J Glob Optim (2011) 51:569–606
DOI 10.1007/s10898-011-9664-7

Generalized McCormick relaxations

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Received: 21 September 2009 / Accepted: 24 January 2011 / Published online: 24 February 2011

Abstract Convex and concave relaxations are used extensively in global optimization algorithms. Among the various techniques available for generating relaxations of a given function, McCormick's relaxations are attractive due to the recursive nature of their definition, which affords wide applicability and easy implementation computationally. Furthermore, these relaxations are typically stronger than those resulting from convexification or linearization procedures. This article leverages the recursive nature of McCormick's relaxations to define a generalized form which both affords a new framework within which to analyze the properties of McCormick's relaxations, and extends the applicability of McCormick's technique to challenging open problems in global optimization. Specifically, relaxations of the parametric solutions of ordinary differential equations are considered in detail, and prospects for relaxations of the parametric solutions of nonlinear algebraic equations are discussed. For the case of ODEs, a complete computational procedure for evaluating convex and concave relaxations of the parametric solutions is described. Through McCormick's composition rule, these relaxations may be used to construct relaxations for very general optimal control problems.

Keywords Convex relaxations · Global optimization · Optimal control

Electronic supplementary material The online version of this article (doi:10.1007/s10898-011-9664-7) contains supplementary material, which is available to authorized users.

This paper is based on work funded by the National Science Foundation under grants CTS-0521962 and CBET-0933095 and by the Chevron University Partnership Program (UPP) with the MIT Energy Initiative.

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Mathematics Subject Classification (2000) 49M20 · 90C26

1 Introduction

Many deterministic techniques for the global solution of nonconvex optimization problems require convex and/or concave relaxations of the participating functions [1,2,12,17,32]. For programs where these functions are known in closed form, there are well known techniques for constructing such relaxations [2,17,32]. However, programs arise frequently in applications where the participating functions are not known explicitly, and their evaluation includes the numerical solution of a system of equations. Among these are programs where it is desired to optimize the performance of a physical system whose state is governed by a set of implicit nonlinear algebraic equations, ordinary differential equations (ODEs), partial differential equations (PDEs) or differential-algebraic equations (DAEs). In each case, the problem can in principle be approximated as a standard nonlinear program (NLP) in which all functions are known explicitly through a discretization scheme with the addition of many variables and constraints [4,6,8,19]. However, this approach increases the dimension of the search space dramatically, so that such reformulations typically exceed the capabilities of global optimization routines for nonconvex programs. At the same time, global optimization is nearly always warranted because there is no way of determining whether or not the parametric solution of a system of implicit algebraic and/or differential equations will be convex, concave or neither. Unfortunately, the situation is most frequently the latter [16].

Without discretization and reduction to a NLP, it is not immediately clear how convex and concave relaxations can be constructed for programs dependent on the solution of an embedded system of equations because the participating functions are not known explicitly. In particular, the dependence of the solutions of the embedded equations (state variables) on the optimization variables is unknown. When the objective and constraints are described by algorithms with a finite number of iterations, known *a priori*, as would result from composition with a linear or otherwise explicit system of algebraic equations, it has been shown that McCormick's relaxation technique can be used recursively to construct the desired convex and concave relaxations [18]. In the case of an implicit nonlinear system of equations, McCormick's composition rule and factorable representation provide a means for constructing the desired convex and concave relaxations of the objective and constraint functions, provided that convex and concave relaxations of the state variables with respect to the optimization variables are available. In this work we extend McCormick's relaxation technique to enable the relaxation of the solutions of implicit nonlinear equations with respect to some parametric dependence (the optimization variables).

Toward this end, generalized McCormick relaxations are introduced. McCormick's relaxation technique is first formalized mathematically (Sect. 3) and a number of useful properties are established. Next, this formulation is generalized in order to make various aspects of the construction of McCormick's relaxations transparent, and to allow the recursive definition of these relaxations to be treated directly (Sect. 4). This generalization has two important implications. First, standard McCormick relaxations can be treated as a special case, which allows many properties of McCormick's relaxations to be proven rigorously, including very strong convergence results which are not apparent through their standard definition. Second, the generalized relaxations provide a powerful framework for developing McCormick-type relaxations for the parametric solutions of equations. Systems of ODEs are considered in detail in Sect. 7 and it is shown that by taking generalized McCormick relaxations of the ODE right-hand side functions, it is possible to construct an auxiliary system of ODEs with solutions which are convex and concave relaxations of the parametric solution of the original ODEs. Furthermore, a complete computational procedure is described for automatically evaluating these relaxations. Finally, it is shown that these relaxations satisfy a number of convergence properties as the parameter space is partitioned, so that they are suitable for implementation in spatial branch-and-bound algorithms [11]. An analogous relaxation theory is discussed briefly for nonlinear algebraic systems in Sect. 6, though a complete procedure for generating relaxations of the parametric solutions remains an open challenge.

2 Preliminaries

The methods in this paper rely heavily on interval analysis. Unless specified otherwise, the term interval is intended to mean a closed, bounded interval in $\mathbb{R}$ or interval vector in $\mathbb{R}^n$. The space of closed, bounded real intervals is denoted by $\mathbb{IR}$ and the space of n-dimensional interval vectors by $\mathbb{IR}^n$. For any $X \subset \mathbb{R}^n$, the set of all interval subsets of X is denoted by $IX \subset \mathbb{IR}^n$. The following definitions and results are adopted from Moore [20].

Definition 1 Let $X \equiv [\mathbf{x}^L, \mathbf{x}^U] \in \mathbb{IR}^n$. Define the *width* of X by $w(X) = \max_i \left(x_i^U - x_i^L\right)$.

Definition 2 The *Hausdorff metric*, denoted d_H, is defined for any $\hat{X}, \tilde{X} \in \mathbb{IR}^n$ by

$$d_H(\hat{X}, \tilde{X}) = \max_i \left(\max\left(|\hat{x}_i^L - \tilde{x}_i^L|, |\hat{x}_i^U - \tilde{x}_i^U|\right)\right).$$

Definition 3 Let $X \subset \mathbb{R}^n$. An interval-valued function $G : IX \to \mathbb{IR}$ is called an *interval extension* of a real-valued function $g : X \to \mathbb{R}$ on X if

$$G([x_1, x_1], \ldots, [x_n, x_n]) = [g(x_1, \ldots, x_n), g(x_1, \ldots, x_n)],$$

for any degenerate interval vector in IX. G is *inclusion monotonic* on X if, for any two intervals $\hat{X}, \tilde{X} \in IX$, $\hat{X} \subset \tilde{X}$ implies that $G(\hat{X}) \subset G(\tilde{X})$.

Theorem 1 *Let $X \subset \mathbb{R}^n$. If G is an inclusion monotonic interval extension of g on X, then $g(\mathbf{x}) \in G(\hat{X}), \forall \mathbf{x} \in \hat{X}$, for every $\hat{X} \in IX$.*

Proof See Moore [20], Theorem 3.1. □

Definition 4 Let $X \subset \mathbb{R}^n$. An interval-valued function $G : IX \to \mathbb{IR}$ is called *Lipschitz* on X if there exists $L \in \mathbb{R}_+$ such that

$$w(G(\hat{X})) \leq Lw(\hat{X}), \quad \forall \hat{X} \in IX.$$

G is said to be *Lipschitz in the Hausdorff metric* on X if there exists $L_H \in \mathbb{R}_+$ such that

$$d_H(G(\hat{X}), G(\tilde{X})) \leq L_H d_H(\hat{X}, \tilde{X}), \quad \forall \hat{X}, \tilde{X} \in IX.$$

Theorem 2 *Consider two sets $X_1, X_2 \subset \mathbb{R}$ and two univariate functions $g_1 : X_1 \to X_2$ and $g_2 : X_2 \to Y \subset \mathbb{R}$. If G_1 is an inclusion monotonic and Lipschitz interval extension of g_1 on X_1, G_2 is an inclusion monotonic and Lipschitz interval extension of g_2 on X_2, and $G_1(X_1) \subset X_2$, then $G_2 \circ G_1$ is an inclusion monotonic and Lipschitz interval extension of $g_2 \circ g_1$ on X_1.*

Proof See Moore [20], Sect. 4.1. □

This work involves the construction of convex and concave relaxations. These are defined below, followed by some results concerning convex and concave functions.

