P}) + w(F_{k,U}(t, \hat{P})) \right) - \left(f_k^{*,L}(t, \hat{P}) - w(F_{k,L}(t, \hat{P})) \right), \\ &= f_k^{*,U}(t, \hat{P}) - f_k^{*,L}(t, \hat{P}) + w(F_{k,U}(t, \hat{P})) + w(F_{k,L}(t, \hat{P})). \end{aligned} \quad (4.4)$$

Since f_k is continuous, the Weierstrass theorem (e.g., [3]) ensures that the infimum and supremum defining $f_k^{*,L}(t, \hat{P})$ and $f_k^{*,U}(t, \hat{P})$, respectively, are attained at some points

$(\mathbf{z}^{*,\min}, \mathbf{p}^{*,\min}) \in \mathcal{B}_k^L(X^B(t, \hat{P})) \times \hat{P}$ and $(\mathbf{z}^{*,\max}, \mathbf{p}^{*,\max}) \in \mathcal{B}_k^U(X^B(t, \hat{P})) \times \hat{P}$, respectively. Specifically, note that $z_k^{*,\min} = x_k^L(t, \hat{P})$ and $z_k^{*,\max} = x_k^U(t, \hat{P})$, so that

$$\begin{aligned} f_k^{*,U}(t, \hat{P}) - f_k^{*,L}(t, \hat{P}) &= f_k(t, (z_1^{*,\max}, \dots, x_k^U(t, \hat{P}), \dots, z_{n_x}^{*,\max}), \mathbf{p}^{*,\max}) \\ &\quad - f_k(t, (z_1^{*,\min}, \dots, x_k^L(t, \hat{P}), \dots, z_{n_x}^{*,\min}), \mathbf{p}^{*,\min}). \end{aligned}$$

Subtracting and adding $f_k(t, (z_1^{*,\max}, \dots, x_k^L(t, \hat{P}), \dots, z_{n_x}^{*,\max}), \mathbf{p}^{*,\max})$ gives

$$\begin{aligned} f_k^{*,U}(t, \hat{P}) - f_k^{*,L}(t, \hat{P}) &= \left[f_k(t, (z_1^{*,\max}, \dots, x_k^U(t, \hat{P}), \dots, z_{n_x}^{*,\max}), \mathbf{p}^{*,\max}) \right. \\ &\quad \left. - f_k(t, (z_1^{*,\max}, \dots, x_k^L(t, \hat{P}), \dots, z_{n_x}^{*,\max}), \mathbf{p}^{*,\max}) \right] \\ &\quad + \left[f_k(t, (z_1^{*,\max}, \dots, x_k^L(t, \hat{P}), \dots, z_{n_x}^{*,\max}), \mathbf{p}^{*,\max}) \right. \\ &\quad \left. - f_k(t, (z_1^{*,\min}, \dots, x_k^L(t, \hat{P}), \dots, z_{n_x}^{*,\min}), \mathbf{p}^{*,\min}) \right]. \end{aligned}$$

Applying (4.2) to the first term on the right and the Lipschitz condition for f_k to the second,

$$f_k^{*,U}(t, \hat{P}) - f_k^{*,L}(t, \hat{P}) \leq \alpha_k w(X_k^B(t, \hat{P})) + L \max \left\{ \max_{i \neq k} w(X_i^B(t, \hat{P})), w(\hat{P}) \right\}.$$

Finally, first-order convergence in diameter of F implies that

$$\begin{aligned} w(F_{k,U}(t, \hat{P})) &\leq \tau_k \max \left\{ \max_{i \neq k} w(X_i^B(t, \hat{P})), w(\hat{P}) \right\}, \\ w(F_{k,L}(t, \hat{P})) &\leq \tau_k \max \left\{ \max_{i \neq k} w(X_i^B(t, \hat{P})), w(\hat{P}) \right\}. \end{aligned}$$

Therefore, (4.4) implies (4.3). To see that this bound can be negative, choose $\alpha_k < 0$ and take $w(X_k^B(t, \hat{P}))$ arbitrarily large. Finally, when the naïve state bounding method is used, $\frac{d}{dt}w(X_k^B(t, \hat{P}))$ is equal to $w(F_k(t, X^B(t, \hat{P}), \hat{P}))$, which must be nonnegative. $\square$

The following example gives a specific case where state bounds from Harrison's method satisfy $\frac{d}{dt}w(X_i^B(t, \hat{P})) < 0$ for some i and some t .

Example 4.11. Consider the simple chemical reaction $A \rightleftharpoons B$, with the ODE model

$$\begin{aligned} \dot{x}_A &= -k_f x_A + k_r x_B, \\ \dot{x}_B &= k_f x_A - k_r x_B, \end{aligned}$$

with $X_{A,0} \equiv [0.8, 1.2]$, $X_{B,0} \equiv [0.1, 0.1]$, $K_f \equiv [15, 20]$, $K_r \equiv [1, 5]$, and $P \equiv K_f \times K_r$. Applying the rules of interval arithmetic, the vector field for Harrison's state bounding system for species A is

$$\begin{aligned} \dot{x}_A^L &= \min\{-k_f^L x_A^L, -k_f^U x_A^L\} + \min\{k_r^L x_B^L, k_r^U x_B^L, k_r^U x_B^U\}, \\ \dot{x}_A^U &= \max\{-k_f^L x_A^U, -k_f^U x_A^U\} + \max\{k_r^L x_B^L, k_r^L x_B^U, k_r^U x_B^L, k_r^U x_B^U\}. \end{aligned}$$

At the initial time, with the provided initial conditions and parameter ranges, we obtain $\dot{x}_A^L(t_0) = -15.9 > -17.5 = \dot{x}_A^U(t_0)$. This means that at the initial time, the bounds for species A are becoming tighter, since $\frac{dw(X_A^B)}{dt}(t_0, \hat{P}) = \dot{x}_A^U - \dot{x}_A^L = -1.6$.

If instead we use the naïve state bounding system, the vector field for species A are

$$\begin{aligned}\dot{x}_A^L &= \min\{-k_f^L x_A^L, -k_f^L x_A^U, -k_f^U x_A^L, -k_f^U x_A^U\} + \min\{k_r^L x_B^L, k_r^L x_B^U, k_r^U x_B^L, k_r^U x_B^U\}, \\ \dot{x}_A^U &= \max\{-k_f^L x_A^L, -k_f^L x_A^U, -k_f^U x_A^L, -k_f^U x_A^U\} + \max\{k_r^L x_B^L, k_r^L x_B^U, k_r^U x_B^L, k_r^U x_B^U\},\end{aligned}$$

which gives $\dot{x}_A^L(t_0) = -23.9 < -1 = \dot{x}_A^U(t_0)$, so the bounds are becoming farther apart.

Next, we build on Proposition 4.9 to establish a bound on the convergence prefactor of Harrison's method using the logarithmic norm. Recall that $w_V(X^B)$ denotes the vector with elements $w(X_k^B)$.

Theorem 4.12. *Let $\mathbf{x}^L, \mathbf{x}^U : I \times \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^{n_x}$ satisfy Harrison's state bounding system and let $X^B(t, \hat{P}) \equiv [\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})]$. Choose any $P' \in \mathbb{I}P$ and assume that $\cup_{t \in I, \hat{P} \in \mathbb{I}P'} X^B(t, \hat{P})$ is contained in a compact set $X' \subset D$. Let $L \in \mathbb{R}_+$ be a Lipschitz constant for $\mathbf{f}$ on $I \times X' \times P'$, and let $\tau_k \in \mathbb{R}_+$ be the prefactor for convergence of F_k in diameter on $I \times X' \times P'$ as per Assumption 4.1. Furthermore, assume there exists $\alpha \in \mathbb{R}^{n_x}$ such that, for all $t \in I$ and $k \in \{1, \dots, n_x\}$,*

$$\begin{aligned}f_k(t, \mathbf{z}^{(1)}, \mathbf{p}) - f_k(t, \mathbf{z}^{(2)}, \mathbf{p}) &\leq \alpha_k(z_k^{(1)} - z_k^{(2)}), \\ \forall(\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \mathbf{p}) &\in \{X' \times X' \times P' : z_j^{(1)} = z_j^{(2)}, \forall j \neq k \text{ and } z_k^{(1)} \geq z_k^{(2)}\}.\end{aligned}$$

Define $\mathbf{S} \in \mathbb{R}^{n_x \times n_x}$ by

$$s_{ij} = \begin{cases} \alpha_i & \text{if } i = j \\ L + 2\tau_i & \text{if } i \neq j \end{cases}$$

Then, for each $(t, \hat{P}) \in I \times \mathbb{I}P'$, the state bounds from Harrison's method satisfy:

1. $\frac{d}{dt} w_V(X^B(t, \hat{P})) \leq \mathbf{S} w_V(X^B(t, \hat{P})) + (2\boldsymbol{\tau} + L\mathbf{1})w(\hat{P})$, where $\mathbf{1}$ is a vector whose components are all 1.
2. If $\mu_\infty(\mathbf{S}) = 0$, then

$$w(X^B(t, \hat{P})) \leq w(X^B(t_0, \hat{P})) + [(t - t_0)(L + 2\|\boldsymbol{\tau}\|_\infty)] w(\hat{P}). \quad (4.5)$$

3. If $\mu_\infty(\mathbf{S}) \neq 0$, then

$$\begin{aligned}w(X^B(t, \hat{P})) &\leq [\exp(\mu_\infty(\mathbf{S})(t - t_0))] w(X^B(t_0, \hat{P})) \\ &\quad - \left[(1 - \exp(\mu_\infty(\mathbf{S})(t - t_0))) \frac{(L + 2\|\boldsymbol{\tau}\|_\infty)}{\mu_\infty(\mathbf{S})} \right] w(\hat{P}).\end{aligned} \quad (4.6)$$

4. If $\alpha_i < -(n_x - 1)|L + 2\tau_i|, \forall i$, then $\mu_\infty(\mathbf{S}) < 0$, the state bounds can grow closer together as time increases, and

$$\lim_{t \rightarrow +\infty} w(X^B(t, \hat{P})) \leq - \left[\frac{(L + 2\|\boldsymbol{\tau}\|_\infty)}{\mu_\infty(\mathbf{S})} \right] w(\hat{P}). \quad (4.7)$$

Proof. Using Proposition 4.9, we have for every k ,

$$\begin{aligned} \frac{d}{dt}w(X_k^B(t, \hat{P})) &\leq \alpha_k w(X_k^B(t, \hat{P})) + (L + 2\tau_k) \max \left\{ w(\hat{P}), \max_{i \neq k} w(X_i^B(t, \hat{P})) \right\}, \\ &\leq \alpha_k w(X_k^B(t, \hat{P})) + (L + 2\tau_k) \left(w(\hat{P}) + \sum_{i \neq k} w(X_i^B(t, \hat{P})) \right). \end{aligned}$$

Thus, by the definition of $\mathbf{S}$,

$$\frac{d}{dt}w_V(X^B(t, \hat{P})) \leq \mathbf{S}w_V(X^B(t, \hat{P})) + (L\mathbf{1} + 2\boldsymbol{\tau})w(\hat{P}), \quad (4.8)$$

which establishes Claim 1. To establish Claim 2, we follow a similar line of reasoning as [60, (1.8)]. The argument is based on the upper right Dini derivative, which is defined for any $\psi : I \rightarrow \mathbb{R}$ by

$$D_t^+ \psi(t) = \limsup_{h \rightarrow 0+} \frac{\psi(t+h) - \psi(t)}{h}, \quad \forall t \in I.$$

With this definition,

$$\begin{aligned} D_t^+ w(X^B(t, \hat{P})) &= D_t^+ \|w_V(X^B(t, \hat{P}))\|_\infty, \\ &= \limsup_{h \rightarrow 0+} \frac{\|w_V(X^B(t+h, \hat{P}))\|_\infty - \|w_V(X^B(t, \hat{P}))\|_\infty}{h}. \end{aligned}$$

The right-hand sides of Harrison's state bounding system are continuous by Assumption 4.1, which implies that $\mathbf{x}^L(\cdot, \hat{P})$ and $\mathbf{x}^U(\cdot, \hat{P})$ are continuously differentiable on I . It follows that $w_V(X^B(\cdot, \hat{P}))$ is differentiable, and hence the approximation $w_V(X^B(t+h, \hat{P})) \approx w_V(X^B(t, \hat{P})) + h \frac{d}{dt}w_V(X^B(t, \hat{P}))$ has an error converging to zero super-linearly as $h \rightarrow 0$. Therefore, $D_t^+ w(X^B(t, \hat{P}))$ is equivalent to

$$\limsup_{h \rightarrow 0+} \frac{\|w_V(X^B(t, \hat{P})) + h \frac{d}{dt}w_V(X^B(t, \hat{P}))\|_\infty - \|w_V(X^B(t, \hat{P}))\|_\infty}{h}. \quad (4.9)$$

If, for every $k \in \{1, \dots, n_x\}$, we can ensure that

$$0 \leq w(X_k^B(t, \hat{P})) + h \frac{d}{dt}w(X_k^B(t, \hat{P})) \quad (4.10)$$

for all sufficiently small h , then (4.8) can be applied to bound (4.9) from above by

$$\begin{aligned} &\limsup_{h \rightarrow 0+} \frac{\|w_V(X^B(t, \hat{P})) + h (\mathbf{S}w_V(X^B(t, \hat{P})) + (L\mathbf{1} + 2\boldsymbol{\tau})w(\hat{P}))\|_\infty - \|w_V(X^B(t, \hat{P}))\|_\infty}{h}, \\ &= \limsup_{h \rightarrow 0+} \frac{\|(\mathbf{I} + h\mathbf{S})w_V(X^B(t, \hat{P})) + h(L\mathbf{1} + 2\boldsymbol{\tau})w(\hat{P})\|_\infty - \|w_V(X^B(t, \hat{P}))\|_\infty}{h}, \\ &\leq \limsup_{h \rightarrow 0+} \frac{\|\mathbf{I} + h\mathbf{S}\|_\infty - 1}{h} \|w_V(X^B(t, \hat{P}))\|_\infty + \|(L\mathbf{1} + 2\boldsymbol{\tau})w(\hat{P})\|_\infty. \end{aligned} \quad (4.11)$$

To verify (4.10), first note that $w(X_k^B(t, \hat{P})) \geq 0$. If $w(X_k^B(t, \hat{P})) > 0$, then (4.10) clearly holds for all sufficiently small h . On the other hand, if $w(X_k^B(t, \hat{P})) = 0$, then $x_k^L(t, \hat{P}) = x_k^U(t, \hat{P})$ and hence $\mathcal{B}_k^L(X^B(t, \hat{P})) = \mathcal{B}_k^U(X^B(t, \hat{P}))$. In this case, the definition of Harrison's state bounding system implies that

$$\frac{d}{dt}w(X_k^B(t, \hat{P})) = f_k^U([t, t], \mathcal{B}_k^U(X^B(t, \hat{P})), \hat{P}) - f_k^L([t, t], \mathcal{B}_k^L(X^B(t, \hat{P})), \hat{P}) \geq 0,$$

and hence (4.10) holds. We conclude that $D_t^+ w(X^B(t, \hat{P}))$ is bounded above by (4.11).