Definition 5 Let X be a convex set in $\mathbb{R}^n$ and $g : X \to \mathbb{R}$. A function $g^c : X \to \mathbb{R}$ is a *convex relaxation*, or *convex underestimator*, of g on X if g^c is convex on X and $g^c(\mathbf{x}) \leq g(\mathbf{x}), \forall \mathbf{x} \in X$. Similarly, a function $g^C : X \to \mathbb{R}$ is a *concave relaxation*, or *concave overestimator*, of g on X if g^C is concave on X and $g^C(\mathbf{x}) \geq g(\mathbf{x}), \forall \mathbf{x} \in X$.

Definition 6 Let X be a convex set in $\mathbb{R}^n$ and $g : X \to \mathbb{R}$. The *convex envelope* of g on X is defined point-wise, for every $\mathbf{x} \in X$, by $g^c_{\text{env}}(\mathbf{x}) = \sup g^c(\mathbf{x})$, where the supremum is taken over every convex relaxation of g on X. Similarly, the *concave envelope* of g on X is defined, for every $\mathbf{x} \in X$, by $g^C_{\text{env}}(\mathbf{x}) = \inf g^C(\mathbf{x})$, where the infimum is taken over every concave relaxation of g on X.

Proposition 1 *Suppose g is a convex function on an interval $[x^L, x^U] \subset \mathbb{R}$ and g attains its infimum at $x^{\min} \in [x^L, x^U]$. Then g is monotone decreasing on $[x^L, x^{\min}]$ and monotone increasing on $[x^{\min}, x^U]$. Similarly, if g is concave on $[x^L, x^U]$ and attains its supremum at $x^{\max} \in [x^L, x^U]$, then g is monotone increasing on $[x^L, x^{\max}]$ and monotone decreasing on $[x^{\max}, x^U]$.*

Proof The proof is elementary. □

McCormick's relaxation technique makes use of the function $\text{mid}(x, y, z)$, defined for any $x, y, z \in \mathbb{R}$ as the middle value of its arguments. For any $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{R}^n$, $\text{mid}(\mathbf{x}, \mathbf{y}, \mathbf{z})$ denotes the vector with elements $\text{mid}(x_i, y_i, z_i)$, $i = 1, \ldots, n$.

3 Standard McCormick relaxations

In previous literature, the presentation of McCormick's relaxation technique has always been algorithmic in nature. However, here we are concerned with establishing several important properties of McCormick's relaxations, including convexity/concavity properties with respect to certain arguments, which are well established, but also nontrivial continuity properties, Lipschitz conditions and convergence properties which are not obviously true. All of these properties will be essential for the development of relaxations for the parametric solutions of ODEs and other applications in Sects. 5, 6 and 7. Since many of these properties are not required by standard applications, they have not been established previously, nor has care been taken to formalize McCormick's technique in a manner which guarantees them. For this reason, this section contains a detailed mathematical development of McCormick's relaxation technique. Throughout, care is taken to define a minimal set of assumptions on the basic elements, the bounding operations and relaxations for univariate intrinsic functions (Definition 7), such that the resulting relaxations have the desired properties. It is found that the necessary properties are either true or can be made so by minor modifications.

Let $S \subset \mathbb{R}^{n_p}$, let $P \equiv [\mathbf{p}^L, \mathbf{p}^U] \subset S$, and let $\mathscr{F} : S \to \mathbb{R}$. McCormick's relaxations (or standard McCormick relaxations) are defined for *factorable* functions, defined as follows.

Definition 7 (Univariate intrinsic function) A function $U : B \to \mathbb{R}$, $B \subset \mathbb{R}$, is called a *univariate intrinsic function* if, for any interval $V \subset B$, an inclusion monotonic interval extension of U on V, a convex relaxation of U on V and a concave relaxation of U on V are known and can be evaluated computationally.

Definition 8 (Factorable function) A function $\mathscr{F} : S \to \mathbb{R}$ is *factorable* if it can be expressed in terms of a finite number of factors $v_1, \ldots, v_m$ such that, given $\mathbf{p} \in S$, $v_i = p_i$ for $i = 1, \ldots, n_p$, and v_k is defined for each $n_p < k \leq m$ as either

(a) $v_k = v_i + v_j$, with $i, j < k$, or
(b) $v_k = v_i v_j$, with $i, j < k$, or
(c) $v_k = U_k(v_i)$, with $i < k$, where $U_k : B_k \to \mathbb{R}$ is a univariate intrinsic function,

and $\mathscr{F}(\mathbf{p}) = v_m(\mathbf{p})$.

Nearly every function that can be represented finitely on a computer is factorable. For any such function, convex and concave relaxations can be obtained by McCormick's relaxation technique. The method associates with each factor v_k the quantities v_k^L, v_k^U, v_k^c and v_k^C (shorthand $v_k^{L/U/c/C}$), which are, respectively, a lower bound on P, an upper bound on P, a convex underestimator on P and a concave overestimator on P. This is done for each factor, and eventually for $\mathscr{F}$ itself, by the following procedure.

Definition 9 (Standard McCormick relaxations $\mathscr{U}$ and $\mathscr{O}$) Denote the McCormick relaxations of $\mathscr{F}$ on $P = [\mathbf{p}^L, \mathbf{p}^U] \subset S$ by the functions $\mathscr{U}, \mathscr{O} : P \to \mathbb{R}$, where for each $\mathbf{p} \in P$, $\mathscr{U}(\mathbf{p})$ and $\mathscr{O}(\mathbf{p})$ are defined by the following procedure:

1. Set $v_i^L = p_i^L$ and $v_i^U = p_i^U$, for all $i = 1, \ldots, n_p$ (denote $V_i \equiv [v_i^L, v_i^U]$).
2. Set $v_i^c = v_i^C = p_i$, for all $i = 1, \ldots, n_p$.
3. Set $k = n_p + 1$.
4. Compute v_k^L, v_k^U and $V_k \equiv [v_k^L, v_k^U]$ according to the definition of v_k, as either

   (a) $v_k^L = v_i^L + v_j^L$ and $v_k^U = v_i^U + v_j^U$, with $i, j < k$, or
   (b) $v_k^L = \min\left(v_i^L v_j^L, v_i^L v_j^U, v_i^U v_j^L, v_i^U v_j^U\right)$ and
   $v_k^U = \max\left(v_i^L v_j^L, v_i^L v_j^U, v_i^U v_j^L, v_i^U v_j^U\right)$, with $i, j < k$, or
   (c) $v_k^L = U_k^L(v_i^L, v_i^U)$ and $v_k^U = U_k^U(v_i^L, v_i^U)$, with $i < k$, where $U_k^{L/U} : \{y, z \in B_k : [y, z] \subset B_k\} \to \mathbb{R}$ form an inclusion monotonic interval extension of U_k on V_i.

5. Compute $\bar{v}_k^c$ and $\bar{v}_k^C$ according to the definition of v_k, as either

   (a) $\bar{v}_k^c = v_i^c + v_j^c$ and $\bar{v}_k^C = v_i^C + v_j^C$, with $i, j < k$, or
   (b) $\bar{v}_k^c = \max(\alpha_i + \alpha_j - v_j^L v_i^L, \beta_i + \beta_j - v_j^U v_i^U)$, and $\bar{v}_k^C = \min(\gamma_i + \gamma_j - v_j^L v_i^U, \delta_i + \delta_j - v_j^U v_i^L)$, where

$$\alpha_i = \min(v_j^L v_i^c, v_j^L v_i^C), \quad \alpha_j = \min(v_i^L v_j^c, v_i^L v_j^C),$$
$$\beta_i = \min(v_j^U v_i^c, v_j^U v_i^C), \quad \beta_j = \min(v_i^U v_j^c, v_i^U v_j^C),$$
$$\gamma_i = \max(v_j^L v_i^c, v_j^L v_i^C), \quad \gamma_j = \max(v_i^U v_j^c, v_i^U v_j^C),$$
$$\delta_i = \max(v_j^U v_i^c, v_j^U v_i^C), \quad \delta_j = \max(v_i^L v_j^c, v_i^L v_j^C),$$

   with $i, j < k$, or
   (c) $\bar{v}_k^c = e_{U_k}(h_k^{\min})$ and $\bar{v}_k^C = E_{U_k}(h_k^{\max})$, where $e_{U_k}, E_{U_k} : V_i \to \mathbb{R}$ are, respectively, convex and concave relaxations of U_k on V_i, $i < k$, and

$$h_k^{\min} = \mathrm{mid}(v_i^c, v_i^C, z_k^{\min}) \quad \text{and} \quad h_k^{\max} = \mathrm{mid}(v_i^c, v_i^C, z_k^{\max}),$$

   where $z_k^{\min}$ is a minimum of e_{U_k} on V_i and $z_k^{\max}$ is a maximum of E_{U_k} on V_i.