Since $\|\cdot\|_\infty$ is directionally differentiable, it follows that $\lim_{h \rightarrow 0^+} \frac{\|\mathbf{I} + h\mathbf{S}\|_\infty - 1}{h}$ exists [60], and is therefore equal to the lim sup, and both are equal to the logarithmic norm $\mu_\infty(\mathbf{S})$ by Definition 2.3. Thus,

$$\begin{aligned} D_t^+ w(X^B(t, \hat{P})) &\leq \mu_\infty(\mathbf{S}) \|w_V(X^B(t, \hat{P}))\|_\infty + (L + \|2\boldsymbol{\tau}\|_\infty)w(\hat{P}), \\ &= \mu_\infty(\mathbf{S})w(X^B(t, \hat{P})) + (L + \|2\boldsymbol{\tau}\|_\infty)w(\hat{P}). \end{aligned} \quad (4.12)$$

Since the function $w(X^B(\cdot, \hat{P})) = \|w_V(X^B(\cdot, \hat{P}))\|_\infty$ is the composition the continuously differentiable function $w_V(X^B(\cdot, \hat{P}))$ and the Lipschitz continuous function $\|\cdot\|_\infty$, $w(X^B(\cdot, \hat{P}))$ is absolutely continuous. It follows that its derivative exists and coincides with $D_t^+ w(X^B(t, \hat{P}))$ for a.e. $t \in I$. Moreover, $D_t^+ w(X^B(\cdot, \hat{P}))$ is Lebesgue integrable on I and satisfies $w(X^B(t, \hat{P})) - w(X^B(t_0, \hat{P})) = \int_{t_0}^t D_s^+ w(X^B(s, \hat{P}))ds$. Thus,

$$\begin{aligned} w(X^B(t, \hat{P})) &\leq w(X^B(t_0, \hat{P})) + \int_{t_0}^t \mu_\infty(\mathbf{S})w(X^B(s, \hat{P})) + (L + 2\|\boldsymbol{\tau}\|_\infty)w(\hat{P})ds, \\ &= w(X^B(t_0, \hat{P})) + (L + 2\|\boldsymbol{\tau}\|_\infty)w(\hat{P})(t - t_0) + \int_{t_0}^t \mu_\infty(\mathbf{S})w(X^B(s, \hat{P}))ds. \end{aligned}$$

If $\mu_\infty(\mathbf{S}) = 0$, we obtain (4.5), which proves Claim 2. If $\mu_\infty(\mathbf{S}) \neq 0$, we apply Lemma 2.2 with $\mu \equiv \mu_\infty(\mathbf{S})$, $\lambda_0 \equiv w(X^B(t_0, \hat{P}))$, $\lambda_1 \equiv (L + 2\|\boldsymbol{\tau}\|_\infty)w(\hat{P})$, and $x \equiv w(X^B(\cdot, \hat{P}))$ to obtain (4.6), and hence Claim 3.

By Proposition 2.4, if $\alpha_i < -(n_x - 1)|L + 2\tau_i|$, $\forall i$, then $\mu_\infty(\mathbf{S}) < 0$. Then, (4.7) clearly follows from (4.6), which proves Claim 4. $\square$

Corollary 4.13. *Let the Hypotheses of Theorem 4.12 hold, and let $\tau_0 \in \mathbb{R}_+$ be the prefactor for convergence in diameter of X_0 on P' (see Assumption 4.1). Then, for each $(t, \hat{P}) \in I \times \mathbb{I}P'$, the state bounds from Harrison's method satisfy:*

1. *If $\mu_\infty(\mathbf{S}) = 0$, then*

$$w(X^B(t, \hat{P})) \leq [\tau_0 + (t - t_0)(L + 2\|\boldsymbol{\tau}\|_\infty)]w(\hat{P}).$$

2. *If $\mu_\infty(\mathbf{S}) \neq 0$, then*

$$w(X^B(t, \hat{P})) \leq \left[\exp(\mu_\infty(\mathbf{S})(t - t_0)) \left(\tau_0 + \frac{(L + 2\|\boldsymbol{\tau}\|_\infty)}{\mu_\infty(\mathbf{S})} \right) - \frac{(L + 2\|\boldsymbol{\tau}\|_\infty)}{\mu_\infty(\mathbf{S})} \right] w(\hat{P}).$$

Proof. Claims 1–2 follow from Claims 2–3 of Theorem 4.12 by noting that $w(X^B(t_0, \hat{P}))$ is equivalent to $w(X_0(\hat{P}))$, which is bounded above by $\tau_0 w(\hat{P})$ for all $\hat{P} \in \mathbb{I}P'$. $\square$

See §6.2 for an application of the convergence-order bounds in Theorem 4.12 and Corollary 4.13 for a chemical kinetics problem.

We close this section with an inclusion monotonicity result for state bounds. As an immediate consequence, we prove that Harrison's bounds are guaranteed to be tighter than the naïve bounds for all $t \in I$ and $\hat{P} \in \mathbb{I}P$. Moreover, this monotonicity result is central to the convergence results for state relaxations presented in the next section.

Theorem 4.14. *Let $\mathbf{u}, \mathbf{o}, \tilde{\mathbf{u}}, \tilde{\mathbf{o}} : I \times \mathbb{I}D \times \mathbb{I}P \rightarrow \mathbb{R}^{n_x}$ and $\mathbf{v}_0, \mathbf{w}_0, \tilde{\mathbf{v}}_0, \tilde{\mathbf{w}}_0 : \mathbb{I}P \rightarrow \mathbb{R}^{n_x}$. Let $\mathbf{v}, \mathbf{w}, \tilde{\mathbf{v}}, \tilde{\mathbf{w}} : I \times \mathbb{I}P \rightarrow \mathbb{R}^{n_x}$ be absolutely continuous on I for each $\hat{P} \in \mathbb{I}P$ and satisfy the following ODEs for a.e. $t \in I$:*

$$\begin{aligned} \dot{\mathbf{v}}(t, \hat{P}) &= \mathbf{u}(t, [\mathbf{v}(t, \hat{P}), \mathbf{w}(t, \hat{P})], \hat{P}), & \mathbf{v}(t_0, \hat{P}) &= \mathbf{v}_0(\hat{P}), \\ \dot{\mathbf{w}}(t, \hat{P}) &= \mathbf{o}(t, [\mathbf{v}(t, \hat{P}), \mathbf{w}(t, \hat{P})], \hat{P}), & \mathbf{w}(t_0, \hat{P}) &= \mathbf{w}_0(\hat{P}), \end{aligned} \quad (4.13)$$

$$\begin{aligned} \dot{\tilde{\mathbf{v}}}(t, \hat{P}) &= \tilde{\mathbf{u}}(t, [\tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P})], \hat{P}), & \tilde{\mathbf{v}}(t_0, \hat{P}) &= \tilde{\mathbf{v}}_0(\hat{P}), \\ \dot{\tilde{\mathbf{w}}}(t, \hat{P}) &= \tilde{\mathbf{o}}(t, [\tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P})], \hat{P}), & \tilde{\mathbf{w}}(t_0, \hat{P}) &= \tilde{\mathbf{w}}_0(\hat{P}). \end{aligned} \quad (4.14)$$

The solutions $\mathbf{v}, \mathbf{w}, \tilde{\mathbf{v}},$ and $\tilde{\mathbf{w}}$ satisfy the inclusion

$$[\mathbf{v}(t, \hat{P}), \mathbf{w}(t, \hat{P})] \subset [\tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P})], \quad \forall (t, \hat{P}) \in I \times \mathbb{I}P, \quad (4.15)$$

provided that the following conditions hold:

1. The initial condition functions $\mathbf{v}_0, \mathbf{w}_0, \tilde{\mathbf{v}}_0,$ and $\tilde{\mathbf{w}}_0$ satisfy

$$[\mathbf{v}_0(\hat{P}), \mathbf{w}_0(\hat{P})] \subset [\tilde{\mathbf{v}}_0(\hat{P}), \tilde{\mathbf{w}}_0(\hat{P})], \quad \forall \hat{P} \in \mathbb{I}P. \quad (4.16)$$

2. The vector fields $\mathbf{u}, \mathbf{o}, \tilde{\mathbf{u}},$ and $\tilde{\mathbf{o}}$ satisfy

$$\begin{aligned} [\mathbf{u}(t, Z, \hat{P}), \mathbf{o}(t, Z, \hat{P})] &\subset [\tilde{\mathbf{u}}(t, Z, \hat{P}), \tilde{\mathbf{o}}(t, Z, \hat{P})], \\ \text{a.e. } t \in (t_0, t_f], \quad \forall (Z, \hat{P}) &\in \mathbb{I}D \times \mathbb{I}P. \end{aligned} \quad (4.17)$$

3. The vector fields $\tilde{\mathbf{u}}$ and $\tilde{\mathbf{o}}$ satisfy

$$\begin{aligned} [\tilde{\mathbf{u}}(t, Z', \hat{P}), \tilde{\mathbf{o}}(t, Z', \hat{P})] &\subset [\tilde{\mathbf{u}}(t, Z, \hat{P}), \tilde{\mathbf{o}}(t, Z, \hat{P})], \\ \text{a.e. } t \in (t_0, t_f], \quad \forall (Z, Z', \hat{P}) &\in \mathbb{I}D \times \mathbb{I}D \times \mathbb{I}P : Z' \subset Z. \end{aligned} \quad (4.18)$$

4. The vector fields $\tilde{\mathbf{u}}$ and $\tilde{\mathbf{o}}$ are locally Lipschitz continuous on $I \times \mathbb{I}D \times \mathbb{I}P$.

Proof. See §A.2. □

Corollary 4.15. *Let $\mathbf{x}^L, \mathbf{x}^U : I \times \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^{n_x}$ be a solution of Harrison's state bounding system and let $\tilde{\mathbf{x}}^L, \tilde{\mathbf{x}}^U : I \times \mathbb{I}P \rightarrow \mathbb{I}\mathbb{R}^{n_x}$ be a solution of the naïve state bounding system. The inclusion $[\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})] \subset [\tilde{\mathbf{x}}^L(t, \hat{P}), \tilde{\mathbf{x}}^U(t, \hat{P})]$ holds for all $(t, \hat{P}) \in I \times \mathbb{I}P$.*

Proof. It suffices to verify the four hypotheses of Theorem 4.14 with $[\mathbf{v}, \mathbf{w}] = [\mathbf{x}^L, \mathbf{x}^U]$ and $[\tilde{\mathbf{v}}, \tilde{\mathbf{w}}] = [\tilde{\mathbf{x}}^L, \tilde{\mathbf{x}}^U]$. Hypothesis 1 is evident. By Assumption 4.1, the inclusion function F is inclusion monotonic. Since $\mathcal{B}_i^L(Z) \subset Z$ and $\mathcal{B}_i^U(Z) \subset Z$, it follows that

$$[f_i^L([t, t], \mathcal{B}_i^L(Z), \hat{P}), f_i^U([t, t], \mathcal{B}_i^U(Z), \hat{P})] \subset [f_i^L([t, t], Z, \hat{P}), f_i^U([t, t], Z, \hat{P})],$$

for all $(t, Z, \hat{P}) \in I \times \mathbb{I}D \times \mathbb{I}P$, which verifies Hypothesis 2. Moreover, inclusion monotonicity of F directly implies Hypothesis 3. Finally, Hypothesis 4 follows from the Lipschitz condition in Assumption 4.1. Specifically, when the right-hand side functions of the naïve state bounding system are restricted to degenerate first arguments $[t, t] \in \mathbb{I}I$, we obtain the needed local Lipschitz property on $I \times \mathbb{I}D \times \mathbb{I}P$. □

5 Convergence of state relaxations

In this section, we analyze the convergence behavior of two auxiliary ODE methods for computing state relaxations for (3.1). The first method, termed the *relaxation amplifying dynamics (RAD) method*, is analogous to the naïve state bounding method analyzed in §4 and was first introduced in [54]. The second method, termed the *relaxation preserving dynamics (RPD) method*, improves upon the RAD method in a manner that is analogous to the improvement of Harrison’s method over the naïve state bounding method [51]. After defining both methods, we first show that RAD has second-order pointwise convergence under appropriate assumptions. Next, we apply the Monotonicity Theorem 4.14 to show that RPD state relaxations are always tighter than those from RAD, which implies that RPD has second-order pointwise convergence as well. Finally, we establish time-varying bounds on the convergence-order prefactors using the logarithmic norm. By analogy to the state bounding results in §4, we show that the RPD method permits the pointwise relaxation error to decrease over time, and we provide sufficient conditions for this to occur. In contrast, such a decrease is impossible for the RAD method.

5.1 Methods for generating state relaxations

Like the naïve and Harrison state bounding methods defined in §4, the RAD and RPD state relaxation methods specify relaxations $\mathbf{x}^{cv}$ and $\mathbf{x}^{cc}$ as the solutions of auxiliary systems of ODEs. Moreover, just as the right-hand sides of the naïve and Harrison state bounding systems are constructed using an inclusion function for right-hand side $\mathbf{f}$ of the original ODEs (3.1), the right-hand sides of the RAD and RPD state relaxation systems are constructed using convex and concave relaxations of $\mathbf{f}$. However, standard convex and concave relaxations are inadequate for this task. Instead, the RAD and RPD systems use a more general construction called a *relaxation function* for $\mathbf{f}$. This construction is based on the concept of *composite relaxations*, which is motivated by the need to relax the composite function $\mathbf{p} \mapsto \mathbf{f}(t, \mathbf{x}(t, \mathbf{p}), \mathbf{p})$ given relaxations of $\mathbf{p} \mapsto \mathbf{x}(t, \mathbf{p})$ on $\hat{P} \in \mathbb{IP}$.

Definition 5.1 (Composite relaxations). Let $\mathbf{h} : D \subset \mathbb{R}^n \rightarrow \mathbb{R}^m$ and let $S \subset D$ be convex. Two functions $\mathbf{u}, \mathbf{o} : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^m$ are called *convex and concave composite relaxations for $\mathbf{h}$ on S* , respectively, if the following condition holds: For any convex set $Q \subset \mathbb{R}^q$ and any functions $\mathbf{s}, \mathbf{s}^{cv}, \mathbf{s}^{cc} : Q \rightarrow \mathbb{R}^n$ such that $\mathbf{s}(Q) \subset S$ and $\mathbf{s}^{cv}$ and $\mathbf{s}^{cc}$ are, respectively, convex and concave relaxations of $\mathbf{s}$ on Q , convex and concave relaxations of the composition $\mathbf{q} \mapsto \mathbf{h}(\mathbf{s}(\mathbf{q}))$ are given by $\mathbf{q} \mapsto \mathbf{u}(\mathbf{s}^{cv}(\mathbf{q}), \mathbf{s}^{cc}(\mathbf{q}))$ and $\mathbf{q} \mapsto \mathbf{o}(\mathbf{s}^{cv}(\mathbf{q}), \mathbf{s}^{cc}(\mathbf{q}))$, respectively.

The definition of a relaxation function also requires the following notation for the space of pairs of intervals $[\mathbf{s}^L, \mathbf{s}^U]$ and $[\mathbf{s}^{cv}, \mathbf{s}^{cc}]$, which are intended to represent, respectively, interval bounds on $\mathbf{s}$ and the values of convex and concave relaxations of $\mathbf{s}$ at a particular point in its domain. We call such pairs *McCormick objects* due to their use in McCormick’s relaxation technique [30] as formalized in [47].

Definition 5.2 ($\mathbb{MR}^n$). Define the space of *McCormick objects*

$$\mathbb{MR}^n \equiv \{S = (S^B, S^C) \in \mathbb{IR}^n \times \mathbb{IR}^n : S^B \cap S^C \neq \emptyset\}. \quad (5.1)$$

Elements of $\mathbb{MR}^n$ are denoted by script capitals. For any $S \in \mathbb{MR}^n$, the notations $S^B, S^C \in \mathbb{IR}^n$ and $\mathbf{s}^L, \mathbf{s}^U, \mathbf{s}^{cv}, \mathbf{s}^{cc} \in \mathbb{R}^n$ will commonly be used to denote the intervals and vectors

satisfying $\mathcal{S} = (S^B, S^C) = ([\mathbf{s}^L, \mathbf{s}^U], [\mathbf{s}^{cv}, \mathbf{s}^{cc}])$. For any $D \subset \mathbb{R}^n$, let $\mathbb{M}D \equiv \{\mathcal{S} \in \mathbb{M}\mathbb{R}^n : S^B \subset D\}$.

Definition 5.3 (Relaxation function). Let $\mathbf{h} : D \subset \mathbb{R}^n \rightarrow \mathbb{R}^m$ and $\mathcal{H} : \mathbb{M}D \rightarrow \mathbb{M}\mathbb{R}^m$. $\mathcal{H}$ is a *relaxation function* for $\mathbf{h}$ on $\mathbb{M}D$ if, for every $\mathcal{S} = (S^B, [\mathbf{s}^{cv}, \mathbf{s}^{cc}]) \in \mathbb{M}D$, $\mathcal{H}(\mathcal{S}) = (H(S^B), [\mathbf{h}^{cv}(\mathcal{S}), \mathbf{h}^{cc}(\mathcal{S})])$, where H is an inclusion function for $\mathbf{h}$ on $\mathbb{M}D$ and the functions $(\mathbf{s}^{cv}, \mathbf{s}^{cc}) \mapsto \mathbf{h}^{cv}((S^B, [\mathbf{s}^{cv}, \mathbf{s}^{cc}]))$ and $(\mathbf{s}^{cv}, \mathbf{s}^{cc}) \mapsto \mathbf{h}^{cc}((S^B, [\mathbf{s}^{cv}, \mathbf{s}^{cc}]))$ are, respectively, convex and concave composite relaxations for $\mathbf{h}$ on S^B . Moreover, $\mathcal{H}$ is *inclusion monotonic* on $\mathbb{M}D$ if, for any $\mathcal{S}, \tilde{\mathcal{S}} \in \mathbb{M}D$, the inclusions $S^B \subset \tilde{S}^B$ and $[\mathbf{s}^{cv}, \mathbf{s}^{cc}] \subset [\tilde{\mathbf{s}}^{cv}, \tilde{\mathbf{s}}^{cc}]$ imply $H(S^B) \subset H(\tilde{S}^B)$ and $[\mathbf{h}^{cv}(\mathcal{S}), \mathbf{h}^{cc}(\mathcal{S})] \subset [\mathbf{h}^{cv}(\tilde{\mathcal{S}}), \mathbf{h}^{cc}(\tilde{\mathcal{S}})]$.

Remark 5.4. A relaxation function $\mathcal{H} = (H, [\mathbf{h}^{cv}, \mathbf{h}^{cc}])$ for $\mathbf{h}$ provides standard convex and concave relaxations of $\mathbf{h}$ on $S \in \mathbb{M}D$ through the definitions (see Lemma 2.4.11 in [47]):

$$\mathbf{h}_{\text{std}}^{cv}(\mathbf{s}) \equiv \mathbf{h}^{cv}((S, [\mathbf{s}, \mathbf{s}]]), \quad \mathbf{h}_{\text{std}}^{cc}(\mathbf{s}) \equiv \mathbf{h}^{cc}((S, [\mathbf{s}, \mathbf{s}]]), \quad \forall \mathbf{s} \in S.$$

More generally, $\mathcal{H}$ provides a scheme of estimators for $\mathbf{h}$ in S through the definitions

$$\mathbf{h}_{\text{schm}}^{cv}(\hat{S}, \mathbf{s}) \equiv \mathbf{h}^{cv}((\hat{S}, [\mathbf{s}, \mathbf{s}]]), \quad \mathbf{h}_{\text{schm}}^{cc}(\hat{S}, \mathbf{s}) \equiv \mathbf{h}^{cc}((\hat{S}, [\mathbf{s}, \mathbf{s}]]), \quad \forall \mathbf{s} \in \hat{S}, \quad \forall \hat{S} \in \mathbb{M}S.$$

However, relaxation functions are more general because $\mathbf{s}^{cv}$ and $\mathbf{s}^{cc}$ need not coincide, which enables the compositions necessary to define the state relaxation systems below.

Remark 5.5. For simplicity of exposition, the definition of a relaxation function here is slightly different than the original definition in [47]. Specifically, if $\mathcal{H}$ is a relaxation function as defined here, then it is also a relaxation function as defined in [47]. If $\mathcal{H}$ is a relaxation function as defined in [47] *and in addition* is inclusion monotonic, then it is a relaxation function as defined here. The presentation in [47] is more general, but the one here avoids some technical developments and is sufficient for the present analysis.

To define the RAD and RPD state relaxation systems, let $\mathcal{X}_0 : \mathbb{M}P \rightarrow \mathbb{M}\mathbb{R}^{n_x}$ and $\mathcal{F} : \mathbb{M}I \times \mathbb{M}D \times \mathbb{M}P \rightarrow \mathbb{M}\mathbb{R}^{n_x}$ denote relaxation functions for $\mathbf{x}_0$ and $\mathbf{f}$ in (3.1), respectively. Moreover, denote $\mathcal{X}_0(\mathcal{P}) = (X_0^B(P^B), [\mathbf{x}_0^{cv}(\mathcal{P}), \mathbf{x}_0^{cc}(\mathcal{P})])$ and $\mathcal{F}(\mathcal{T}, \mathcal{X}, \mathcal{P}) = (F^B(T^B, X^B, P^B), [\mathbf{f}^{cv}(\mathcal{T}, \mathcal{X}, \mathcal{P}), \mathbf{f}^{cc}(\mathcal{T}, \mathcal{X}, \mathcal{P})])$ for every $(\mathcal{T}, \mathcal{X}, \mathcal{P}) \in \mathbb{M}I \times \mathbb{M}D \times \mathbb{M}P$.

Assumption 5.6. $\mathcal{F}$ and $\mathcal{X}_0$ are inclusion monotonic and locally Lipschitz continuous on their domains with respect to the metric

$$d_M(\mathcal{Y}, \mathcal{Z}) \equiv \max \left\{ d_H(Y^B, Z^B), d_H(Y^C, Z^C) \right\}, \quad \forall \mathcal{Y}, \mathcal{Z} \in \mathbb{M}\mathbb{R}^n.$$

Remark 5.7. By Theorem 2.5.12 in [47], the Lipschitz condition in Assumption 5.6 is equivalent to the assumption that the four functions

$$\begin{aligned} (\mathbf{p}^L, \mathbf{p}^U) &\mapsto \mathbf{x}_0^L([\mathbf{p}^L, \mathbf{p}^U]), & (\mathbf{p}^L, \mathbf{p}^U, \mathbf{p}^{cv}, \mathbf{p}^{cc}) &\mapsto \mathbf{x}_0^{cv}([\mathbf{p}^L, \mathbf{p}^U], [\mathbf{p}^{cv}, \mathbf{p}^{cc}]), \\ (\mathbf{p}^L, \mathbf{p}^U) &\mapsto \mathbf{x}_0^U([\mathbf{p}^L, \mathbf{p}^U]), & (\mathbf{p}^L, \mathbf{p}^U, \mathbf{p}^{cv}, \mathbf{p}^{cc}) &\mapsto \mathbf{x}_0^{cc}([\mathbf{p}^L, \mathbf{p}^U], [\mathbf{p}^{cv}, \mathbf{p}^{cc}]), \end{aligned}$$

are all locally Lipschitz continuous in the conventional, real-valued sense, and similarly for $\mathbf{f}^L, \mathbf{f}^U, \mathbf{f}^{cv}, \mathbf{f}^{cc}$.

Remark 5.8. If $\mathbf{f}$ and $\mathbf{x}_0$ are factorable functions, then, under some mild technical conditions, $\mathcal{F}$ and $\mathcal{X}_0$ satisfying Assumption 5.6 can be automatically obtained from their *natural McCormick extensions* as described in [47] (see Theorems 2.5.40 and 2.4.32). This construction is based on the generalized McCormick relaxation technique originally proposed in [55].

In the definitions of the RAD and RPD methods below, we only require elements of $\mathbb{M}P$ of the form $(\hat{P}, [\mathbf{p}, \mathbf{p}])$, which we denote with the shorthand $\hat{\mathcal{P}}_{\mathbf{p}}$, and elements of $\mathbb{M}I$ of the form $([t, t], [t, t])$, which we denote simply by t . By a slight abuse of notation, we will also use $\hat{\mathcal{P}}_{\mathbf{p}}$ as shorthand for the point $(\hat{P}, \mathbf{p}) \in \mathbb{I}P \times P$ (recall that state relaxations are defined as mappings from $I \times \mathbb{I}P \times P$ into $\mathbb{R}^{n_x}$ in Definition 3.2).

Definition 5.9 (Cut). Define $\text{Cut} : \mathbb{M}\mathbb{R}^n \rightarrow \mathbb{M}\mathbb{R}^n$ by $\text{Cut}(\mathcal{S}) \equiv (S^B, S^B \cap S^C)$.

Definition 5.10 (Relaxation amplifying dynamics (RAD) [54]). Let $\mathbf{x}^L, \mathbf{x}^U : I \times \mathbb{I}P \rightarrow \mathbb{R}^{n_x}$ be state bounds for (3.1) and let $X^B(t, \hat{P}) \equiv [\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})]$. The *relaxation amplifying dynamics (RAD) method* computes state relaxations for (3.1) on $\hat{P} \in \mathbb{I}P$ as the solution of the following auxiliary ODEs for all $i \in \{1, \dots, n_x\}$, which we refer to as the *RAD system*:

$$\begin{aligned} \dot{x}_i^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}) &= f_i^{cv}(t, \text{Cut}(X^B(t, \hat{P}), [\mathbf{x}^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{x}^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}})]), \hat{\mathcal{P}}_{\mathbf{p}}), \\ \dot{x}_i^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}}) &= f_i^{cc}(t, \text{Cut}(X^B(t, \hat{P}), [\mathbf{x}^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{x}^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}})]), \hat{\mathcal{P}}_{\mathbf{p}}), \\ x_i^{cv}(t_0, \hat{\mathcal{P}}_{\mathbf{p}}) &= x_{0,i}^{cv}(\hat{\mathcal{P}}_{\mathbf{p}}), \\ x_i^{cc}(t_0, \hat{\mathcal{P}}_{\mathbf{p}}) &= x_{0,i}^{cc}(\hat{\mathcal{P}}_{\mathbf{p}}). \end{aligned}$$

The RPD method defined next improves on the RAD method using the key insight of Harrison's method through the interval functions $\mathcal{B}_i^L$ and $\mathcal{B}_i^U$ (Definition 4.4). However, for technical reasons, the validity of this improvement requires the state relaxations to remain within the state bounds for all time. Thus, the RPD system is formulated as a hybrid system that ensures $\mathbf{x}^{cv}(t, \hat{P}), \mathbf{x}^{cc}(t, \hat{P}) \in X^B(t, \hat{P})$ for all $t \in I$ and $\hat{P} \in \mathbb{I}P$.

Definition 5.11 (Relaxation preserving dynamics (RPD) [47, 51]). Let $\mathbf{x}^L, \mathbf{x}^U : I \times \mathbb{I}P \rightarrow \mathbb{R}^{n_x}$ be state bounds for (3.1) and let $X^B(t, \hat{P}) \equiv [\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})]$. The *relaxation preserving dynamics (RPD) method* computes state relaxations for (3.1) on $\hat{P} \in \mathbb{I}P$ as the solution of the following auxiliary ODEs for all $i \in \{1, \dots, n_x\}$, which we refer to as the *RPD system*:

$$\begin{aligned} \dot{x}_i^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}) &= \begin{cases} f_i^{cv}(t, \text{Cut}(X^B, \mathcal{B}_i^L([\mathbf{x}^{cv}, \mathbf{x}^{cc}])), \hat{\mathcal{P}}_{\mathbf{p}}) & \text{if } b_i^{cv} = 0, \\ \max\{\dot{x}_i^L, f_i^{cv}(t, \text{Cut}(X^B, \mathcal{B}_i^L([\mathbf{x}^{cv}, \mathbf{x}^{cc}])), \hat{\mathcal{P}}_{\mathbf{p}})\} & \text{if } b_i^{cv} = 1, \end{cases} \\ \dot{x}_i^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}}) &= \begin{cases} f_i^{cc}(t, \text{Cut}(X^B, \mathcal{B}_i^U([\mathbf{x}^{cv}, \mathbf{x}^{cc}])), \hat{\mathcal{P}}_{\mathbf{p}}) & \text{if } b_i^{cc} = 0, \\ \min\{\dot{x}_i^U, f_i^{cc}(t, \text{Cut}(X^B, \mathcal{B}_i^U([\mathbf{x}^{cv}, \mathbf{x}^{cc}])), \hat{\mathcal{P}}_{\mathbf{p}})\} & \text{if } b_i^{cc} = 1, \end{cases} \\ x_i^{cv}(t_0, \hat{\mathcal{P}}_{\mathbf{p}}) &= x_{0,i}^{cv}(\hat{\mathcal{P}}_{\mathbf{p}}), \\ x_i^{cc}(t_0, \hat{\mathcal{P}}_{\mathbf{p}}) &= x_{0,i}^{cc}(\hat{\mathcal{P}}_{\mathbf{p}}). \end{aligned}$$

Above, all state bounds and relaxations appearing in the right-hand side functions are evaluated at $(t, \hat{P})$ and $(t, \hat{\mathcal{P}}_{\mathbf{p}})$, respectively, and b_i^{cv} and b_i^{cc} are Boolean variables satisfying

$$b_i^{cv} = \begin{cases} 0 & \text{if } x_i^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}) > x_i^L(t, \hat{P}) \\ 1 & \text{if } x_i^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}) \leq x_i^L(t, \hat{P}) \end{cases}, \quad b_i^{cc} = \begin{cases} 0 & \text{if } x_i^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}}) < x_i^U(t, \hat{P}) \\ 1 & \text{if } x_i^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}}) \geq x_i^U(t, \hat{P}) \end{cases}.$$

For any $\hat{P} \in \mathbb{I}P$, if state bounds $X^B(t, \hat{P})$ are available on all of I and $X^B(t, \hat{P}) \subset D$, $\forall t \in I$, then the RAD system is guaranteed to have a unique solution on I for every $\mathbf{p} \in P$, and this parametric solution provides valid state relaxations for (3.1). This was proven originally in [54]. A more recent presentation that is consistent with the notation

and terminology used here can be found in [47]. Similarly, if a solution of the RPD system exists on I for some $\hat{P} \in \mathbb{I}P$ and every $\mathbf{p} \in \hat{P}$, then it is unique and provides valid state relaxations for (3.1) [47, 51].

Remark 5.12. For a detailed numerical example highlighting the differences in the calculated right-hand sides for RAD and RPD (Definitions 5.10–5.11), see Example 5.23.

Remark 5.13. For simplicity, the RAD and RPD systems presented above differ slightly from those presented in [47]. Here, the right-hand sides of the RAD system are only defined for $\mathcal{X}(t, \hat{\mathcal{P}}_{\mathbf{p}}) \in \mathbb{M}D$, which requires that

$$\mathbf{x}^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}) \leq \mathbf{x}^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \quad [\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})] \cap [\mathbf{x}^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{x}^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}})] \neq \emptyset. \quad (5.2)$$

In [47], RAD is stated with a Lipschitz extension of the right-hand sides used here that is defined even when (5.2) is violated. However, since every solution of that system produces valid state relaxations (Theorem 7.3.4, [47]), it follows (5.2) must hold. Thus, any such solution is also a solution of RAD as defined here. Moreover, the Lipschitz condition in Assumption 5.6 implies that the solution of RAD is unique, so our statement here is equivalent. The analogous simplifications have also been made to the RPD system. Moreover, the statement of RPD in [47] includes additional logical conditions to prevent $\mathbf{x}^{cv}$ from crossing $\mathbf{x}^U$ and $\mathbf{x}^{cc}$ from crossing $\mathbf{x}^L$. However, it is shown in Lemmas 7.5.3 and 7.5.6 in [47] that any solution of this more complicated system is also a solution of RPD as defined here, and moreover satisfies $\mathbf{x}^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{x}^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}}) \in X^B(t, \hat{P}), \forall t \in I$. Furthermore, the Lipschitz condition in Assumption 5.6 implies that the solution of RPD is unique (Theorem 1, Chapter 2, §10 in [12]), so our statement here is again equivalent.

Remark 5.14. It is more precise to refer to the systems in Definitions 5.10–5.11 as specific *implementations* of the RAD and RPD theories for ODEs. The original definitions of the terms RAD and RPD in [51] are more general in that they apply to other types of dynamic systems as well (e.g., semi-explicit differential-algebraic equations [50]). However, for simplicity we will use the terms RAD and RPD here to refer specifically to the methods in Definitions 5.10–5.11.

5.2 Convergence-order results

We begin by establishing the pointwise convergence order of the RAD method. It is necessary to assume a certain convergence property of the relaxation function $\mathcal{F}$, defined next.