6. Compute v_k^c and v_k^C as $v_k^c = \mathrm{mid}\left(v_k^L, v_k^U, \bar{v}_k^c\right)$ and $v_k^C = \mathrm{mid}\left(v_k^L, v_k^U, \bar{v}_k^C\right)$.
7. If $k = m$, got to 8. Otherwise, assign $k := k + 1$ and go to 4.
8. Set $\mathscr{U}(\mathbf{p}) = v_m^c(\mathbf{p})$ and $\mathscr{O}(\mathbf{p}) = v_m^C(\mathbf{p})$.

Remark 1 The functions $U_k^{L/U}$, e_{U_k} and E_{U_k} are available for many common univariate functions (e^x, $\sin(x)$, x^n, $-x$, etc.). Many of the most common, along with the appropriate values for $z_k^{\min}$ and $z_k^{\max}$, are compiled in Sect. II of Online Resource 1. e_{U_k} and E_{U_k} are often taken to be the convex and concave envelopes of U_k on V_i, which are usually simple to construct for these univariate functions. The nature of the functions $U_k^{L/U}$, e_{U_k} and E_{U_k} and their effects on the properties of $\mathscr{U}$ and $\mathscr{O}$ will be formalized through a series of assumptions in Sect. 3.1.

Remark 2 In McCormick's original work [17], Step 6 in Definition 9 is not performed; i.e. $v_k^c = \bar{v}_k^c$ and $v_k^C = \bar{v}_k^C$. However, Proposition 2 shows that this step is valid and can actually result in tighter relaxations. Step 6 is necessary for Lemma 1 below, which is in turn required for many results in later sections (Sect. I of Online Resource 1 contains examples where omitting this step results in violations of Lemma 1 and Theorem 4). Also note that, in McCormick's original work, the bounds $v_k^{L/U}$ are not always computed using natural interval extensions [20], though this is the case in Definition 9 and it is the only case treated in this work.

The McCormick relaxations of $\mathscr{F}$ on P are not always guaranteed to exist because a domain violation may occur in Step 4c or 5c of Definition 9. The assumption that such a violation does not occur is fundamental to the analysis to follow and is formalized below.

Assumption 1 $\mathscr{F}$ can be represented on P by a factorization with the property that, for each k such that $n_p < k \leq m$ and v_k is defined by Definition 8(c), $V_i \subset B_k$.

In general, the factorable representation of a function is not unique, and if a particular factorization does not satisfy the condition of Assumption 1, another often does. In any reference to the factors of $\mathscr{F}$ in the remainder of this article, it is always assumed that the condition of Assumption 1 is satisfied. Under Assumption 1, the validity of McCormick's relaxation technique is well established and is formalized in Proposition 2 below. First, the notations v_k and $v_k^{c/C}$ require some clarification. Note that, in the following definition, P is regarded as fixed, so that each V_k, $1 \leq k \leq m$ is also fixed and independent of $\mathbf{p} \in P$.

Definition 10 (Step and cumulative mappings) Let the *cumulative mapping* v_k be the mapping $v_k : P \to \mathbb{R}$ defined for each $\mathbf{p} \in P$ by the value $v_k(\mathbf{p})$ when the factors of $\mathscr{F}$ are computed recursively, as per Definition 8, beginning from $\mathbf{p}$. Define the cumulative mappings $v_k^{c/C} : P \to \mathbb{R}$ in an analogous manner by Definition 9. For any $n < k \leq m$, let the *step mapping* v_k be a mapping of the form $v_k : V_i(\times V_j) \to \mathbb{R}$, with arguments v_i (v_j), defined by the expression given in Definition 8(a), (b), or (c), and define the step mappings $v_k^{c/C} : V_i \times V_i(\times V_j \times V_j) \to \mathbb{R}$, with arguments $v_i^{c/C}$ $(v_j^{c/C})$, in an analogous manner by Definition 9.

Note that the McCormick relaxations $\mathscr{U}$ and $\mathscr{O}$ are the cumulative mappings v_m^c and v_m^C, respectively. The domain of definition of the step mappings $v_k^{c/C}$ is justified by the following lemma.

Lemma 1 $v_k^{c/C}(\mathbf{p}) \in V_k$ *for all* $k = 1, \ldots, m$ *and every* $\mathbf{p} \in P$.

Proof The result is a trivial consequence of Step 6 in Definition 9. □

Proposition 2 *Choose any* $n_p < k \leq m$ *and consider the definition of* v_k*, by either* (a), (b) *or* (c) *in Definition* (8)*, and the corresponding definitions of* $v_k^{c/C}$*, by Step* 6 *and either Step* 5a, *5b or 5c in Definition 9. Suppose that, for every $i < k$, the values $v_i^{L/U}$ are valid upper and lower bounds on the image of P under the cumulative mapping v_i, and that the cumulative mappings $v_i^{c/C}$ are valid convex and concave relaxations of the cumulative mapping v_i on P. If v_k is defined by Definition 8(c), suppose further that $[v_i^L, v_i^U] \subset B_k$. Then the values $v_k^{L/U}$ are valid upper and lower bounds on the image of P under the cumulative mapping v_k, and the cumulative mappings $v_k^{c/C}$ are valid convex and concave relaxations of the cumulative mapping v_k on P.*

Proof The expressions in steps 4a and 4b in Definition 9 are inclusion monotonic interval extensions of the step mappings v_k defined by (a) and (b) in Definition 8, respectively [20, Chap. 2, Lemma 4.1]. Furthermore, for each v_k defined by (c) in Definition 8, $U_k^{L/U}$ are defined such that $[U_k^L, U_k^U]$ is an inclusion monotonic interval extension of U_k on $V_i \subset B_k$. Therefore, regardless of the definition of v_k, $v_k(\mathbf{p}) \in [v_k^L, v_k^U]$ for all $\mathbf{p} \in P$ by Theorem 1 and the hypothesis that $v_i(\mathbf{p}) \in [v_i^L, v_i^U]$ for all $\mathbf{p} \in P$ and every $i < k$. For proof that $\bar{v}_k^c$ and $\bar{v}_k^C$ are, respectively, convex and concave relaxations of the cumulative mapping v_k on P, see [17]. Then, for any $\mathbf{p} \in P$, $\bar{v}_k^c(\mathbf{p}) \leq v_k(\mathbf{p}) \leq v_k^U$, so that $v_k^c(\mathbf{p}) = \text{mid}\left(v_k^L, v_k^U, \bar{v}_k^c(\mathbf{p})\right) = \max(v_k^L, \bar{v}_k^c(\mathbf{p})) \leq v_k(\mathbf{p})$, and the maximum of two convex functions is convex. Similarly, $v_k^L \leq v_k(\mathbf{p}) \leq \bar{v}_k^C(\mathbf{p})$, so that $v_k^C(\mathbf{p}) = \text{mid}\left(v_k^L, v_k^U, \bar{v}_k^C(\mathbf{p})\right) = \min(v_k^U, \bar{v}_k^C(\mathbf{p})) \geq v_k(\mathbf{p})$, and the minimum of two concave functions is concave. □

The hypotheses of Proposition 2 are clearly satisfied for $k = n_p + 1$. Then, since $\mathscr{U} = v_m^c$ and $\mathscr{O} = v_m^C$, Assumption 1 and induction on Proposition 2 show that $\mathscr{U}$ and $\mathscr{O}$ are, respectively, convex and concave relaxations of $\mathscr{F}$ on P.

3.1 Assumptions on $U_k^{L/U}$, e_{U_k} and E_{U_k}

To prove that the McCormick relaxations $\mathscr{U}$ and $\mathscr{O}$ have particular properties, more information about the relaxations e_{U_k} and E_{U_k} and the bounding operations $U_k^{L/U}$ is needed. One way to achieve this is simply to compile a list of all permissible univariate functions, along with the corresponding bounding operations and convex and concave relaxations. Such a list can be found in Sect. II of Online Resource 1. However, in the interest of flexibility, this work instead makes a minimal set of assumptions on e_{U_k}, E_{U_k} and $U_k^{L/U}$. This approach is more involved, but has the advantage that new univariate functions may be added in an informed manner, such that no desired properties are lost. In Sect. III of Online Resource 1, it is shown that all of these assumptions hold for the univariate functions treated in Sect. II of that document.

Assumption 2 For each k such that $n_p < k \leq m$ and v_k is defined by Definition 8(c), e_{U_k} and E_{U_k} are continuous functions on V_i.

The next assumption is a stronger version of the previous. It will be required only for certain results and will be asserted directly wherever it is required.

Assumption 3 For each k such that $n_p < k \leq m$ and v_k is defined by Definition 8(c), e_{U_k} and E_{U_k} are Lipschitz on V_i.

The remaining assumptions concern the properties of $U_k^{L/U}$, e_{U_k} and E_{U_k} on nested subintervals of V_i. By definition $U_k^{L/U}$ are functions of the bounds $v_i^{L/U}$. It is assumed that the values of e_{U_k} and E_{U_k} at any given $z \in V_i$ are also constructed by some procedure which takes the bounds v_i^L and v_i^U as inputs. That is, if two distinct sets are considered, V_i^1 and V_i^2, it is sensible to refer to the convex relaxation of U_k constructed over V_i^1, denoted $e^1_{U_k}$, and the convex relaxation of U_k constructed over V_i^2, denoted $e^2_{U_k}$. This manner of constructing e_{U_k} and E_{U_k} is useful when McCormick's relaxations are used to construct successively refined approximations of a function on an interval P by generating relaxations on successively finer partitions of P, as is done in branch-and-bound global optimization algorithms. The following assumptions are required for the results in Sect. 3.3.

Assumption 4 For each k such that $n_p < k \leq m$ and v_k is defined by Definition 8(c), define the interval-valued function H_k for each interval $[v_i^{L,\ell}, v_i^{U,\ell}] = V_i^\ell \subset V_i$ by

$$H_k(V_i^\ell) \equiv [U_k^L(v_i^{L,\ell}, v_i^{U,\ell}), U_k^U(v_i^{L,\ell}, v_i^{U,\ell})].$$

H_k is a Lipschitz interval function on V_i, i.e. $\exists L \in \mathbb{R}$ such that

$$U_k^U(v_i^{L,\ell}, v_i^{U,\ell}) - U_k^L(v_i^{L,\ell}, v_i^{U,\ell}) \leq L(v_i^{U,\ell} - v_i^{L,\ell}), \quad \forall [v_i^{L,\ell}, v_i^{U,\ell}] \subset V_i.$$

Assumption 5 Consider any two intervals, V_i^1 and V_i^2, such that $V_i^2 \subset V_i^1 \subset V_i$. For every k such that $n < k \leq m$ and v_k is defined by Definition 8(c), denote the convex and concave relaxations of U_k constructed over V_i^ℓ by $e^\ell_{U_k}$ and $E^\ell_{U_k}$, respectively. $e^\ell_{U_k}$ and $E^\ell_{U_k}$ are constructed such that $e^2_{U_k}(z) \geq e^1_{U_k}(z)$ and $E^2_{U_k}(z) \leq E^1_{U_k}(z)$, $\forall z \in V_i^2$.

Assumption 4 is true whenever the corresponding univariate function is Lipschitz on V_i and $U_k^{L/U}$ return the exact bounds of U_k on any subinterval of V_i [20, Lemma 4.2]. Assumption 5 is always true when $e^\ell_{U_k}$ and $E^\ell_{U_k}$ are taken as the convex and concave envelopes of U_k on V_i^ℓ. Provided that Assumption 1 holds, every $U_k^{L/U}$, e_{U_k} and E_{U_k} listed in Sect. II of Online Resource 1 satisfies Assumptions 4 [20, Lemma 4.2], 2, 3 and 5 (See Sect. III of Online Resource 1).

3.2 Properties of McCormick relaxations

Lemma 2 *For any k such that $n_p < k \leq m$, with $v_k^{c/C}$ defined by Definition 9 Step 6 and Step 5a, 5b or 5c, suppose that the cumulative mappings $v_i^{c/C}$ ($v_j^{c/C}$) are continuous on P. Then the cumulative mappings $v_k^{c/C}$ are continuous on P.*

Proof By Assumption 2 and Definition 9, the step mappings $v_k^{c/C}$ are continuous on $V_i \times V_i(\times V_j \times V_j)$. The hypothesis and Lemma 1 ensures that the cumulative mappings $v_k^{c/C}$ are defined by compositions of continuous functions on all of P and are therefore continuous there.

Lemma 3 *For any k such that $n_p < k \leq m$, with $v_k^{c/C}$ defined by Definition 9 Step 6 and Step 5a, 5b or 5c, suppose that the cumulative mappings $v_i^{c/C}$ ($v_j^{c/C}$) are Lipschitz on P. Then, under Assumption 3, the cumulative mappings $v_k^{c/C}$ are Lipschitz on P.*

Proof If the step mappings $v_k^{c/C}$ are defined by Step 6 and Step 5c in Definition 9, then Assumption 3 ensures that $\bar{v}_k^{c/C}$ are Lipschitz on V_i, and the Lipschitz property is clearly retained after composition with the mid function in Step 6. If $v_k^{c/C}$ are defined by Step 6 and Step 5a or 5b, then it is clear by inspection that they are compositions of functions which are Lipschitz on all of $\mathbb{R}^4$ (addition, constant multiplication, min, max), and hence on $V_i \times V_i \times V_j \times V_j$. Now Lemma 1 ensures that the cumulative mappings $v_k^{c/C}$ are defined by compositions of Lipschitz functions on all of P and are therefore Lipschitz there. □

Theorem 3 *The McCormick relaxations $\mathscr{U}$ and $\mathscr{O}$ are continuous on P. Under Assumption 3, they are Lipschitz on P.*

Proof Clearly, the cumulative mappings $v_k^{c/C}$ are continuous and Lipschitz on P for any $k \leq n_p$. Since $\mathscr{U}$ and $\mathscr{O}$ are the cumulative mappings v_m^c and v_m^C, respectively, finite induction on Lemma 2 proves continuity on P. Under Assumption 3, finite induction on Lemma 3 proves the Lipschitz condition on P. □

3.3 McCormick relaxations on sequences of intervals

The primary motivation for constructing convex and concave relaxations is for their use in branch-and bound global optimization algorithms [11,32]. There, convex and concave relaxations are used to obtain lower and/or upper bounds on the range of a nonconvex function on an interval P. These bounds are then successively refined by partitioning the interval into a number of subintervals and constructing convex and concave relaxations valid on each of these subintervals. In such applications, it is important to understand the relationship between relaxations generated on a nested and convergent sequence of subintervals of P. From these relationships, one can infer the limiting behavior of the relaxations when the partition of P is refined infinitely, which has important consequences for the convergence of global optimization algorithms.

In this section, relaxations on subintervals of P are investigated. The superscript ℓ is used to index subintervals $P^\ell \subset P$, and also relaxations valid on subintervals of P; i.e. $\mathscr{U}^\ell$ and $\mathscr{O}^\ell$ denote the McCormick relaxations of $\mathscr{F}$ constructed as in Definition 9 with P^ℓ in place of P. We consider a nested and convergent sequence of subintervals, $\{P^\ell\} \to P^*$, where P^* is by necessity a subinterval of P. The aim of this analysis is to prove that a branch-and-bound global optimization algorithm with a bounding operation based on convex and/or concave relaxations generated by a particular procedure converges to within a specified tolerance finitely. The reader is referred to Chapter IV in [11] for a detailed discussion of the convergence of branch-and-bound algorithms and the requisite properties of bounding operations (see Definition IV.4 and Theorem IV.3). Here, we claim that the following properties of convex and concave relaxations are sufficient for this application.

Definition 11 (Partition monotonic) Let $g : P \to \mathbb{R}$. A procedure which, given any subinterval $P^\ell \subset P$, generates convex and concave relaxations of g on P^ℓ, respectively $g^{c.\ell}$ and $g^{C,\ell}$, is *partition monotonic* if, for any subintervals $P^2 \subset P^1 \subset P$, $g^{c,2}(\mathbf{p}) \geq g^{c,1}(\mathbf{p})$ and $g^{C,2}(\mathbf{p}) \leq g^{C,1}(\mathbf{p})$, $\forall \mathbf{p} \in P^2$.