Definition 5.15 ((γ_1, γ_2) -convergence). Let $D \subset \mathbb{R}^n$ be bounded and let $\mathcal{H} : \mathbb{M}D \rightarrow \mathbb{M}\mathbb{R}^m$ satisfy $\mathcal{H}(\mathcal{S}) = (H^B(S^B), H^C(\mathcal{S})), \forall \mathcal{S} = (S^B, S^C) \in \mathbb{M}D$. We say that $\mathcal{H}$ has (γ_1, γ_2) -convergence on $\mathbb{M}D$ if $\exists \tau_{BB}, \tau_{CC}, \tau_{CB} \in \mathbb{R}_+$ such that

$$w(H^B(S^B)) \leq \tau_{BB} w(S^B)^{\gamma_1}, \quad (5.3)$$

$$w(H^C(\mathcal{S})) \leq \tau_{CC} w(S^C)^{\gamma_1} + \tau_{CB} w(S^B)^{\gamma_2}, \quad \forall \mathcal{S} \in \mathbb{M}D. \quad (5.4)$$

Remark 5.16. Recall from Remark 5.4 that relaxation functions define schemes of estimators when evaluated with S^C degenerate. Considering such arguments, it is straightforward to show that (γ_1, γ_2) -convergence on $\mathbb{M}D$ implies pointwise convergence in D of order γ_2 (Definition 2.18).

Assumption 5.17. For any compact $P' \subset P$ and $X' \subset D$, the relaxation functions $\mathcal{F}$ and $\mathcal{X}_0$ have $(1, 2)$ -convergence on $\mathbb{M}I \times \mathbb{M}X' \times \mathbb{M}P'$ and $\mathbb{M}P'$, respectively.

In §A.3, we show that natural McCormick extensions [47] have $(1, 2)$ -convergence on compact subsets of their domains. Since they also satisfy Assumption 5.6 (see Remark 5.8), they therefore satisfy all of the assumptions required for the following results. In the remainder of this section, we make the following assumptions about the state bounds used in the RAD and RPD systems.

Assumption 5.18. State bounds $\mathbf{x}^L, \mathbf{x}^U : I \times \mathbb{M}P \rightarrow \mathbb{R}^{n_x}$ for (3.1) are available and are continuously differentiable in I for each fixed $\hat{P} \in \mathbb{M}P$. Moreover, denoting $X^B(t, \hat{P}) \equiv [\mathbf{x}^L(t, \hat{P}), \mathbf{x}^U(t, \hat{P})]$, there exists a compact set $P' \subset P$ such that $\cup_{t \in I, \hat{P} \in \mathbb{M}P'} X^B(t, \hat{P})$ is contained in a compact set $X' \subset D$, and such that X^B converges in diameter on P' with order at least one, uniformly on I .

Theorem 5.19. Let $P' \subset P$ and $X' \subset D$ be as in Assumption 5.18. Let $\mathbf{x}^{cv}, \mathbf{x}^{cc} : I \times \mathbb{M}P' \times P' \rightarrow \mathbb{R}^{n_x}$ be the solution of the RAD state relaxation system and let $X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}) \equiv [\mathbf{x}^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{x}^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}})]$. Then X^C has pointwise convergence in P' of order 2, uniformly on I . Specifically, if $\tau_{CC}, \tau_{CB} \in \mathbb{R}_+$ and $\tau_{0,CC}, \tau_{0,CB} \in \mathbb{R}_+$ are $(1, 2)$ -convergence prefactors for $\mathcal{F}$ and $\mathcal{X}_0$ on $\mathbb{M}I \times \mathbb{M}X' \times \mathbb{M}P'$ and $\mathbb{M}P'$, respectively, then $\exists \tau \in \mathbb{R}_+$ such that

$$w(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) \leq (\tau_{0,CB} + \tau(t_f - t_0)) \exp(\tau_{CC}(t - t_0)) w(\hat{P})^2, \quad (5.5)$$

for all $t \in I$ and $\hat{\mathcal{P}}_{\mathbf{p}} = (\hat{P}, [\mathbf{p}, \mathbf{p}]) \in \mathbb{M}P' \times P'$.

Proof. For every $i \in \{1, \dots, n_x\}$ and every $\hat{\mathcal{P}}_{\mathbf{p}} = (\hat{P}, [\mathbf{p}, \mathbf{p}]) \in \mathbb{M}P'$, Definition 5.10 gives,

$$\begin{aligned} w(X_i^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) &= x_i^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}}) - x_i^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}) \\ &= x_{0,i}^{cc}(\hat{\mathcal{P}}_{\mathbf{p}}) - x_{0,i}^{cv}(\hat{\mathcal{P}}_{\mathbf{p}}) \\ &\quad + \int_{t_0}^t f_i^{cc}(s, \text{Cut}(X^B(s, \hat{P}), X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})), \hat{\mathcal{P}}_{\mathbf{p}}) \\ &\quad - f_i^{cv}(s, \text{Cut}(X^B(s, \hat{P}), X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})), \hat{\mathcal{P}}_{\mathbf{p}}) \, ds, \\ &= w(X_{0,i}^C(\hat{\mathcal{P}}_{\mathbf{p}})) + \int_{t_0}^t w(F_i^C(s, \text{Cut}(X^B(s, \hat{P}), X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})), \hat{\mathcal{P}}_{\mathbf{p}})) \, ds. \end{aligned}$$

By Assumption 5.17, $\mathcal{X}_0$ and $\mathcal{F}$ have $(1, 2)$ -convergence on $\mathbb{M}P'$ and $\mathbb{M}I \times \mathbb{M}X' \times \mathbb{M}P'$, respectively. Thus, $\exists \tau_{0,CC}, \tau_{0,CB} \geq 0$ with

$$w(X_{0,i}^C(\hat{\mathcal{P}}_{\mathbf{p}})) \leq \tau_{0,CC} w([\mathbf{p}, \mathbf{p}]) + \tau_{0,CB} w(\hat{P})^2 = \tau_{0,CB} w(\hat{P})^2, \quad \forall \hat{\mathcal{P}}_{\mathbf{p}} \in \mathbb{M}P'. \quad (5.6)$$

Moreover, $\exists \tau_{CC}, \tau_{CB} \in \mathbb{R}_+$ such that

$$\begin{aligned} &w(F_i^C(s, \text{Cut}(X^B(s, \hat{P}), X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})), \hat{\mathcal{P}}_{\mathbf{p}})) \\ &\leq \tau_{CB} \max \left\{ w(X^B(t, \hat{P})), w(\hat{P}) \right\}^2 + \tau_{CC} \max \left\{ w(X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})), w([\mathbf{p}, \mathbf{p}]) \right\}, \end{aligned}$$

for all $s \in I$ and $\hat{\mathcal{P}}_{\mathbf{p}} \in \mathbb{M}P'$. Combined with convergence in diameter of X^B on P' of at least order 1, this implies that $\exists \tau \in \mathbb{R}_+$ such that

$$w\left(F_i^C(s, \text{Cut}(X^B(s, \hat{P}), X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})), \hat{\mathcal{P}}_{\mathbf{p}})\right) \leq \tau w(\hat{P})^2 + \tau_{CC} w(X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})),$$

for all $s \in I$ and $\hat{\mathcal{P}}_{\mathbf{p}} \in \mathbb{M}P'$. Combining these inequalities gives

$$\begin{aligned} w\left(X_i^C(t, \hat{\mathcal{P}}_{\mathbf{p}})\right) &\leq \tau_{0,CB} w(\hat{P})^2 + \int_{t_0}^t \tau w(\hat{P})^2 + \tau_{CC} w(X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})) ds, \\ &\leq \tau_{0,CB} w(\hat{P})^2 + \tau(t_f - t_0) w(\hat{P})^2 + \int_{t_0}^t \tau_{CC} w(X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})) ds, \end{aligned}$$

for all $t \in I$ and $\hat{\mathcal{P}}_{\mathbf{p}} \in \mathbb{M}P'$. Taking the maximum over i , we obtain

$$w\left(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})\right) \leq \tau_{0,CB} w(\hat{P})^2 + \tau(t_f - t_0) w(\hat{P})^2 + \int_{t_0}^t \tau_{CC} w(X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})) ds,$$

for all $t \in I$ and $\hat{\mathcal{P}}_{\mathbf{p}} \in \mathbb{M}P'$. Applying the Gronwall-Bellman inequality gives (5.5). $\square$

To establish second-order pointwise convergence of the RPD method, we first show that the RPD relaxations are guaranteed to be tighter than those produced by the RAD method.

Theorem 5.20. *Let $P' \subset P$ be as in Assumption 5.18. Let $\mathbf{x}^{cv}, \mathbf{x}^{cc} : I \times \mathbb{M}P' \times P' \rightarrow \mathbb{R}^{n_x}$ and $\tilde{\mathbf{x}}^{cv}, \tilde{\mathbf{x}}^{cc} : I \times \mathbb{M}P' \times P' \rightarrow \mathbb{R}^{n_x}$ be the solutions of the RPD and RAD state relaxation systems, respectively. Then $[\mathbf{x}^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{x}^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}})] \subset [\tilde{\mathbf{x}}^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \tilde{\mathbf{x}}^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}})]$ with $\hat{\mathcal{P}}_{\mathbf{p}} = (\hat{P}, \mathbf{p})$ for all $(t, \hat{P}) \in I \times \mathbb{M}P'$ and $\mathbf{p} \in \hat{P}$.*

Proof. Choose any $\hat{P} \in \mathbb{M}P'$ and $\mathbf{p} \in \hat{P}$. It suffices to verify the four hypotheses of Theorem 4.14 with the definitions

$$\begin{aligned} [\tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P})] &\equiv [\tilde{\mathbf{x}}^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \tilde{\mathbf{x}}^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}})], \\ [\mathbf{v}(t, \hat{P}), \mathbf{w}(t, \hat{P})] &\equiv [\mathbf{x}^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{x}^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}})]. \end{aligned} \tag{5.7}$$

With these definitions, the ODEs in the statement of Theorem 4.14 can be identified with those of the RAD and RPD systems in Definitions 5.10 and 5.11. From this, we note that the right-hand sides of the ODEs in the statement of Theorem 4.14 satisfy

$$\begin{aligned} \tilde{u}_i(t, Z, \hat{P}) &= f_i^{cv}(t, \text{Cut}(X^B(t, \hat{P}), [\mathbf{z}^{cv}, \mathbf{z}^{cc}]), \hat{\mathcal{P}}_{\mathbf{p}}), \\ \tilde{o}_i(t, Z, \hat{P}) &= f_i^{cc}(t, \text{Cut}(X^B(t, \hat{P}), [\mathbf{z}^{cv}, \mathbf{z}^{cc}]), \hat{\mathcal{P}}_{\mathbf{p}}), \\ u_i(t, Z, \hat{P}) &\geq f_i^{cv}(t, \text{Cut}(X^B(t, \hat{P}), \mathcal{B}_i^L([\mathbf{z}^{cv}, \mathbf{z}^{cc}])), \hat{\mathcal{P}}_{\mathbf{p}}), \\ o_i(t, Z, \hat{P}) &\leq f_i^{cc}(t, \text{Cut}(X^B(t, \hat{P}), \mathcal{B}_i^U([\mathbf{z}^{cv}, \mathbf{z}^{cc}])), \hat{\mathcal{P}}_{\mathbf{p}}), \end{aligned}$$

for all $(t, Z) \in I \times \mathbb{M}D$.

Since the RAD and RPD systems have the same initial conditions, Hypothesis 1 of Theorem 4.14 holds. By Assumption 5.6, $\mathcal{F}$ is inclusion monotonic. Since $\mathcal{B}_i^L(Z) \subset Z$, it follows that

$$\begin{aligned} \tilde{u}_i(t, Z, \hat{P}) &= f_i^{cv}(t, \text{Cut}(X^B(t, \hat{P}), [\mathbf{z}^{cv}, \mathbf{z}^{cc}]), \hat{\mathcal{P}}_{\mathbf{p}}) \\ &\leq f_i^{cv}(t, \text{Cut}(X^B(t, \hat{P}), \mathcal{B}_i^L([\mathbf{z}^{cv}, \mathbf{z}^{cc}])), \hat{\mathcal{P}}_{\mathbf{p}}) \\ &\leq u_i(t, Z, \hat{P}), \end{aligned}$$

for all $(t, [\mathbf{z}^{cv}, \mathbf{z}^{cc}], \hat{P}) \in I \times \mathbb{I}D \times \mathbb{I}P$. Making the analogous argument for $\tilde{o}_i$, this verifies Hypothesis 2. Moreover, inclusion monotonicity of $\mathcal{F}$ directly implies Hypothesis 3. Finally, Hypothesis 4 follows from the Lipschitz condition in Assumption 5.6. $\square$

Corollary 5.21. *Let $P' \subset P$ be as in Assumption 5.18. Let $\mathbf{x}^{cv}, \mathbf{x}^{cc} : I \times \mathbb{I}P' \times P' \rightarrow \mathbb{R}^{n_x}$ be a solution of the RPD state relaxation system and let $X^C(t, \hat{P}_{\mathbf{p}}) \equiv [\mathbf{x}^{cv}(t, \hat{P}_{\mathbf{p}}), \mathbf{x}^{cc}(t, \hat{P}_{\mathbf{p}})]$. Then X^C has pointwise convergence in P' of order 2, uniformly on I . Specifically, (5.5) holds for all $t \in I$ and $\hat{P}_{\mathbf{p}} = (\hat{P}, \mathbf{p}) \in \mathbb{I}P' \times P'$.*

Proof. For every $\hat{P} \in \mathbb{I}P'$, Assumption 5.18 ensures that $X^B(t, \hat{P}) \subset D$, $\forall t \in I$, and it follows that the RAD system has a unique solution on $I \times \hat{P}$ (see Theorem 7.3.4 and Lemma 7.6.7 in [47]). Let $\tilde{\mathbf{x}}^{cv}, \tilde{\mathbf{x}}^{cc} : I \times \mathbb{I}P' \times P' \rightarrow \mathbb{R}^{n_x}$ be the solution of the RAD state relaxation system and denote $\tilde{X}^C(t, \hat{P}_{\mathbf{p}}) \equiv [\tilde{\mathbf{x}}^{cv}(t, \hat{P}_{\mathbf{p}}), \tilde{\mathbf{x}}^{cc}(t, \hat{P}_{\mathbf{p}})]$. By Theorem 5.20, $w(X^C(t, \hat{P}_{\mathbf{p}})) \leq w(\tilde{X}^C(t, \hat{P}_{\mathbf{p}}))$ for all $t \in I$ and $\hat{P}_{\mathbf{p}} \in \mathbb{I}P' \times P'$. Thus, the result follows directly from Theorem 5.19. $\square$

We have now established second-order pointwise convergence for both the RAD and RPD methods, and provided an upper bound on the convergence prefactor in (5.5). However, this prefactor grows exponentially with time. In the remainder of this section, we show that this exponential bound need not be sharp for the RPD method, and we provide a potentially sharper bound based on the logarithmic norm. When the appropriate logarithmic norm is negative, we show that the pointwise relaxation error for RPD can decrease over time, and the convergence prefactor is bounded as $t \rightarrow +\infty$. In contrast, the error for the RAD method can only increase with time. The following result is analogous to the result of Proposition 4.9 for state bounds.

Proposition 5.22. *Let $P' \subset P$ and $X' \subset D$ be as in Assumption 5.18. Let $\mathbf{x}^{cv}, \mathbf{x}^{cc} : I \times \mathbb{I}P' \times P' \rightarrow \mathbb{R}^{n_x}$ satisfy the RPD state relaxation system and let*

$$X^C(t, \hat{P}_{\mathbf{p}}) \equiv [\mathbf{x}^{cv}(t, \hat{P}_{\mathbf{p}}), \mathbf{x}^{cc}(t, \hat{P}_{\mathbf{p}})].$$

If, for some $(t, k, \hat{P}) \in I \times \{1, \dots, n_x\} \times \mathbb{I}P'$, $\exists \alpha_k \in \mathbb{R}$ such that

$$\begin{aligned} f_k(t, \mathbf{z}^{(1)}, \mathbf{p}) - f_k(t, \mathbf{z}^{(2)}, \mathbf{p}) &\leq \alpha_k (z_k^{(1)} - z_k^{(2)}), \\ \forall (\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \mathbf{p}) &\in X^B(t, \hat{P}) \times X^B(t, \hat{P}) \times \hat{P} : z_j^{(1)} = z_j^{(2)}, \forall j \neq k \text{ and } z_k^{(1)} \geq z_k^{(2)}, \end{aligned} \quad (5.8)$$

then there exist constants $\tilde{\tau}_{CB,k}, \tilde{\tau}_{CC,k} \in \mathbb{R}_+$, independent of $(t, \hat{P}) \in I \times \mathbb{I}P'$, such that

$$\begin{aligned} \frac{d}{dt} w(X_k^C(t, \hat{P}_{\mathbf{p}})) &\leq \alpha_k w(X_k^C(t, \hat{P}_{\mathbf{p}})) + \tilde{\tau}_{CB,k} w(\hat{P})^2 \\ &\quad + \tilde{\tau}_{CC,k} \max_{i \neq k} w(X_i^C(t, \hat{P}_{\mathbf{p}})), \quad \forall \mathbf{p} \in \hat{P}. \end{aligned} \quad (5.9)$$

If $\alpha_k < 0$, this bound can be negative. Furthermore, for the RAD method, it is not possible to obtain $\frac{d}{dt} w(X_k^C(t, \hat{P}_{\mathbf{p}})) < 0$.