Definition 12 (Partition convergent, degenerate perfect) A procedure as in Definition 11 is *partition convergent* if, for any nested and convergent sequence of subintervals of P, $\{P^\ell\} \to P^*$, the sequences $\{g^{c,\ell}\}$ and $\{g^{C,\ell}\}$ converge to $g^{c,*}$ and $g^{C,*}$ uniformly on P^*, where $g^{c,*}$ and $g^{C,*}$ denote the relaxations generated on P^*. A procedure is *degenerate perfect* if the condition $P^* = [\mathbf{p}, \mathbf{p}]$ for any $\mathbf{p} \in P$ implies that $g^{c,*}(\mathbf{p}) = g(\mathbf{p}) = g^{C,*}(\mathbf{p})$.

In this section, it is shown that McCormick's relaxation procedure is partition monotonic and degenerate perfect. In fact, it is also partition convergent, but this result is more natural in the generalized framework of the next section and is proven in Sect. 5.1, albeit under strengthened assumptions. Nonetheless, it is not difficult to show a weaker convergence condition here, and this is in fact enough to warrant the use of McCormick relaxations in branch-and-bound algorithms (see Theorem 5). Before proving partition monotonicity, it is necessary to establish two important properties of natural interval extensions adapted from Moore [20].

Lemma 4 *Choose any K, $1 \leq K \leq m$, and let the interval mapping $H(P^\ell) \equiv [v_K^{L,\ell}, v_K^{U,\ell}]$ be defined, for any interval $P^\ell \subset P$, by the procedure in Definition 9, beginning with P^ℓ. H is an inclusion monotonic and Lipschitz interval extension of the cumulative mapping v_K on P.*

Proof Pick any subintervals of P, $P^2 \subset P^1 \subset P$. First note that $V_i^2 \subset V_i^1 \subset V_i$ and $v_i^{U,1} - v_i^{L,1} = p_i^{U,1} - p_i^{L,1} \leq L_i w(P^1)$ for all $i = 1, \ldots, n_p$ with $L_i = 1$ (the choice of $\ell = 1$ in the Lipschitz condition is arbitrary). For an arbitrary k, suppose this is true for all $i < k$, each with some $L_i \in \mathbb{R}_+$. If $v_k^{L/U}$ is defined by 4a or 4b in Definition 9, then the natural interval extension of the step mapping v_k is both inclusion monotonic and Lipschitz on any interval subset of $\mathbb{R}^2$ ([20], Chapt. 3 and Lemma 4.1), so these properties hold on $V_i \times V_j$. If $v_k^{L/U}$ is defined by 4c, these properties still hold on V_i by Definition 9 and Assumption 4. Now, because the cumulative mapping v_k is a composition of the step mapping v_k with the cumulative mapping $v_i(v_j)$, and because the cumulative mapping $v_i(v_j)$ maps any point in P^2 to $V_i^2 \subset V_i^1 \subset V_i(V_j^2 \subset V_j^1 \subset V_j)$, Theorem 2 can be applied to show that $V_k^2 \subset V_k^1$ and $v_k^{U,1} - v_k^{L,1} \leq L_k(p_k^{U,1} - p_k^{L,1})$ for some $L_k \in \mathbb{R}$. By finite induction, this must be true for all k, and hence for $k = K$. □

Lemma 5 *Choose any subinterval $P^2 \subset P$ and any k such that $n_p < k \leq m$. Consider the definitions of $\bar{v}_k^{c/C}$ by Step 5a, 5b or 5c in Definition 9, and define $\bar{v}_k^{c/C,1}$ and $\bar{v}_k^{c/C,2}$ by the same expressions with $v_i^{c/C/L/U}$ replaced by $v_i^{c/C/L/U,1}$ and $v_i^{c/C/L/U,2}$, respectively, for each $i < k$ in the definitions of $\bar{v}_k^{c/C}$. Suppose that for every such i, $V_i^2 \subset V_i^1$, and for every $\mathbf{p} \in P^2$, $v_i^{c/C,1}(\mathbf{p}) \in V_i^1$, $v_i^{c/C,2}(\mathbf{p}) \in V_i^2$, and $v_i^{c,1}(\mathbf{p}) \leq v_i^{c,2}(\mathbf{p}) \leq v_i^{C,2}(\mathbf{p}) \leq v_i^{C,1}(\mathbf{p})$. Then $\bar{v}_k^{c,2}(\mathbf{p}) \geq \bar{v}_k^{c,1}(\mathbf{p})$ and $\bar{v}_k^{C,2}(\mathbf{p}) \leq \bar{v}_k^{C,1}(\mathbf{p})$ for all $\mathbf{p} \in P^2$.*

Proof The result is shown in three cases, depending on the definition of $\bar{v}_k^{c/C,\ell}$. In every case, Definitions 9 and 3 ensure that $V_k^2 \subset V_k^1$.

(a) Suppose $\bar{v}_k^{c/C,\ell}$ are defined by 5a in Definition 9. Then

$$\bar{v}_k^{c,1}(\mathbf{p}) = v_i^{c,1}(\mathbf{p}) + v_j^{c,1}(\mathbf{p}) \leq v_i^{c,2}(\mathbf{p}) + v_j^{c,2}(\mathbf{p}) = \bar{v}_k^{c,2}(\mathbf{p}), \quad \forall \mathbf{p} \in P^2,$$

and a similar argument holds for $\bar{v}_k^{C,\ell}$.

(b) Suppose $\bar{v}_k^{c/C,\ell}$ are defined by 5b in Definition 9. The proof is presented for $\bar{v}_k^{c,\ell}$; the proof for $\bar{v}_k^{C,\ell}$ is analogous. Choose any $\mathbf{p} \in P^2$ and define the quantities

$$\bar{\alpha}_i^\ell(\mathbf{p}) = \begin{cases} v_i^{c,\ell}(\mathbf{p}) & \text{if } v_j^{L,\ell} \geq 0 \\ v_i^{C,\ell}(\mathbf{p}) & \text{otherwise} \end{cases}, \bar{\alpha}_j^\ell(\mathbf{p}) = \begin{cases} v_j^{c,\ell}(\mathbf{p}) & \text{if } v_i^{L,\ell} \geq 0 \\ v_j^{C,\ell}(\mathbf{p}) & \text{otherwise} \end{cases},$$

$$\bar{\beta}_i^\ell(\mathbf{p}) = \begin{cases} v_i^{c,\ell}(\mathbf{p}) & \text{if } v_j^{U,\ell} \geq 0 \\ v_i^{C,\ell}(\mathbf{p}) & \text{otherwise} \end{cases}, \quad \bar{\beta}_j^\ell(\mathbf{p}) = \begin{cases} v_j^{c,\ell}(\mathbf{p}) & \text{if } v_i^{U,\ell} \geq 0 \\ v_j^{C,\ell}(\mathbf{p}) & \text{otherwise} \end{cases}.$$

By comparison to 5b, it can be seen that the result is established by proving the following inequalities.

$$\begin{aligned}
\bar{v}_k^{c,1}(\mathbf{p}) &= \max\Big(v_j^{L,1}\bar{\alpha}_i^1(\mathbf{p}) + v_i^{L,1}\bar{\alpha}_j^1(\mathbf{p}) - v_j^{L,1}v_i^{L,1}, v_j^{U,1}\bar{\beta}_i^1(\mathbf{p}) \\
&\quad + v_i^{U,1}\bar{\beta}_j^1(\mathbf{p}) - v_j^{U,1}v_i^{U,1}\Big) \\
&\leq \max\Big(v_j^{L,1}\bar{\alpha}_i^2(\mathbf{p}) + v_i^{L,1}\bar{\alpha}_j^2(\mathbf{p}) - v_j^{L,1}v_i^{L,1}, v_j^{U,1}\bar{\beta}_i^2(\mathbf{p}) \\
&\quad + v_i^{U,1}\bar{\beta}_j^2(\mathbf{p}) - v_j^{U,1}v_i^{U,1}\Big) \\
&\leq \max\Big(v_j^{L,2}\bar{\alpha}_i^2(\mathbf{p}) + v_i^{L,2}\bar{\alpha}_j^2(\mathbf{p}) - v_j^{L,2}v_i^{L,2}, v_j^{U,2}\bar{\beta}_i^2(\mathbf{p}) \\
&\quad + v_i^{U,2}\bar{\beta}_j^2(\mathbf{p}) - v_j^{U,2}v_i^{U,2}\Big) \\
&= \bar{v}_k^{c,2}(\mathbf{p}).
\end{aligned}$$

In general, $\max(y, z) \leq \max(z', y')$ if $y \leq y'$ and $z \leq z'$, so to establish the previous inequalities, it suffices to show that

$$\begin{aligned}
v_j^{L,1}\bar{\alpha}_i^1(\mathbf{p}) + v_i^{L,1}\bar{\alpha}_j^1(\mathbf{p}) - v_j^{L,1}v_i^{L,1} &\leq v_j^{L,1}\bar{\alpha}_i^2(\mathbf{p}) + v_i^{L,1}\bar{\alpha}_j^2(\mathbf{p}) - v_j^{L,1}v_i^{L,1} \\
&\leq v_j^{L,2}\bar{\alpha}_i^2(\mathbf{p}) + v_i^{L,2}\bar{\alpha}_j^2(\mathbf{p}) - v_j^{L,2}v_i^{L,2} \quad \text{and} \quad (1) \\
v_j^{U,1}\bar{\beta}_i^1(\mathbf{p}) + v_i^{U,1}\bar{\beta}_j^1(\mathbf{p}) - v_j^{U,1}v_i^{U,1} &\leq v_j^{U,1}\bar{\beta}_i^2(\mathbf{p}) + v_i^{U,1}\bar{\beta}_j^2(\mathbf{p}) - v_j^{U,1}v_i^{U,1} \\
&\leq v_j^{U,2}\bar{\beta}_i^2(\mathbf{p}) + v_i^{U,2}\bar{\beta}_j^2(\mathbf{p}) - v_j^{U,2}v_i^{U,2}. \quad (2)
\end{aligned}$$

Consider the first inequality in (1). If $\bar{\alpha}_i^1(\mathbf{p}) = v_i^{c,1}(\mathbf{p})$, then $v_j^{L,1} \geq 0$. $\bar{\alpha}_i^2(\mathbf{p})$ is either $v_i^{c,2}(\mathbf{p})$ or $v_i^{C,2}(\mathbf{p})$, so the inequality $v_i^{c,1}(\mathbf{p}) \leq v_i^{c,2}(\mathbf{p}) \leq v_i^{C,2}(\mathbf{p})$ shows that $v_j^{L,1}\bar{\alpha}_i^1(\mathbf{p}) \leq v_j^{L,1}\bar{\alpha}_i^2(\mathbf{p})$. Alternatively, if $\bar{\alpha}_i^1(\mathbf{p}) = v_i^{C,1}(\mathbf{p})$, then $v_j^{L,1} < 0$ and the inequality $v_i^{C,1}(\mathbf{p}) \geq v_i^{C,2}(\mathbf{p}) \geq v_i^{c,2}(\mathbf{p})$ again implies that $v_j^{L,1}\bar{\alpha}_i^1(\mathbf{p}) \leq v_j^{L,1}\bar{\alpha}_i^2(\mathbf{p})$. By an analogous argument, it can be shown that $v_i^{L,1}\bar{\alpha}_j^1(\mathbf{p}) \leq v_i^{L,1}\bar{\alpha}_j^2(\mathbf{p})$, and so the first inequality in (1) is satisfied.

Now consider the second inequality in (1). This inequality considers variation in the bounds, while $\bar{\alpha}_i^2(\mathbf{p})$ and $\bar{\alpha}_j^2(\mathbf{p})$ are fixed. The expression

$$v_j^{L,\ell}\bar{\alpha}_i^2(\mathbf{p}) + v_i^{L,\ell}\bar{\alpha}_j^2(\mathbf{p}) - v_j^{L,\ell}v_i^{L,\ell}$$

can be arranged in the following two ways,

$$v_j^{L,\ell}(\bar{\alpha}_i^2(\mathbf{p}) - v_i^{L,\ell}) + v_i^{L,\ell}\bar{\alpha}_j^2(\mathbf{p}) \quad \text{and} \quad v_j^{L,\ell}\bar{\alpha}_i^2(\mathbf{p}) + v_i^{L,\ell}(\bar{\alpha}_j^2(\mathbf{p}) - v_j^{L,\ell}).$$

For either $\ell = 1$ or 2, the hypothesis of the theorem state that $v_i^{c/C,2}(\mathbf{p}) \in V_i^2 \subset V_i^1$ and $v_j^{c/C,2}(\mathbf{p}) \in V_j^2 \subset V_j^1$, so the quantities in parentheses in the these expressions must be nonnegative. Therefore, the first rearrangement shows that the expression is monotone increasing with respect to $v_j^{L,\ell}$, and the second shows that the same is true of $v_i^{L,\ell}$. Combining these facts with the hypothesis that $v_j^{L,1} \leq v_j^{L,2}$ and $v_i^{L,1} \leq v_i^{L,2}$ gives

$$\begin{aligned}
&v_j^{L,1}(\bar{\alpha}_i^2(\mathbf{p}) - v_i^{L,1}) + v_i^{L,1}\bar{\alpha}_j^2(\mathbf{p}) \leq v_j^{L,2}(\bar{\alpha}_i^2(\mathbf{p}) - v_i^{L,1}) + v_i^{L,1}\bar{\alpha}_j^2(\mathbf{p}) \quad \text{and} \\
&v_j^{L,2}\bar{\alpha}_i^2(\mathbf{p}) + v_i^{L,1}(\bar{\alpha}_j^2(\mathbf{p}) - v_j^{L,2}) \leq v_j^{L,2}\bar{\alpha}_i^2(\mathbf{p}) + v_i^{L,2}(\bar{\alpha}_j^2(\mathbf{p}) - v_j^{L,2}),
\end{aligned}$$

which can be combined to prove the second inequality in (1). The inequalities in (2) are proven in an analogous manner.

(c) Suppose $\bar{v}_k^{c/C,\ell}$ are defined by 5c in Definition 9. The proof is presented for $\bar{v}_k^{c,\ell}$; the proof for $\bar{v}_k^{C,\ell}$ is analogous. Choose any $\mathbf{p} \in P^2$. The result will be established through the chain of inequalities

$$e^1_{U_k}(h_k^{min,1}(\mathbf{p})) \leq e^1_{U_k}(h_k^{min,2}(\mathbf{p})) \leq e^2_{U_k}(h_k^{min,2}(\mathbf{p})). \tag{3}$$

Note that $h_k^{min,2}(\mathbf{p}) \in V_k^2$, so the second inequality is true by Assumption 5. It remains to show the first.

By definition, $z_k^{min,1}$ is a minimum of $e^1_{U_k}$ on V_i^1, so if $h_k^{min,1}(\mathbf{p}) = z_k^{min,1}$, then the first inequality in (3) must be satisfied because $h_k^{\min,2}(\mathbf{p}) \in V_i^1$. Suppose $h_k^{min,1}(\mathbf{p}) = v_i^{c,1}(\mathbf{p})$. The definition of the mid function and the fact that $v_i^{c,1}(\mathbf{p}) \leq v_i^{C,1}(\mathbf{p})$ require that $z_k^{min,1} \leq v_i^{c,1}(\mathbf{p}) \leq v_i^{C,1}(\mathbf{p})$, so $h_k^{min,1}(\mathbf{p})$ is to the right of $z_k^{min,1}$. Since $e^1_{U_k}$ is convex on V_i, it is monotonically increasing to the right of $z_k^{min,1}$ by Proposition 1. But $v_i^{c,1}(\mathbf{p}) \leq v_i^{c,2}(\mathbf{p}) \leq v_i^{C,2}(\mathbf{p})$, so if $h_k^{min,2}(\mathbf{p})$ is $v_i^{c,2}(\mathbf{p})$ or $v_i^{C,2}(\mathbf{p})$, then the first inequality in (3) holds. Further, if $h_k^{min,2}(\mathbf{p}) = z_k^{min,2}$, the definition of the mid function requires that $v_i^{c,2}(\mathbf{p}) \leq z_k^{min,2} \leq v_i^{C,2}(\mathbf{p})$, so $z_k^{min,2}$ is to the right of $h_k^{min,1}(\mathbf{p})$ and the first inequality in (3) still holds.