Proof. Choose any $\hat{P} \in \mathbb{I}P'$ and $\mathbf{p} \in \hat{P}$. By Definition 5.11,

$$\begin{aligned} \frac{d}{dt} w(X_k^C(t, \hat{P}_{\mathbf{p}})) &= \frac{d}{dt} (x_k^{cc}(t, \hat{P}_{\mathbf{p}}) - x_k^{cv}(t, \hat{P}_{\mathbf{p}})), \\ &\leq f_k^{cc}(t, \text{Cut}(X^B(t, \hat{P}), \mathcal{B}_k^U(X^C(t, \hat{P}_{\mathbf{p}}))), \hat{P}_{\mathbf{p}}) \\ &\quad - f_k^{cv}(t, \text{Cut}(X^B(t, \hat{P}), \mathcal{B}_k^L(X^C(t, \hat{P}_{\mathbf{p}}))), \hat{P}_{\mathbf{p}}). \end{aligned}$$

Since $X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}) \subset X^B(t, \hat{P}) \subset D$ [47, Lemma 7.5.3], the Cut functions can be removed above. Moreover, the points $\bar{\mathbf{x}}(t, \hat{\mathcal{P}}_{\mathbf{p}}) \equiv (x_1(t, \mathbf{p}), \dots, x_k^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \dots, x_{n_x}(t, \mathbf{p}))$ and $\underline{\mathbf{x}}(t, \hat{\mathcal{P}}_{\mathbf{p}}) \equiv (x_1(t, \mathbf{p}), \dots, x_k^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \dots, x_{n_x}(t, \mathbf{p}))$ are guaranteed to be in D . Thus, we may subtract and add the terms $f_k(t, \bar{\mathbf{x}}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{p})$ and $f_k(t, \underline{\mathbf{x}}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{p})$ to obtain

$$\begin{aligned} \frac{d}{dt} w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) &\leq [f_k^{cc}(t, (X^B(t, \hat{P}), \mathcal{B}_k^U(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))), \hat{\mathcal{P}}_{\mathbf{p}}) - f_k(t, \bar{\mathbf{x}}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{p})] \\ &\quad + [f_k(t, \bar{\mathbf{x}}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{p}) - f_k(t, \underline{\mathbf{x}}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{p})] \\ &\quad + [f_k(t, \underline{\mathbf{x}}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{p}) - f_k^{cv}(t, (X^B(t, \hat{P}), \mathcal{B}_k^L(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))), \hat{\mathcal{P}}_{\mathbf{p}})]. \end{aligned} \quad (5.10)$$

Since $\mathcal{F}$ is a relaxation function for $\mathbf{f}$ and $\bar{\mathbf{x}}(t, \hat{\mathcal{P}}_{\mathbf{p}}) \in \mathcal{B}_k^U(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))$, the first term on the right is bounded above by

$$[f_k^{cc}(t, (X^B(t, \hat{P}), \mathcal{B}_k^U(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))), \hat{\mathcal{P}}_{\mathbf{p}}) - f_k^{cv}(t, (X^B(t, \hat{P}), \mathcal{B}_k^L(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))), \hat{\mathcal{P}}_{\mathbf{p}})].$$

But, by Assumption 5.17, $\mathcal{F}_k$ has $(1, 2)$ -convergence on $\mathbb{M}I \times \mathbb{M}X' \times \mathbb{M}P'$ with some prefactors $\tau_{BB,k}, \tau_{CB,k}, \tau_{CC,k} \in \mathbb{R}_+$, and by Assumption 5.18, X^B has convergence in diameter of order at least one with some prefactor $\tau_B \in \mathbb{R}_+$, uniformly on I . Thus, this quantity is bounded from above by

$$\begin{aligned} &\tau_{CB,k} \max \left\{ w(X^B(t, \hat{P})), w(\hat{P}) \right\}^2 + \tau_{CC,k} \max \left\{ w(\mathcal{B}_k^U(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))), w([\mathbf{p}, \mathbf{p}]) \right\} \\ &\leq \tau_{CB,k} \max \left\{ \tau_B w(\hat{P}), w(\hat{P}) \right\}^2 + \tau_{CC,k} w(\mathcal{B}_k^U(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))), \\ &= \max \left\{ \tau_{CB,k} \tau_B^2, \tau_{CB,k} \right\} w(\hat{P})^2 + \tau_{CC,k} \max_{i \neq k} w(X_i^C(t, \hat{\mathcal{P}}_{\mathbf{p}})). \end{aligned}$$

An analogous argument shows that this is an upper bound for the third term on the right-hand side of (5.10) as well as the first. Now, applying (5.8) to the middle term, (5.10) gives

$$\begin{aligned} \frac{d}{dt} w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) &\leq 2 \max \left\{ \tau_{CB,k} \tau_B^2, \tau_{CB,k} \right\} w(\hat{P})^2 + 2\tau_{CC,k} \max_{i \neq k} w(X_i^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) \\ &\quad + \alpha_k w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})), \end{aligned} \quad (5.11)$$

which verifies (5.9). The constant α_k , which can be negative, multiplies $w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))$, which must be nonnegative, so that there can be a negative contribution to the change in size of $w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))$. If a system has $\alpha_k < 0$, then if $x_k^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}})$ and $x_k^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}})$ are sufficiently far apart relative to the diameters of $\hat{P}$ and $X_i^C(t, \hat{\mathcal{P}}_{\mathbf{p}})$, $\forall i \neq k$, the overall sum can be negative. For RAD, the relaxation function of f_k takes the same arguments for the convex and concave relaxations, so that $\frac{dw(X_k^C)}{dt}(t, \hat{\mathcal{P}}_{\mathbf{p}}) \geq 0$ always. $\square$

Example 5.23. Consider again the very simple chemical reaction $A \rightleftharpoons B$, with the ODE model

$$\begin{aligned} \dot{x}_A &= -k_f x_A + k_r x_B, \\ \dot{x}_B &= k_f x_A - k_r x_B. \end{aligned}$$

Let $\mathcal{X}_{A,0} \equiv ([0.8, 1.2], [0.8, 1.2])$, $\mathcal{X}_{B,0} \equiv ([0.1, 0.1], [0.1, 0.1])$, $\mathcal{K}_f \equiv ([15, 20], [17.5, 17.5])$, $\mathcal{K}_r \equiv ([1, 5], [3, 3])$, and $\mathcal{P} \equiv \mathcal{K}_f \times \mathcal{K}_r$. Using the facts

$$\begin{aligned} 0 &\leq x_A^L(t_0), \quad 0 \leq x_B^L(t_0), \quad 0 \leq x_A^{cv}(t_0), \quad 0 \leq x_B^{cv}(t_0), \\ 0 &\leq k_f^L, \quad 0 \leq k_r^L, \quad k_f^{cv} = k_f^{cc}, \quad k_r^{cv} = k_r^{cc}, \end{aligned}$$

and applying the rules of the natural McCormick extension, the vector fields for the RPD for species A at t_0 are:

$$\begin{aligned} u_A &= -\min\{k_f^{cc} x_A^L + k_f^U x_A^{cv} - k_f^U x_A^L, k_f^{cc} x_A^U + k_f^L x_A^{cv} - k_f^L x_A^U\} \\ &\quad + \max\{k_r^{cv} x_B^L + k_r^L x_B^{cv} - k_r^L x_B^L, k_r^{cv} x_B^U + k_r^U x_B^{cv} - k_r^U x_B^U\}, \\ o_A &= -\max\{k_f^{cv} x_A^L + k_f^L x_A^{cc} - k_f^L x_A^L, k_f^{cv} x_A^U + k_f^U x_A^{cc} - k_f^U x_A^U\} \\ &\quad + \min\{k_r^{cc} x_B^L + k_r^U x_B^{cc} - k_r^U x_B^L, k_r^{cc} x_B^U + k_r^L x_B^{cc} - k_r^L x_B^U\}, \\ \dot{x}_A^{cv} &= \max\{u_A, \dot{x}_A^L\}, \\ \dot{x}_A^{cc} &= \min\{o_A, \dot{x}_A^U\}, \end{aligned}$$

where we have omitted the arguments to preserve readability and $(\dot{x}_A^L, \dot{x}_A^U)$ are computed using Harrison's method as in Example 4.11. At the initial time, we obtain

$$\begin{aligned} u_A &= -\min\{17.5 \cdot 0.8 + 20 \cdot 0.8 - 20 \cdot 0.8, 17.5 \cdot 1.2 + 15 \cdot 0.8 - 15 \cdot 1.2\} \\ &\quad + \max\{3 \cdot 0.1 + 1 \cdot 0.1 - 1 \cdot 0.1, 3 \cdot 0.1 + 5 \cdot 0.1 - 5 \cdot 0.1\}, \\ o_A &= -\max\{17.5 \cdot 0.8 + 15 \cdot 1.2 - 15 \cdot 0.8, 17.5 \cdot 1.2 + 20 \cdot 1.2 - 20 \cdot 1.2\} \\ &\quad + \min\{3 \cdot 0.1 + 5 \cdot 0.1 - 5 \cdot 0.1, 3 \cdot 0.1 + 1 \cdot 0.1 - 1 \cdot 0.1\}, \\ \dot{x}_A^{cv} &= \max\{-13.7, -15.9\} = -13.7, \\ \dot{x}_A^{cc} &= \min\{-20.7, -17.5\} = -20.7. \end{aligned}$$

This means that at the initial time, the relaxations for species A are becoming tighter, since

$$\frac{dw(X_A^C)}{dt}(t_0, \hat{\mathcal{P}}_{\mathbf{P}}) = f_{A,\text{RPD}}^{cc} - f_{A,\text{RPD}}^{cv} = -7.$$

If we use RAD, the vector fields at t_0 are:

$$\begin{aligned} \dot{x}_A^{cv} &= -\min\{k_f^{cc} x_A^L + k_f^U \underbrace{x_A^{cc}} - k_f^U x_A^L, k_f^{cc} x_A^U + k_f^L \underbrace{x_A^{cc}} - k_f^L x_A^U\} \\ &\quad + \max\{k_r^{cv} x_B^L + k_r^L x_B^{cv} - k_r^L x_B^L, k_r^{cv} x_B^U + k_r^U x_B^{cv} - k_r^U x_B^U\}, \\ \dot{x}_A^{cc} &= -\max\{k_f^{cv} x_A^L + k_f^L \underbrace{x_A^{cv}} - k_f^L x_A^L, k_f^{cv} x_A^U + k_f^U \underbrace{x_A^{cv}} - k_f^U x_A^U\} \\ &\quad + \min\{k_r^{cc} x_B^L + k_r^U x_B^{cc} - k_r^U x_B^L, k_r^{cc} x_B^U + k_r^L x_B^{cc} - k_r^L x_B^U\}, \end{aligned}$$

where we have again omitted the arguments and the changed terms are highlighted using braces below. At the initial time, we obtain

$$\begin{aligned} \dot{x}_A^{cv} &= -\min\{17.5 \cdot 0.8 + 20 \cdot \underbrace{1.2} - 20 \cdot 0.8, 17.5 \cdot 1.2 + 15 \cdot \underbrace{1.2} - 15 \cdot 1.2\} \\ &\quad + \max\{3 \cdot 0.1 + 1 \cdot 0.1 - 1 \cdot 0.1, 3 \cdot 0.1 + 5 \cdot 0.1 - 5 \cdot 0.1\}, \\ \dot{x}_A^{cc} &= -\max\{17.5 \cdot 0.8 + 15 \cdot \underbrace{0.8} - 15 \cdot 0.8, 17.5 \cdot 1.2 + 20 \cdot \underbrace{0.8} - 20 \cdot 1.2\} \\ &\quad + \min\{3 \cdot 0.1 + 5 \cdot 0.1 - 5 \cdot 0.1, 3 \cdot 0.1 + 1 \cdot 0.1 - 1 \cdot 0.1\}, \\ \dot{x}_A^{cv} &= -20.7, \\ \dot{x}_A^{cc} &= -13.7. \end{aligned}$$

Thus, we have $\frac{dw(X_{A,RAD}^C)}{dt}(t_0) = f_{A,RAD}^{cc} - f_{A,RAD}^{cv} = +7$, so the relaxations are becoming farther apart with time.

Next, we build on Proposition 5.22 to establish a bound on the convergence prefactor of the RPD method using the logarithmic norm. The following Lemma is required.

Lemma 5.24. *Let $P' \subset P$ be as in Assumption 5.18, let $\mathbf{x}^{cv}, \mathbf{x}^{cc} : I \times \mathbb{I}P' \times P' \rightarrow \mathbb{R}^{n_x}$ satisfy the RPD state relaxation system, and let $X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}) \equiv [\mathbf{x}^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}), \mathbf{x}^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}})]$. For every $k \in \{1, \dots, n_x\}$, every $\hat{\mathcal{P}}_{\mathbf{p}} = (\hat{P}, \mathbf{p}) \in \mathbb{I}P' \times P'$, and a.e. $t \in I$, $\exists \delta > 0$ such that*

$$0 \leq w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) + h \frac{d}{dt} w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})), \quad \forall h \in (0, \delta]. \quad (5.12)$$

Proof. Choose any $k, \hat{\mathcal{P}}_{\mathbf{p}} \in \mathbb{I}P' \times P'$, and $t \in I$. If $w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) > 0$, then (5.12) clearly holds for all sufficiently small h . Otherwise, we must have $w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) = 0$ and it suffices to show that $\frac{d}{dt} w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) \geq 0$. From the definition of the RPD system, $\frac{d}{dt} w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))$ satisfies one of the following four equations at a.e. $t \in I$:

$$\begin{aligned} \frac{d}{dt} w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) &= f_k^{cc}(t, (X^B(t, \hat{P}), \mathcal{B}_k^U(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})), \hat{\mathcal{P}}_{\mathbf{p}})) \\ &\quad - f_k^{cv}(t, (X^B(t, \hat{P}), \mathcal{B}_k^L(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})), \hat{\mathcal{P}}_{\mathbf{p}})), \\ \frac{d}{dt} w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) &= f_k^{cc}(t, (X^B(t, \hat{P}), \mathcal{B}_k^U(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})), \hat{\mathcal{P}}_{\mathbf{p}})) - \dot{x}_k^L(t, \hat{P}), \\ \frac{d}{dt} w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) &= \dot{x}_k^U(t, \hat{P}) - f_k^{cv}(t, (X^B(t, \hat{P}), \mathcal{B}_k^L(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})), \hat{\mathcal{P}}_{\mathbf{p}})), \\ \frac{d}{dt} w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) &= \dot{x}_k^U(t, \hat{P}) - \dot{x}_k^L(t, \hat{P}). \end{aligned}$$

In the first case, note that $w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) = 0$ implies

$$\mathcal{B}_k^L(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) = \mathcal{B}_k^U(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) = X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}). \quad (5.13)$$

Moreover, since $\mathbf{x}(t, \mathbf{p}) \in X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})$ and $\mathcal{F}_k$ is a relaxation function for $\mathbf{f}_k$,

$$\begin{aligned} f_k^{cv}(t, (X^B(t, \hat{P}), X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})), \hat{\mathcal{P}}_{\mathbf{p}}) &\leq f_k(t, \mathbf{x}(t, \mathbf{p}), \mathbf{p}), \\ &\leq f_k^{cc}(t, (X^B(t, \hat{P}), X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})), \hat{\mathcal{P}}_{\mathbf{p}}). \end{aligned}$$