Now suppose that $h_k^{min,1}(\mathbf{p}) = v_i^{C,1}(\mathbf{p})$. The definition of the mid function and the fact that $v_i^{c,1}(\mathbf{p}) \leq v_i^{C,1}(\mathbf{p})$ require that $z_k^{min,1} \geq v_i^{C,1}(\mathbf{p}) \geq v_i^{c,1}(\mathbf{p})$, so $h_k^{min,1}(\mathbf{p})$ is now to the left of $z_k^{min,1}$. By the convexity of $e^1_{U_k}$, it is monotonically decreasing to the left of $z_k^{min,1}$ by Proposition 1. But, by hypothesis, $v_i^{C,1}(\mathbf{p}) \geq v_i^{C,2}(\mathbf{p}) \geq v_i^{c,2}(\mathbf{p})$, so if $h_k^{min,2}(\mathbf{p})$ is $v_i^{c,2}(\mathbf{p})$ or $v_i^{C,2}(\mathbf{p})$, then the first inequality in (3) holds. Further, if $h_k^{min,2}(\mathbf{p}) = z_k^{min,2}$, the definition of the mid function requires that $v_i^{c,2}(\mathbf{p}) \leq z_k^{min,2} \leq v_i^{C,2}(\mathbf{p})$, so $z_k^{min,2}$ is to the left of $h_k^{min,1}(\mathbf{p})$ and the first inequality in (3) still holds. Since $\mathbf{p}$ was chosen arbitrarily, the result holds for all $\mathbf{p} \in P^2$.

Theorem 4 *McCormick relaxations are partition monotonic.*

Proof Choose any subintervals $P^2 \subset P^1 \subset P$ and any $\mathbf{p} \in P^2$. $V_k^2 \subset V_k^1$ for all $k = 1, \ldots, m$ by Lemma 4. Further, the conclusions of Lemma 1 and Proposition 2 hold with P^ℓ in place of P, so that $v_k^{L,\ell} \leq v_k^{c,\ell}(\mathbf{p}) \leq v_k^{C,\ell}(\mathbf{p}) \leq v_k^{U,\ell}$, $\forall \mathbf{p} \in P^\ell$, for every $k = 1, \ldots, m$ and $\ell = 1, 2$. Now, for any $1 \leq i \leq n_p$, $v_i^{c,2}(\mathbf{p}) \geq v_i^{c,1}(\mathbf{p})$ and $v_i^{C,2}(\mathbf{p}) \leq v_i^{C,1}(\mathbf{p})$, $\forall \mathbf{p} \in P^2$, by definition. Choose any k and suppose these inequalities hold for all $i < k$. Then the hypotheses of Lemma 5 are satisfied, which, combined with $V_k^2 \subset V_k^1$, gives $\max(v_k^{L,2}, \bar{v}_k^{c,2}(\mathbf{p})) \geq \max(v_k^{L,1}, \bar{v}_k^{c,1}(\mathbf{p}))$, $\forall \mathbf{p} \in P^2$. But, as in the proof of Proposition 2,

$$v_k^{c,\ell}(\mathbf{p}) = \text{mid}(v_k^{L,\ell}, v_k^{U,\ell}, \bar{v}_k^{c,\ell}(\mathbf{p})) = \max(v_k^{L,\ell}, \bar{v}_k^{c,\ell}(\mathbf{p})), \quad \forall \mathbf{p} \in P^2,$$

for both $\ell = 1, 2$, so that $v_k^{c,2}(\mathbf{p}) \geq v_k^{c,1}(\mathbf{p})$, $\forall \mathbf{p} \in P^2$. An analogous argument shows that $v_k^{C,2}(\mathbf{p}) \leq v_k^{C,1}(\mathbf{p})$, $\forall \mathbf{p} \in P^2$. Now, by finite induction, these inequalities hold for all $k = 1, \ldots, m$. But $\mathscr{U}^\ell(\mathbf{p}) = v_m^{c,\ell}(\mathbf{p})$ and $\mathscr{O}^\ell(\mathbf{p}) = v_m^{C,\ell}(\mathbf{p})$, $\ell = 1, 2$. □

Consider a nested sequence of subintervals of P, $\{P^\ell\}$, converging to a degenerate interval $[\mathbf{p}, \mathbf{p}]$. For McCormick relaxations to be useful in branch-and-bound optimization algorithms, it is necessary that the sequences of relaxations satisfy $\{\mathscr{U}^\ell(\mathbf{p})\} \to \mathscr{F}(\mathbf{p})$ and

$\{\mathscr{O}^{\ell}(\mathbf{p})\}\to\mathscr{F}(\mathbf{p})$. That is, the values of the relaxations at $\mathbf{p}$ converge to the exact function value. The above monotonicity theorem guarantees that the sequence $\{\mathscr{U}^{\ell}(\mathbf{p})\}$ is increasing and bounded above by $\mathscr{F}(\mathbf{p})$, and that the sequence $\{\mathscr{O}^{\ell}(\mathbf{p})\}$ is decreasing and bounded below by $\mathscr{F}(\mathbf{p})$, but it does not imply that the relaxation values get arbitrarily close to the function value. In other words, the sequences are guaranteed to converge, but not necessarily to $\mathscr{F}(\mathbf{p})$. To ensure that the limit of both of these sequences is in fact $\mathscr{F}(\mathbf{p})$, the Lipschitz property shown in Lemma 4 is required.

Theorem 5 *McCormick relaxations are degenerate perfect. Moreover, for any nested sequence of subintervals of P satisfying $\{P^{\ell}\}\to[\mathbf{p},\mathbf{p}]$, $\mathbf{p}\in P$, $\{\mathscr{U}^{\ell}(\mathbf{p})\}\to\mathscr{F}(\mathbf{p})$ and $\{\mathscr{O}^{\ell}(\mathbf{p})\}\to\mathscr{F}(\mathbf{p})$.*

Proof Lemma 4 with $K=m$, the definition of an interval extension (Definition 2) and Lemma 1 guarantee that McCormick relaxations are degenerate perfect. Consider any sequence of subintervals as in the hypothesis. It is clear that $\{w(P^{\ell})\}\to 0$. Then Lemma 4 with $K=m$ gives $v_m^{U,\ell}-v_m^{L,\ell}\leq Lw(P^{\ell})$ for some $L\in\mathbb{R}_{+}$, so that $\{v_m^{U,\ell}-v_m^{L,\ell}\}\to 0$. But $v_m^{L,\ell}\leq\mathscr{U}^{\ell}(\mathbf{p})\leq\mathscr{F}(\mathbf{p})\leq\mathscr{O}^{\ell}(\mathbf{p})\leq v_m^{U,\ell}$, so the result holds. □

4 Generalized mccormick relaxations

In this section, a more general notion of McCormick relaxations is formulated. This generalization allows many important properties to be established which are quite inaccessible in the standard framework. Moreover, this formulation allows complex uses of McCormick's technique which have previously not been explored. There are two distinctive features of this formulation. First, the initial relaxations, $v_i^{c/C}$ for $i=1,\ldots,n_p$, are taken as arguments separate from the value of $\mathbf{p}$. This allows for compositions with previously constructed relaxations which may not be compatible with the procedure given in Definition 9. Essentially, such a relaxation behaves like an intermediate $v_k^{c/C}$ in Definition 9; taking relaxations of previous factors as input and composing with later factors. The second feature of the generalized McCormick relaxations is that the dependence on the bounds is made explicit, which enables a more natural treatment of their properties on sequences of intervals. The presentation below is abstract, but powerful, and requires slightly stronger assumptions on the bounding operations and relaxations for univariate intrinsic functions. Nonetheless, all assumptions are again found to hold for all univariate functions listed in Sect. II of Online Resource 1.

For flexibility, the generalized McCormick relaxations are formulated without reference to any particular functional form, but rather with respect to a generic collection of factors $\mathscr{V}$ with domain S_Φ. Accordingly, the generalized relaxations carry no inherent meaning; they only take on significance as valid relaxations for a particular application when the factors and domain are specified appropriately and the proper inputs are given.

Definition 13 **(S_Φ, Φ, $\mathscr{V}$)** Let $S_\Phi\subset\mathbb{R}^n$, let $\Phi\subset S_\Phi$, and let $\mathscr{V}$ be a collection of m factors such that, given any $\boldsymbol{\phi}\in\Phi$, $v_k=\phi_k$ for each $v_k\in\mathscr{V}$ with $k=1,\ldots,n$, and for each k such that $n<k\leq m$, $v_k\in\mathscr{V}$ is defined by either (a), (b) or (c) in Definition 8.