Together, these facts imply $\frac{d}{dt} w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) \geq 0$. The second case can only occur if $x_k^L(t, \hat{P}) = x_k^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}) = x_k^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}})$, and under these conditions $\frac{d}{dt} w(X_k^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) \geq 0$ for a.e. $t \in I$ by Lemma 7.5.6 in [47]. The third case is analogous to the second. Finally, the fourth case can only occur if $x_k^L(t, \hat{P}) = x_k^{cv}(t, \hat{\mathcal{P}}_{\mathbf{p}}) = x_k^{cc}(t, \hat{\mathcal{P}}_{\mathbf{p}}) = x_k^U(t, \hat{P})$. Since $x_k^U(s, \hat{P}) - x_k^L(s, \hat{P}) \geq 0, \forall s \in I$, it is a contradiction to have $\dot{x}_k^U(t, \hat{P}) - \dot{x}_k^L(t, \hat{P}) < 0$ in this case. In particular, if $\dot{x}_k^U(t, \hat{P}) - \dot{x}_k^L(t, \hat{P}) = -\alpha < 0$, then continuity of the derivatives implies that we can choose $h > 0$ so small that $\dot{x}_k^U(s, \hat{P}) - \dot{x}_k^L(s, \hat{P}) \leq -\alpha/2$ for all $s \in [t, t+h]$. But then the Fundamental Theorem of Calculus gives

$$0 \leq x_k^U(t+h, \hat{P}) - x_k^L(t+h, \hat{P}) = \int_t^{t+h} \dot{x}_k^U(s, \hat{P}) - \dot{x}_k^L(s, \hat{P}) ds \leq -(\alpha/2)h,$$

which is a contradiction. $\square$

Theorem 5.25. Let $P' \subset P$ and $X' \subset D$ be as in Assumption 5.18, let $\mathbf{x}^{cv}, \mathbf{x}^{cc} : I \times \mathbb{I}P' \times P' \rightarrow \mathbb{R}^{n_x}$ satisfy the RPD state relaxation system, and let $X^C(t, \hat{P}_{\mathbf{p}}) \equiv [\mathbf{x}^{cv}(t, \hat{P}_{\mathbf{p}}), \mathbf{x}^{cc}(t, \hat{P}_{\mathbf{p}})]$. Suppose $\exists \alpha_k \in \mathbb{R}$ such that, for all $(t, k, \hat{P}) \in I \times \{1, \dots, n_x\} \times \mathbb{I}P'$,

$$\begin{aligned} f_k(t, \mathbf{z}^{(1)}, \mathbf{p}) - f_k(t, \mathbf{z}^{(2)}, \mathbf{p}) &\leq \alpha_k(z_k^{(1)} - z_k^{(2)}), \\ \forall (\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \mathbf{p}) \in X' \times X' \times P' : z_j^{(1)} &= z_j^{(2)}, \forall j \neq k \text{ and } z_k^{(1)} \geq z_k^{(2)}. \end{aligned} \quad (5.14)$$

Noting that this hypothesis implies (5.9) for all $(t, k, \hat{P}) \in I \times \{1, \dots, n_x\} \times \mathbb{I}P'$, let $\tilde{\tau}_{CB,k}, \tilde{\tau}_{CC,k} \in \mathbb{R}_+$ satisfy (5.9) for all $(t, \hat{P}) \in I \times \mathbb{I}P'$. Define $\mathbf{S} \in \mathbb{R}^{n_x \times n_x}$ by

$$S_{ij} = \begin{cases} \alpha_i & \text{if } i = j \\ \tilde{\tau}_{CC,i} & \text{if } i \neq j \end{cases}$$

Then, for each $(t, \hat{P}) \in I \times \mathbb{I}P'$ and $\mathbf{p} \in \hat{P}$, the state relaxations satisfy:

1. $\frac{d}{dt} w_V(X^C(t, \hat{P}_{\mathbf{p}})) \leq \mathbf{S} w_V(X^C(t, \hat{P}_{\mathbf{p}})) + \tilde{\tau}_{CB} w(\hat{P})^2$.
2. If $\mu_\infty(\mathbf{S}) = 0$, then

$$w(X^C(t, \hat{P}_{\mathbf{p}})) \leq w(X^C(t_0, \hat{P}_{\mathbf{p}})) + [(t - t_0) \|\tilde{\tau}_{CB}\|_\infty] w(\hat{P})^2. \quad (5.15)$$

3. If $\mu_\infty(\mathbf{S}) \neq 0$, then

$$\begin{aligned} w(X^C(t, \hat{P}_{\mathbf{p}})) &\leq [\exp(\mu_\infty(\mathbf{S})(t - t_0))] w(X^C(t_0, \hat{P}_{\mathbf{p}})) \\ &\quad - \left[(1 - \exp(\mu_\infty(\mathbf{S})(t - t_0))) \frac{\|\tilde{\tau}_{CB}\|_\infty}{\mu_\infty(\mathbf{S})} \right] w(\hat{P})^2. \end{aligned} \quad (5.16)$$

4. If $\alpha_i < -(n_x - 1) \|\tilde{\tau}_{CB,i}\|$, $\forall i$, then $\mu_\infty(\mathbf{S}) < 0$, the state relaxations can grow closer together as time increases, and

$$\lim_{t \rightarrow +\infty} w(X^C(t, \hat{P}_{\mathbf{p}})) \leq -\frac{\|\tilde{\tau}_{CB}\|_\infty}{\mu_\infty(\mathbf{S})} w(\hat{P})^2. \quad (5.17)$$

Proof. Using Proposition 5.22, we have for every k ,

$$\begin{aligned} \frac{d}{dt} w(X_k^C(t, \hat{P}_{\mathbf{p}})) &\leq \alpha_k w(X_k^C(t, \hat{P}_{\mathbf{p}})) + \tilde{\tau}_{CB,k} w(\hat{P})^2 + \tilde{\tau}_{CC,k} \max_{i \neq k} w(X_i^C(t, \hat{P}_{\mathbf{p}})), \\ &\leq \alpha_k w(X_k^C(t, \hat{P}_{\mathbf{p}})) + \tilde{\tau}_{CB,k} w(\hat{P})^2 + \tilde{\tau}_{CC,k} \sum_{i \neq k} w(X_i^C(t, \hat{P}_{\mathbf{p}})). \end{aligned}$$

Thus, by the definition of $\mathbf{S}$

$$\frac{d}{dt} w_V(X^C(t, \hat{P}_{\mathbf{p}})) \leq \mathbf{S} w_V(X^C(t, \hat{P}_{\mathbf{p}})) + \tilde{\tau}_{CB} w(\hat{P})^2, \quad (5.18)$$

which establishes Claim 1. To establish Claim 2, we again consider the upper right Dini derivative as in [60, (1.8)]:

$$\begin{aligned} D_t^+ w(X^C(t, \hat{P}_{\mathbf{p}})) &= D_t^+ \left\| w_V(X^C(t, \hat{P}_{\mathbf{p}})) \right\|_\infty, \\ &= \limsup_{h \rightarrow 0^+} \frac{\left\| w_V(X^C(t+h, \hat{P}_{\mathbf{p}})) \right\|_\infty - \left\| w_V(X^C(t, \hat{P}_{\mathbf{p}})) \right\|_\infty}{h}. \end{aligned}$$

Due to discontinuities in the right-hand sides of the RPD system, $\mathbf{x}^{cv}(\cdot, \hat{\mathcal{P}}_{\mathbf{p}})$ and $\mathbf{x}^{cc}(\cdot, \hat{\mathcal{P}}_{\mathbf{p}})$ need not be differentiable on I . However, they are absolutely continuous, and hence differentiable at a.e. $t \in I$. Thus, for a.e. $t \in I$, $w_V(X^C(\cdot, \hat{\mathcal{P}}_{\mathbf{p}}))$ is differentiable, and hence the Taylor approximation $w_V(X^C(t+h, \hat{\mathcal{P}}_{\mathbf{p}})) \approx w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) + h \frac{d}{dt} w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))$ has an error converging to zero super-linearly as $h \rightarrow 0$. Therefore, for a.e. $t \in I$, $D_t^+ w(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))$ is equivalent to

$$\limsup_{h \rightarrow 0+} \frac{\|w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) + h \frac{d}{dt} w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))\|_{\infty} - \|w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))\|_{\infty}}{h}. \quad (5.19)$$

Moreover, for a.e. $t \in I$, Lemma 5.24 ensures that this Taylor approximation is nonnegative for sufficiently small h . It follows that (5.18) can be applied to bound (5.19) from above by

$$\begin{aligned} & \limsup_{h \rightarrow 0+} \frac{\|w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) + h (\mathbf{S} w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) + \tilde{\tau}_{CB} w(\hat{P})^2)\|_{\infty} - \|w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))\|_{\infty}}{h}, \\ &= \limsup_{h \rightarrow 0+} \frac{\|(\mathbf{I} + h\mathbf{S})w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) + h\tilde{\tau}_{CB} w(\hat{P})^2\|_{\infty} - \|w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))\|_{\infty}}{h}, \\ &\leq \limsup_{h \rightarrow 0+} \frac{\|\mathbf{I} + h\mathbf{S}\|_{\infty} - 1}{h} \|w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))\|_{\infty} + \|\tilde{\tau}_{CB} w(\hat{P})^2\|_{\infty}. \end{aligned} \quad (5.20)$$

Since $\|\cdot\|_{\infty}$ is directionally differentiable, it follows that $\lim_{h \rightarrow 0+} \frac{\|\mathbf{I} + h\mathbf{S}\|_{\infty} - 1}{h}$ exists [60], and is therefore equal to the lim sup, and both are equal to the logarithmic norm $\mu_{\infty}(\mathbf{S})$ by Definition 2.3. Thus,

$$D_t^+ w(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) \leq \mu_{\infty}(\mathbf{S}) \|w_V(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))\|_{\infty} + \|\tilde{\tau}_{CB}\|_{\infty} w(\hat{P})^2, \quad (5.21)$$

for a.e. $t \in I$. Since $w(X^C(\cdot, \hat{\mathcal{P}}_{\mathbf{p}})) = \|w_V(X^C(\cdot, \hat{\mathcal{P}}_{\mathbf{p}}))\|_{\infty}$ is the composition of the absolutely continuous function $w_V(X^C(\cdot, \hat{\mathcal{P}}_{\mathbf{p}}))$ and the Lipschitz continuous function $\|\cdot\|_{\infty}$, $w(X^C(\cdot, \hat{\mathcal{P}}_{\mathbf{p}}))$ is absolutely continuous. It follows that its derivative exists and coincides with $D_t^+ w(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}}))$ for a.e. $t \in I$. Moreover, $D_t^+ w(X^C(\cdot, \hat{\mathcal{P}}_{\mathbf{p}}))$ is Lebesgue integrable on I and satisfies $w(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) - w(X^C(t_0, \hat{\mathcal{P}}_{\mathbf{p}})) = \int_{t_0}^t D_s^+ w(X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})) ds$. Thus,

$$\begin{aligned} w(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})) &\leq w(X^C(t_0, \hat{\mathcal{P}}_{\mathbf{p}})) + \int_{t_0}^t \mu_{\infty}(\mathbf{S}) w(X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})) + \|\tilde{\tau}_{CB}\|_{\infty} w(\hat{P})^2 ds, \\ &= w(X^C(t_0, \hat{\mathcal{P}}_{\mathbf{p}})) + \|\tilde{\tau}_{CB}\|_{\infty} (t - t_0) w(\hat{P})^2 + \int_{t_0}^t \mu_{\infty}(\mathbf{S}) w(X^C(s, \hat{\mathcal{P}}_{\mathbf{p}})) ds. \end{aligned}$$

If $\mu_{\infty}(\mathbf{S}) = 0$, we obtain (5.15), which proves Claim 2. If $\mu_{\infty}(\mathbf{S}) \neq 0$, we apply Lemma 2.2 with $\mu \equiv \mu_{\infty}(\mathbf{S})$, $\lambda_0 \equiv w(X^C(t_0, \hat{\mathcal{P}}_{\mathbf{p}}))$, $\lambda_1 \equiv \|\tilde{\tau}_1\|_{\infty} w(\hat{P})^2$, and $x \equiv w(X^C(\cdot, \hat{\mathcal{P}}_{\mathbf{p}}))$ to obtain (5.16), and hence Claim 3.

By Proposition 2.4, if $\alpha_i < -(n_x - 1)|\tilde{\tau}_{CB,i}|$, $\forall i$, then $\mu_{\infty}(\mathbf{S}) < 0$. Then, (5.17) clearly follows from (5.16), which proves Claim 4. $\square$

Corollary 5.26. *Let the hypotheses of Theorem 5.25 hold and let $\tau_{CB,0}, \tau_{CC,0} \in \mathbb{R}_+$ be the prefactors for (1, 2)-convergence of $\mathcal{X}_0$ on $\mathbb{M}^{P'}$ as per Assumption 5.17. Then, for each $(t, \hat{P}) \in I \times \mathbb{I}^{P'}$ and each $\mathbf{p} \in \hat{P}$, the state relaxations from the RPD method satisfy:*

1. If $\mu_\infty(\mathbf{S}) = 0$, then

$$w\left(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})\right) \leq [\tau_{CB,0} + (t - t_0)\|\tilde{\tau}_{CB}\|_\infty] w(\hat{P})^2. \quad (5.22)$$

2. If $\mu_\infty(\mathbf{S}) \neq 0$, then

$$w\left(X^C(t, \hat{\mathcal{P}}_{\mathbf{p}})\right) \leq \left[\exp(\mu_\infty(\mathbf{S})(t - t_0)) \left(\tau_{CB,0} + \frac{\|\tilde{\tau}_{CB}\|_\infty}{\mu_\infty(\mathbf{S})} \right) - \frac{\|\tilde{\tau}_{CB}\|_\infty}{\mu_\infty(\mathbf{S})} \right] w(\hat{P})^2.$$

Proof. Claims 1–2 follow from Claims 2–3 of Theorem 5.25 by noting that $w(X^C(t_0, \hat{\mathcal{P}}_{\mathbf{p}}))$ is equivalent to $w(X_0^C(\hat{\mathcal{P}}_{\mathbf{p}}))$, which is bounded above by $\tau_{CB,0}w(\hat{P})^2$ for all $\hat{P} \in \mathbb{I}P'$. $\square$

See §6.2 for an application of the convergence-order bounds in Theorem 5.25 and Corollary 5.26 to a chemical kinetics problem.

6 Numerical results and discussion

6.1 Overall numerical performance of RAD and RPD in global dynamic optimization

In [44, Chapter 2], the numerical performance of a variety of global dynamic optimization algorithms was assessed on a suite of test problems. Two of the relaxation methods tested were RAD and RPD. The test suite was solved with a variety of bounding, relaxation, domain reduction, and optimization methods. There are 26 pairs of tabular data from [44] for which RAD and RPD are both used on the same test problem with all other options being identical. To give an idea of the relative cost per node, for the present paper, we calculated the CPU time divided by the number of lower bounding problem evaluations (the lower-bounding problems are the dominant cost). RPD took on average of 2.9 times longer per lower-bounding problem. Despite the higher cost per lower-bounding problem, the average *speedup of overall* CPU time for RPD relative to RAD was 3.6. This analysis of the overall speedup, however, does not fully illustrate how much better RPD can be. There were several test problems in [44] for which only RPD was used, because the very long CPU times of RAD made it impractical to allow them to solve to guaranteed global optimality.

6.2 An illustrative numerical example

Consider the global parameter estimation problem posed in [11, 58, 61] for the first-order reversible chain reaction $A \rightleftharpoons B \rightleftharpoons C$. The ODE model is:

$$\begin{aligned} \dot{x}_1 &= -p_1x_1 + p_2x_2, \\ \dot{x}_2 &= p_1x_1 - (p_2 + p_3)x_2 + p_4x_3, \\ \dot{x}_3 &= p_3x_2 - p_4x_3, \end{aligned} \quad (6.1)$$

with $\mathbf{x}(t_0) = (1, 0, 0)$, $\mathbf{p} \in P = [0, 10]^2 \times [10, 50]^2$, and $t \in [0, 0.5]$. It can be shown that the solution must satisfy $\mathbf{x}(t, \mathbf{p}) \in [0, 1]^3$ for all $(t, \mathbf{p}) \in I \times P$. The parameter estimation problem is to find the values of $\mathbf{p} = (p_1, \dots, p_4)$ that minimize a sum-of-squared-errors objective function h using experimental data from [11, Example 2]. To study the empirical convergence behavior of the RAD and RPD methods for this problem, we constructed a

nested sequence of intervals $\hat{P} \in \mathbb{I}P$ converging to the global minimum and plotted the relaxation error $\min_{\mathbf{p} \in \hat{P}} h(\mathbf{p}) - \min_{\mathbf{p} \in \hat{P}} h^{cv}(\hat{P}_{\mathbf{p}})$ for both methods as a function of $w(\hat{P})$. On log-log axes, we refer to the steepest slope of a line bounding this curve from above as the *empirical convergence order* of the method. To investigate the effect of t on the convergence behavior, we repeated these calculations for two modified problems where t_f is shortened from 0.5 to 0.3, and then to 0.1, omitting later time points from the sum-of-squared-errors objective h as needed.

For both RAD and RPD, state bounds were provided using Harrison's method. Moreover, before calculating h^{cv} , the state relaxations were first intersected with the state bounds to produce the best possible enclosure; i.e., $X^C(t, \hat{P}_{\mathbf{p}}) := X^C(t, \hat{P}_{\mathbf{p}}) \cap X^B(t, \hat{P})$, $\forall \mathbf{p} \in \hat{P}$. We expect the state bounds to be tighter than the state relaxations in two situations. First, since Harrison's bounds have $w(X^B(t, \hat{P})) \sim O(w(\hat{P}))$, while both RAD and RPD have $w(X^C(t, \hat{P}_{\mathbf{p}})) \sim O(w(\hat{P})^2)$, $\forall \mathbf{p} \in \hat{P}$, Harrison's bounds may be expected to be tighter for large $w(\hat{P})$. More specifically, there is a *critical diameter* $w_{\text{crit}}(t)$ (possibly infinite) such that $w(X^B(t, \hat{P})) \leq w(X^C(t, \hat{P}_{\mathbf{p}}))$ for all $w(\hat{P}) \geq w_{\text{crit}}(t)$. Second, the convergence-order prefactor for Harrison's method satisfies the improved bound established in Corollary 4.13, while the RAD relaxations obey the simple prefactor bound in Theorem 5.19, which grows exponentially with time. Thus, Harrison's bounds may be significantly tighter than RAD relaxations for large t . Indeed, if the RAD prefactor bound increases exponentially faster than that of Harrison's method, then $w_{\text{crit}}(t)$ may decrease exponentially with time. In contrast, this will not occur for the RPD method, since RPD also satisfies an improved prefactor bound as per Corollary 5.26.

Figure 6.1 shows that the relaxation error converges as $w(\hat{P}) \rightarrow 0$ using both RAD and RPD. However, for each fixed $w(\hat{P})$, the errors increase with increasing t_f . With $t_f = 0.1$, Figure 6.1 shows second-order empirical convergence for both methods, as expected. However, with $t_f = 0.5$, the empirical convergence order of RAD is reduced to first-order. Of course, RAD must exhibit second-order convergence for small enough $w(\hat{P})$ by Theorem 5.19. The first-order trend in Figure 6.1 occurs because the state bounds are tighter than the RAD relaxations for all $\hat{P}$ at $t_f = 0.5$ (i.e., $w(\hat{P}) \geq w_{\text{crit}}(t_f)$), and Harrison's bounds have first-order convergence in diameter. As discussed above, Harrison's bounds dominate in this case due to a smaller convergence prefactor, which in turn results from a more modest growth of the prefactor with time. On the other hand, the RPD method demonstrates second-order convergence at all times shown because its prefactor also grows more slowly than that of RAD, as per Corollary 5.26. Thus, although RAD and RPD have the same pointwise convergence order, their behaviors differ in consequential ways. Indeed, this example shows that $w_{\text{crit}}(t_f)$ may become so small for RAD relaxations that second-order convergence is never observed in practice. In the context of global dynamic optimization, this implies that RAD will be unable to avoid the cluster problem [10, 67], leading to large computational burden relative to RPD.

7 Conclusion

Convergence behavior of bounds and relaxations is pivotal to the success of deterministic global optimization algorithms. We proved that relaxations generated by relaxation-amplifying dynamics (RAD) [54] and relaxation-preserving dynamics (RPD) [51] both obey second-order convergence bounds. We also illustrated how they can behave very differently from each other in practice, despite both obeying a second-order convergence bound. Nu-

Fig. 6.1 Empirically, the relaxations of the objective function for a test problem using RAD converge in P with order 2 at short integration times ($t \in [0, 0.1]$), but with order less than 1 at longer integration times. Relaxations based on RPD consistently converge in P with order 2.

merically, we have found that relaxations generated using RAD give empirical first-order convergence in some test problems and empirical second-order convergence in others. On the other hand, relaxations generated using RPD give second-order empirical convergence most of the time. For RAD, the convergence-order bound for the state bounds grows more slowly with time than the convergence-order bound for the state relaxations, leading to a critical parameter interval diameter that decreases as time increases. This critical diameter is the locus of intersection of the first- and second-order convergence bounds. For intervals smaller than the critical diameter, the second-order bound is dominant; otherwise the first-order bound is. Because for RAD with Harrison bounds, the critical diameter decreases with time, longer time horizons increase the likelihood that RAD will display empirical first-order convergence even for very small intervals in parameter space. Even without the changeover in empirical convergence between first- and second-order at some critical parameter interval diameter, our analysis predicts that RPD could potentially perform much better, simply based on the potentially much smaller convergence prefactor. It was recently shown that a sufficiently small convergence prefactor can eliminate the cluster problem of global optimization [67].

8 Acknowledgments

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A Supporting lemmas and proofs

A.1 Proof of Lemma 2.2

Proof. If $\mu = 0$, the result is trivial. Now consider $\mu \neq 0$. Define

$$v(s) \equiv \exp(\mu(t_0 - s)) \int_{t_0}^s \mu x(r) dr, \quad \forall s \in I. \quad (\text{A.1})$$

Differentiating gives

$$v'(s) = \mu \exp(\mu(t_0 - s)) \left(x(s) - \int_{t_0}^s \mu x(r) dr \right), \quad \forall s \in I.$$

Since $\mu \neq 0$,

$$\frac{v'(s)}{\mu} = \underbrace{\exp(\mu(t_0 - s))}_{\geq 0} \underbrace{\left(x(s) - \int_{t_0}^s \mu x(r) dr \right)}_{\leq \lambda_0 + \lambda_1(s - t_0)}, \quad \forall s \in I,$$

where the bound on the second term comes from (2.1). Therefore,

$$\frac{v'(s)}{\mu} \leq \exp(\mu(t_0 - s))(\lambda_0 + \lambda_1(s - t_0)), \quad \forall s \in I.$$

Note that $v(t_0) = 0$ and integrate:

$$\begin{aligned} \frac{v(t)}{\mu} &= \int_{t_0}^t \frac{v'(s)}{\mu} ds \leq \int_{t_0}^t \exp(\mu(t_0 - s))(\lambda_0 + \lambda_1(s - t_0)) ds, \\ &= \frac{\lambda_0 \mu + \lambda_1 - \exp(\mu(t_0 - t))(\lambda_0 \mu + \lambda_1 + \lambda_1 \mu(t - t_0))}{\mu^2}, \quad \forall t \in I. \end{aligned}$$

Substitute in the definition for v from (A.1):

$$\exp(\mu(t_0 - t)) \int_{t_0}^t x(s) ds \leq \frac{\lambda_0 \mu + \lambda_1 - \exp(\mu(t_0 - t))(\lambda_0 \mu + \lambda_1 + \lambda_1 \mu(t - t_0))}{\mu^2}, \quad \forall t \in I.$$

Multiply by $\exp(\mu(t - t_0))$:

$$\int_{t_0}^t x(s) ds \leq \frac{(\lambda_0 \mu + \lambda_1) \exp(\mu(t - t_0)) - (\lambda_0 \mu + \lambda_1 + \lambda_1 \mu(t - t_0))}{\mu^2}, \quad \forall t \in I.$$

Differentiate the above inequality to obtain

$$x(t) \leq \left(\lambda_0 + \frac{\lambda_1}{\mu} \right) \exp(\mu(t - t_0)) - \frac{\lambda_1}{\mu}, \quad \forall t \in I.$$

□

A.2 Proof of Theorem 4.14

The following argument follows a similar line of reasoning to [47, Corollary 3.3.6] and [47, Proof of Theorem 3.3.2], but is sufficiently different that we prove it in full.

Proof. Fix any $\hat{P} \in \mathbb{I}P$. Since solutions to (4.13) and (4.14) are assumed to exist,

$$\mathbf{v}(t, \hat{P}), \mathbf{w}(t, \hat{P}), \tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P}) \in D, \quad \forall t \in I.$$

Since, in addition, the intervals in Hypotheses 1 and 2 of Theorem 4.14 are proper,

$$\mathbf{v}(t, \hat{P}) \leq \mathbf{w}(t, \hat{P}) \quad \text{and} \quad \tilde{\mathbf{v}}(t, \hat{P}) \leq \tilde{\mathbf{w}}(t, \hat{P}), \quad \forall t \in I.$$

We need to prove that $\tilde{\mathbf{v}}(t, \hat{P}) \leq \mathbf{v}(t, \hat{P})$ and $\mathbf{w}(t, \hat{P}) \leq \tilde{\mathbf{w}}(t, \hat{P})$, $\forall t \in I$, which holds at t_0 by Hypothesis 1. Suppose (to arrive at a contradiction) $\exists t \in I$ such that either $v_i(t, \hat{P}) < \tilde{v}_i(t, \hat{P})$ or $w_i(t, \hat{P}) > \tilde{w}_i(t, \hat{P})$ for at least one $i \in \{1, \dots, n_x\}$ and define

$$t_1 \equiv \inf\{t \in I : v_i(t, \hat{P}) < \tilde{v}_i(t, \hat{P}) \text{ or } w_i(t, \hat{P}) > \tilde{w}_i(t, \hat{P}), \text{ for at least one } i\}.$$

Applying [47, Lemma 3.3.5] with the definition $\delta(t) \equiv (\tilde{\mathbf{v}}(t, \hat{P}) - \mathbf{v}(t, \hat{P}), \mathbf{w}(t, \hat{P}) - \tilde{\mathbf{w}}(t, \hat{P}))$, we obtain the following fact:

- For any $t_4 \in (t_1, t_f]$, $\varepsilon > 0$, and $\beta \in \mathbb{R}_+$, there exists $j \in \{1, \dots, n_x\}$, an absolutely continuous and non-decreasing function $\rho : [t_1, t_4] \rightarrow \mathbb{R}$, and numbers $t_2, t_3 \in [t_1, t_4]$ with $t_2 < t_3$ such that

$$0 < \rho(t) \leq \varepsilon, \quad \forall t \in [t_1, t_4] \quad \text{and} \quad \dot{\rho}(t) > \beta \rho(t), \quad \text{a.e. } t \in [t_1, t_4], \quad (\text{A.2})$$

$$\tilde{\mathbf{v}}(t, \hat{P}) - \mathbf{1}\rho(t) < \mathbf{v}(t, \hat{P}) \quad \text{and} \quad \mathbf{w}(t, \hat{P}) < \tilde{\mathbf{w}}(t, \hat{P}) + \mathbf{1}\rho(t), \quad \forall t \in [t_2, t_3], \quad (\text{A.3})$$

where $\mathbf{1}$ is a vector with all components equal to 1, and

$$\begin{aligned} v_j(t_2, \hat{P}) &= \tilde{v}_j(t_2, \hat{P}), \quad v_j(t_3, \hat{P}) = \tilde{v}_j(t_3, \hat{P}) - \rho(t_3), \\ \text{and } v_j(t, \hat{P}) &< \tilde{v}_j(t, \hat{P}), \quad \forall t \in (t_2, t_3) \end{aligned} \quad (\text{A.4})$$

$$\begin{aligned} \left(\text{or } w_j(t_2, \hat{P}) &= \tilde{w}_j(t_2, \hat{P}), \quad w_j(t_3, \hat{P}) = \tilde{w}_j(t_3, \hat{P}) + \rho(t_3), \right. \\ \text{and } w_j(t, \hat{P}) &> \tilde{w}_j(t, \hat{P}), \quad \forall t \in (t_2, t_3) \Big). \end{aligned} \quad (\text{A.5})$$

To apply this fact, we choose $\varepsilon > 0$ small enough that

$$K \equiv [\tilde{\mathbf{v}}(t_1, \hat{P}), \tilde{\mathbf{w}}(t_1, \hat{P})] + 2\varepsilon[-\mathbf{1}, \mathbf{1}] \subset D, \quad (\text{A.6})$$

which is possible because D is open and $[\tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P})] \subset D$, $\forall t \in I$, by the existence of a solution to (4.14). Next, we choose $\beta = L$, where L is the larger of the two Lipschitz constants for $\tilde{\mathbf{u}}$ and $\tilde{\mathbf{o}}$ on $I \times \mathbb{I}K \times \mathbb{I}\hat{P}$. Such an L exists by Hypothesis 4 (see also Remark 4.2). Finally, we choose t_4 sufficiently small that

$$[\tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P})] \subset [\tilde{\mathbf{v}}(t_1, \hat{P}), \tilde{\mathbf{w}}(t_1, \hat{P})] + \varepsilon[-\mathbf{1}, \mathbf{1}], \quad \forall t \in (t_1, t_4]. \quad (\text{A.7})$$

Now, suppose (A.4) holds (the proof is analogous if instead (A.5) holds). We know from (A.3) that

$$[\mathbf{v}(t, \hat{P}), \mathbf{w}(t, \hat{P})] \subset [\tilde{\mathbf{v}}(t, \hat{P}) - \rho(t)\mathbf{1}, \tilde{\mathbf{w}}(t, \hat{P}) + \rho(t)\mathbf{1}], \quad \forall t \in [t_2, t_3].$$

By (4.17), (4.18), and the inclusion above, we have

$$\begin{aligned} u_j(t, [\mathbf{v}(t, \hat{P}), \mathbf{w}(t, \hat{P})], \hat{P}) &\geq \tilde{u}_j(t, [\tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P})], \hat{P}), \\ &\geq \tilde{u}_j(t, [\tilde{\mathbf{v}}(t, \hat{P}) - \rho(t)\mathbf{1}, \tilde{\mathbf{w}}(t, \hat{P}) + \rho(t)\mathbf{1}], \hat{P}), \quad \text{a.e. } t \in [t_2, t_3]. \end{aligned} \quad (\text{A.8})$$

Above, $[\tilde{\mathbf{v}}(t, \hat{P}) - \rho(t)\mathbf{1}, \tilde{\mathbf{w}}(t, \hat{P}) + \rho(t)\mathbf{1}]$ is guaranteed to be a subset of K , and hence of D , by (A.2), (A.7), and (A.6). Thus, Lipschitz continuity of $\tilde{u}_j$ on $I \times \mathbb{I}K \times \mathbb{I}\hat{P}$ gives

$$\tilde{u}_j(t, [\tilde{\mathbf{v}}(t, \hat{P}) - \rho(t)\mathbf{1}, \tilde{\mathbf{w}}(t, \hat{P}) + \rho(t)\mathbf{1}], \hat{P}) \geq \tilde{u}_j(t, [\tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P})], \hat{P}) - L\rho(t). \quad (\text{A.9})$$

Combining (A.8) and (A.9),

$$u_j(t, [\mathbf{v}(t, \hat{P}), \mathbf{w}(t, \hat{P})], \hat{P}) \geq \tilde{u}_j(t, [\tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P})], \hat{P}) - L\rho(t), \quad \text{a.e. } t \in [t_2, t_3].$$

Adding $\dot{\rho}(t)$ to both sides,

$$\begin{aligned} u_j(t, [\mathbf{v}(t, \hat{P}), \mathbf{w}(t, \hat{P})], \hat{P}) + \dot{\rho}(t) &\geq \tilde{u}_j(t, [\tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P})], \hat{P}) - L\rho(t) + \dot{\rho}(t), \\ &> \tilde{u}_j(t, [\tilde{\mathbf{v}}(t, \hat{P}), \tilde{\mathbf{w}}(t, \hat{P})], \hat{P}), \quad \text{a.e. } t \in [t_2, t_3], \end{aligned}$$

where the second inequality follows from (A.2) with $\beta = L$. By [47, Theorem 3.3.3], this implies that $(\tilde{v}_j(\cdot, \hat{P}) - v_j(\cdot, \hat{P}) - \rho)$ is non-increasing on $[t_2, t_3]$, so that

$$\tilde{v}_j(t_3, \hat{P}) - v_j(t_3, \hat{P}) - \rho(t_3) \leq \tilde{v}_j(t_2, \hat{P}) - v_j(t_2, \hat{P}) - \rho(t_2).$$

But, by (A.4), this implies that $0 \leq -\rho(t_2)$, which contradicts (A.2). $\square$

A.3 (1,2)-Convergence of natural McCormick extensions

In this section, we establish the $(1, 2)$ -convergence of natural McCormick extensions [47, Definition 2.4.31] as required by Assumption 5.17. To begin, we show that $(1, 2)$ -convergence is composable.

Theorem A.1. *Let $D_x \subset \mathbb{R}^n$ and let $\mathcal{F} : \mathbb{M}D_x \rightarrow \mathbb{M}\mathbb{R}^m$ have the form $\mathcal{F}(\mathcal{X}) = (F^B(X^B), F^C(\mathcal{X}))$, $\forall \mathcal{X} = (X^B, X^C) \in \mathbb{M}D_x$. Moreover, let $F^B(X^B) \subset D_y \subset \mathbb{R}^m$ for all $X^B \in \mathbb{I}D_x$, and let $\mathcal{G} : \mathbb{M}D_y \rightarrow \mathbb{M}\mathbb{R}^q$ have the form $\mathcal{G}(\mathcal{Y}) = (G^B(Y^B), G^C(\mathcal{Y}))$. If $\mathcal{F}$ and $\mathcal{G}$ have $(1, 2)$ -convergence on $\mathbb{M}D_x$ and $\mathbb{M}D_y$, respectively, then $\mathcal{G} \circ \mathcal{F}$ has $(1, 2)$ -convergence on $\mathbb{M}D_x$.*

Proof. Applying $(1, 2)$ -convergence for $\mathcal{G}$ and $\mathcal{F}$ sequentially, we obtain for any $\mathcal{X} \in \mathbb{M}D_x$,

$$w(G^B \circ F^B(X^B)) \leq \tau_{BB}^G w(F^B(X^B)) \quad (\text{A.10})$$

$$\leq \tau_{BB}^G \tau_{BB}^F w(X^B), \quad (\text{A.11})$$

$$w(G^C \circ \mathcal{F}(\mathcal{X})) \leq \tau_{CC}^G w(F^C(\mathcal{X})) + \tau_{CB}^G w(F^B(X^B))^2, \quad (\text{A.12})$$

$$\leq \tau_{CC}^G (\tau_{CC}^F w(X^C) + \tau_{CB}^F w(X^B)^2) + \tau_{CB}^G (\tau_{BB}^F w(X^B))^2, \quad (\text{A.13})$$

$$\leq \tau_{CC}^G \tau_{CC}^F w(X^C) + (\tau_{CC}^G \tau_{CB}^F + \tau_{CB}^G (\tau_{BB}^F)^2) w(X^B)^2. \quad (\text{A.14})$$

$\square$

Recall that a function is *factorable* if it can be written as a finite recursive sequence of basic operations including addition, multiplication, and composition with univariate functions from a standard library (e.g., $\frac{1}{x}$, e^x , x^n , etc.) Natural McCormick extensions are constructed for such functions by recursively applying simple relaxation rules for each basic operation in this sequence (see [47] for a precise definition). Specifically, these rules are relaxation functions for the basic operations. In light of Theorem A.1, it follows that, in order to establish $(1, 2)$ -convergence of natural McCormick extensions, it suffices to establish $(1, 2)$ -convergence of the relaxation functions for addition, multiplication, and univariate composition.

A.3.1 Addition

Definition A.2. McCormick addition $+$: $\mathbb{MR} \times \mathbb{MR} \rightarrow \mathbb{MR}$ is defined by

$$+(\mathcal{X}, \mathcal{Y}) = \mathcal{X} + \mathcal{Y} = (X^B + Y^B, (X^B \cap X^C) + (Y^B \cap Y^C)). \quad (\text{A.15})$$

Lemma A.3. McCormick addition has (1,2)-convergence on $\mathbb{MR} \times \mathbb{MR}$.

Proof. Choose any $(\mathcal{X}, \mathcal{Y}) \in \mathbb{MR} \times \mathbb{MR}$ and let $\mathcal{Z} = +(\mathcal{X}, \mathcal{Y})$. Then,

$$w(Z^B) = w(X^B) + w(Y^B) \leq 2 \max(w(X^B), w(Y^B)) = 2w(X^B \times Y^B) \quad (\text{A.16})$$

and

$$\begin{aligned} w(Z^C) &= w(X^B \cap X^C) + w(Y^B \cap Y^C) \leq w(X^C) + w(Y^C), \\ &\leq 2 \max(w(X^C), w(Y^C)), \\ &= 2w(X^C \times Y^C). \end{aligned} \quad (\text{A.17})$$

□

A.3.2 Multiplication

The following definition of McCormick's multiplication rule is nonstandard but facilitates our convergence arguments. It is shown in [47, §2.4.2] that this definition is equivalent except that the Cut function is not applied to $\mathcal{X}$ and $\mathcal{Y}$ in McCormick's original work [30].

Definition A.4. McCormick multiplication $\times$: $\mathbb{MR} \times \mathbb{MR} \rightarrow \mathbb{MR}$ is defined by

$$\times(\mathcal{X}, \mathcal{Y}) = \mathcal{X}\mathcal{Y} = (X^B Y^B, [z^{cv}, z^{cc}]),$$

where $X^B Y^B$ denotes standard interval multiplication [33] and

$$\begin{aligned} z^{cv} &= \max \left(\left[y^L \bar{X}^C + x^L \bar{Y}^C - x^L y^L \right]^L, \left[y^U \bar{X}^C + x^U \bar{Y}^C - x^U y^U \right]^L \right), \\ z^{cc} &= \min \left(\left[y^L \bar{X}^C + x^U \bar{Y}^C - y^L x^U \right]^U, \left[y^U \bar{X}^C + x^L \bar{Y}^C - y^U x^L \right]^U \right). \end{aligned}$$

Above, $\bar{X} = \text{Cut}(\mathcal{X})$, $\bar{Y} = \text{Cut}(\mathcal{Y})$, and the notations $[\cdot]^L$ and $[\cdot]^U$ refer to the lower and upper bounds of the interval-valued quantity in brackets, respectively.

Lemma A.5. McCormick multiplication is (1,2)-convergent on $\mathbb{MK}$ for any compact $K \subset \mathbb{R} \times \mathbb{R}$.

Proof. Choose any compact $K \subset \mathbb{R} \times \mathbb{R}$. The existence of $\tau_{BB} \geq 0$ such that $w(X^B Y^B) \leq \tau_{BB} w(X^B \times Y^B)$ for all $(X^B, Y^B) \in \mathbb{MK}$ is well known [33]. Choose any $(\mathcal{X}, \mathcal{Y}) \in \mathbb{MK}$ and let $\mathcal{Z} = \times(\mathcal{X}, \mathcal{Y})$. We have $w(Z^C) = z^{cc} - z^{cv}$. There are four cases to consider. For the first case,

$$w(Z^C) = \left[y^L \bar{X}^C + x^U \bar{Y}^C - y^L x^U \right]^U - \left[y^L \bar{X}^C + x^L \bar{Y}^C - x^L y^L \right]^L.$$

Writing $r^U = w(R) + r^L$ for $R = [y^L \bar{X}^C + x^U \bar{Y}^C - y^L x^U]$ on the right,

$$\begin{aligned} w(Z^C) &= w \left(\left[y^L \bar{X}^C + x^U \bar{Y}^C - y^L x^U \right] \right) \\ &\quad + \left[y^L \bar{X}^C + x^U \bar{Y}^C - y^L x^U \right]^L - \left[y^L \bar{X}^C + x^L \bar{Y}^C - x^L y^L \right]^L, \\ &= w \left(\left[y^L \bar{X}^C + x^U \bar{Y}^C \right] \right) \\ &\quad + \left[y^L \bar{X}^C \right]^L + \left[x^U \bar{Y}^C \right]^L - y^L x^U - \left[y^L \bar{X}^C \right]^L - \left[x^L \bar{Y}^C \right]^L + x^L y^L, \\ &\leq |y^L| w(\bar{X}^C) + |x^U| w(\bar{Y}^C) + \left[x^U \bar{Y}^C \right]^L - y^L x^U - \left[x^L \bar{Y}^C \right]^L + x^L y^L, \\ &= |y^L| w(\bar{X}^C) + |x^U| w(\bar{Y}^C) + \left[x^U \bar{Y}^C - y^L x^U \right]^L - \left[x^L \bar{Y}^C - x^L y^L \right]^L, \\ &\leq |y^L| w(X^C) + |x^U| w(Y^C) + \left[x^U (\bar{Y}^C - y^L) \right]^L - \left[x^L (\bar{Y}^C - y^L) \right]^L. \end{aligned}$$

Noting that $\bar{Y}^C \subset Y^B$, it follows that every element of $\bar{Y}^C - y^L$ is nonnegative and bounded above by $w(Y^B)$. Thus, $\exists q_1, q_2 \in (\bar{Y}^C - y^L)$, both bounded between 0 and $w(Y^B)$, satisfying

$$\begin{aligned} w(Z^C) &\leq |y^L|w(X^C) + |x^U|w(Y^C) + x^U q_1 - x^L q_2, \\ &= |y^L|w(X^C) + |x^U|w(Y^C) + (x^L + w(X^B))q_1 - x^L q_2, \\ &= |y^L|w(X^C) + |x^U|w(Y^C) + x^L(q_1 - q_2) + w(X^B)q_1, \\ &\leq |y^L|w(X^C) + |x^U|w(Y^C) + |x^L|w(\bar{Y}^C - y^L) + w(X^B)w(Y^B), \\ &\leq |y^L|w(X^C) + (|x^U| + |x^L|)w(Y^C) + w(X^B)w(Y^B), \\ &\leq (|y^L| + |x^U| + |x^L|) \max(w(X^C), w(Y^C)) + \max(w(X^B)^2, w(Y^B)^2), \\ &\leq 3 \max\{|x^L|, |x^U|, |y^L|\} w(X^C \times Y^C) + w(X^B \times Y^B)^2, \\ &\leq 3(\max_{x \in K} |x|) w(X^C \times Y^C) + w(X^B \times Y^B)^2. \end{aligned}$$

Similar arguments hold in the remaining three cases. $\square$

A.3.3 Univariate Functions

Let $\mathcal{L}$ be a library of univariate functions $u : B \subset \mathbb{R} \rightarrow \mathbb{R}$ that are permissible in the definition of a factorable function. The construction of the natural McCormick extension requires the following assumption.

Assumption A.6. For every $u : B \subset \mathbb{R} \rightarrow \mathbb{R}$ in $\mathcal{L}$, the following objects are available:

1. An inclusion function $U^B : \mathbb{B} \rightarrow \mathbb{B}$.
2. A scheme of estimators $(u^{cv}, u^{cc}) : \mathbb{B} \times B \rightarrow \mathbb{R} \times \mathbb{R}$.
3. Functions $x^{\min}, x^{\max} : \mathbb{B} \rightarrow \mathbb{R}$ such that $x^{\min}(X)$ and $x^{\max}(X)$ are a minimum of $u^{cv}(X, \cdot)$ and a maximum of $u^{cc}(X, \cdot)$ on X , respectively.

Definition A.7. For every $u : B \subset \mathbb{R} \rightarrow \mathbb{R}$ in $\mathcal{L}$, the McCormick univariate composition rule $\mathcal{U} : \mathbb{M}B \rightarrow \mathbb{M}\mathbb{R}$ is defined by

$$\mathcal{U}(\mathcal{X}) = (U^B(X^B), [u^{cv}(X^B, \text{mid}(x^{cv}, x^{cc}, x^{\min}(X^B))), u^{cc}(X^B, \text{mid}(x^{cv}, x^{cc}, x^{\max}(X^B)))]),$$

where the mid function selects the middle value of its arguments.

Note that $\mathcal{X} \in \mathbb{M}B$ implies that either $x^{cv} \in X^B$ or $x^{cc} \in X^B$, or both. By definition, $x^{\min}(X^B)$ and $x^{\max}(X^B)$ are both also in X^B , so that, in both uses of the mid function above, at least two of the three arguments lie in X^B . Thus, mid chooses an element of X^B , and hence of B , so that $\mathcal{U}(\mathcal{X})$ is defined.

The following assumptions are required to establish (1,2)-convergence of $\mathcal{U}$ and are standard in the convergence literature (see Theorem 8 in [4]).

Assumption A.8. For every $u : B \subset \mathbb{R} \rightarrow \mathbb{R}$ in $\mathcal{L}$ and any compact $K \subset B$:

1. u is Lipschitz continuous on K .
2. The inclusion function U^B converges in diameter in K with order at least one.
3. The scheme of estimators (u^{cv}, u^{cc}) converges pointwise in K with order at least 2.

Lemma A.9. $\mathcal{U} : \mathbb{M}B \rightarrow \mathbb{M}\mathbb{R}$ is (1,2)-convergent on $\mathbb{M}K$ for any compact $K \subset B$.

Proof. Choose any compact $K \subset B$. By Assumption A.8, there exists $\tau_{BB} \geq 0$ such that $w(U^B(X^B)) \leq \tau_{BB}w(X^B)$, $\forall X^B \in \mathbb{B}K$. Let $L \in \mathbb{R}_+$ be a Lipschitz constant for u on K and let $\tau \in \mathbb{R}_+$ be the pointwise convergence-order prefactor for $\mathcal{U}$ in K as per Assumption A.8. Choose any $\mathcal{X} \in \mathbb{M}K$. Since both of the points $\text{mid}(x^{cv}, x^{cc}, x^{\min}(X^B))$ and $\text{mid}(x^{cv}, x^{cc}, x^{\max}(X^B))$ are in X^C , it follows that

$$|\text{mid}(x^{cv}, x^{cc}, x^{\max}(X^B)) - \text{mid}(x^{cv}, x^{cc}, x^{\min}(X^B))| \leq w(X^C). \quad (\text{A.18})$$

Then,

$$\begin{aligned} w(U^C(\mathcal{X})) &= |u^{cc}(X^B, \text{mid}(x^{cv}, x^{cc}, x^{\max}(X^B))) - u^{cv}(X^B, \text{mid}(x^{cv}, x^{cc}, x^{\min}(X^B)))|, \\ &\leq |u^{cc}(X^B, \text{mid}(x^{cv}, x^{cc}, x^{\max}(X^B))) - u(\text{mid}(x^{cv}, x^{cc}, x^{\max}(X^B)))| \\ &\quad + |u(\text{mid}(x^{cv}, x^{cc}, x^{\max}(X^B))) - u(\text{mid}(x^{cv}, x^{cc}, x^{\min}(X^B)))| \\ &\quad + |u(X^B, \text{mid}(x^{cv}, x^{cc}, x^{\min}(X^B))) - u^{cv}(X^B, \text{mid}(x^{cv}, x^{cc}, x^{\min}(X^B)))|, \\ &\leq \tau w(X^B)^2 + Lw(X^C) + \tau w(X^B)^2. \end{aligned} \quad (\text{A.19})$$

$\square$

Combining the results of §A.3.1-A.3.3 with the Composition Theorem A.1, it is straightforward to show that the natural McCormick extension $\mathcal{F} : \mathbb{MD} \rightarrow \mathbb{MR}^m$ of a factorable function $\mathbf{f} : D \rightarrow \mathbb{R}^m$ has $(1, 2)$ -convergence on any compact $K \subset D$, as required by Assumption 5.17.

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