Recall that, for any v_k defined by Definition 8(c), B_k denotes the domain of the univariate intrinsic function U_k. For generality, we extend this notation to all $n<k\leq m$ by defining $B_k=\mathbb{R}^2$ for all v_k defined by Definition 8(a) or (b).

Definition 14 **($\mathbf{y}_k^\circ, \mathbf{y}^\circ, \tilde{B}_k, \tilde{\Phi}$)** Let $\mathbf{y}_k^\circ = (y_k^L, y_k^U, y_k^c, y_k^C)$, $\mathbf{y}^\circ = (\mathbf{y}_1^\circ, \ldots, \mathbf{y}_n^\circ)$, and define the following sets:

$$\tilde{B}_k \equiv \left\{\mathbf{y}_i^\circ(, \mathbf{y}_j^\circ) \in \mathbb{R}^4 : \; y_i^{c/C} \in [y_i^L, y_i^U],\; (y_j^{c/C} \in [y_j^L, y_j^U],)\; [y_i^L, y_i^U](\times[y_j^L, y_j^U]) \subset B_k)\right\},$$

$$\tilde{\Phi} \equiv \left\{\mathbf{y}^\circ \in \mathbb{R}^{4n} : \; y_i^{c/C} \in [y_i^L, y_i^U],\; i = 1, \ldots, n,\; [y_1^L, y_1^U] \times \cdots \times [y_n^L, y_n^U] \subset \Phi\right\}.$$

Definition 15 (Generalized McCormick relaxations $\tilde{\mathscr{U}}$ and $\tilde{\mathscr{O}}$) Define the Generalized McCormick relaxations of the factors $\mathscr{V}$ on Φ as the functions $\tilde{\mathscr{U}}, \tilde{\mathscr{O}} : \tilde{\Phi} \to \mathbb{R}$ where, for each $\mathbf{y}^\circ \in \tilde{\Phi}$, $\tilde{\mathscr{U}}(\mathbf{y}^\circ)$ and $\tilde{\mathscr{O}}(\mathbf{y}^\circ)$ are defined by the following procedure:

1. Set $v_i^L = y_i^L$ and $v_i^U = y_i^U$ for all $i = 1, \ldots, n$.
2. Set $v_i^c = y_i^c$ and $v_i^C = y_i^C$ for all $i = 1, \ldots, n$.
3. Set $k = n + 1$.
4. Define v_k^L and v_k^U according to the definition of v_k, as in Step 4 of Definition 9.
5. Define $\bar{v}_k^c$ and $\bar{v}_k^C$ according to the definition of v_k, as in Step 5 of Definition 9.
6. Define v_k^c and v_k^C as $v_k^c = \text{mid}\left(v_k^L, v_k^U, \bar{v}_k^c\right)$ and $v_k^C = \text{mid}\left(v_k^L, v_k^U, \bar{v}_k^C\right)$.
7. If $k = m$, go to 8. Otherwise, assign $k := k + 1$ and go to 4.
8. Set $\tilde{\mathscr{U}}(\mathbf{y}^\circ) = v_m^c(\mathbf{y}^\circ)$ and $\tilde{\mathscr{O}}(\mathbf{y}^\circ) = v_m^C(\mathbf{y}^\circ)$.

This definition is truly a generalization of Definition 9, since the standard McCormick relaxations of $\mathscr{F}$ can be recovered by letting $\mathscr{V}$ be the set of factors describing $\mathscr{F}$, letting $n = n_p$ and $\Phi = P$, and evaluating $\tilde{\mathscr{U}}$ and $\tilde{\mathscr{O}}$ for each $\mathbf{p} \in P$ at $\mathbf{y}^\circ \equiv (p_1^L, p_1^U, p_1, p_1, \ldots, p_n^L, p_n^U, p_n, p_n)$. This relationship is explored in Sect. 5.1.

The following basic assumption, analogous to Assumption 1, is required to ensure that $\tilde{\mathscr{U}}$ and $\tilde{\mathscr{O}}$ are well-defined.

Assumption 6 For any $v_k \in \mathscr{V}$ defined by Definition 8(c), $V_i(\mathbf{y}^\circ) \subset B_k$ for all $\mathbf{y}^\circ \in \tilde{\Phi}$.

If Φ is an interval, then inclusion monotonicity implies that Assumption 6 holds if and only if, for each $v_k \in \mathscr{V}$ defined by Definition 8(c), $V_i(\mathbf{y}^\circ) \subset B_k$ for some $\mathbf{y}^\circ \in \tilde{\Phi}$ satisfying $[y_1^L, y_1^U] \times \cdots \times [y_n^L, y_n^U] = \Phi$.

As with the standard relaxations in Sect. 3, it will be helpful to define step and cumulative mappings for the generalized McCormick relaxations. In this case, the step mappings $v_k^{c/C}$ are complicated by the need to incorporate dependence on the bounds of previous factors explicitly, while the corresponding cumulative mappings are complicated by the need to introduce explicit dependence on both initial bounds and initial relaxation values. Moreover, mappings associated with the bounds themselves are needed.

Definition 16 (Generalized step and cumulative mappings) For each $v_k \in \mathscr{V}$, let the *generalized cumulative mapping* v_k be the mapping $v_k : \Phi \to \mathbb{R}$, defined for each $\boldsymbol{\phi} \in \Phi$ by the value $v_k(\boldsymbol{\phi})$ when the factors $\mathscr{V}$ are computed recursively beginning from $\boldsymbol{\phi}$, as in Definition 13. Define the generalized cumulative mappings $v_k^{L/U/c/C} : \tilde{\Phi} \to \mathbb{R}$ in an analogous manner by Definition 15. For each $n < k \le m$, let the *generalized step mapping* v_k be a mapping of the form $v_k : B_k \to \mathbb{R}$, with arguments $v_i(v_j)$, defined by Definition 13 and the expressions in Definition 8(a), (b), or (c), and define the generalized step mappings $v_k^{L/U/c/C} : \tilde{B}_k \to \mathbb{R}$, with arguments $v_i^{L/U/c/C}(v_j^{L/U/c/C})$, in an analogous manner by Definition 15.

Strictly, the generalized step and cumulative mappings $v_k^{L/U}$ only depend on the bounds of the previous factors, not the relaxation values. However, defining these mappings on $\tilde{B}_k$ and

$\tilde{\Phi}$ is convenient and poses no mathematical difficulty. Note that $\tilde{\mathscr{U}}$ and $\tilde{\mathscr{O}}$ are the generalized cumulative mappings v_m^c and v_m^C, respectively, analogous to the situation with the standard relaxations in Sect. 3.

Let $\mathbf{v}_i^\circ(\mathbf{y}^\circ) \equiv (v_i^L(\mathbf{y}^\circ), v_i^U(\mathbf{y}^\circ), v_i^c(\mathbf{y}^\circ), v_i^C(\mathbf{y}^\circ))$. Combined with Assumption 6, the following lemma shows that, for each $n < k \leq m$ and each $\mathbf{y}^\circ \in \tilde{\Phi}$, $(\mathbf{v}_i^\circ(\mathbf{y}^\circ), \mathbf{v}_j^\circ(\mathbf{y}^\circ)) \in \tilde{B}_k$, $\left[\text{or } \mathbf{v}_i^\circ(\mathbf{y}^\circ) \in \tilde{B}_k\right]$, which justifies the domain of definition of the generalized step mappings.

Lemma 6 $v_k^{c/C}(\mathbf{y}^\circ) \in V_k(\mathbf{y}^\circ)$ *for all* $k = 1, \ldots, m$ *and every* $\mathbf{y}^\circ \in \tilde{\Phi}$.

Proof Choose any $\mathbf{y}^\circ \in \tilde{\Phi}$. The result is obviously true for any $k = 1, \ldots, n$ by the definition of $\tilde{\Phi}$. For all other k, the result follows from Step 6 in Definition 15. □

The next definition makes the dependence of the relaxations e_{U_k} and E_{U_k} on the bounds y_i^L and y_i^U explicit. All of the univariate relaxations in Sect. II of Online Resource 1 are given in this generalized form.

Definition 17 ($\tilde{e}_{U_k}, \tilde{E}_{U_k}$) For each $v_k \in \mathscr{V}$ defined by Definition 8(c), let the functions $\tilde{e}_{U_k}, \tilde{E}_{U_k} : \tilde{B}_k \to \mathbb{R}$ be defined by

$$\tilde{e}_{U_k}(\mathbf{y}_i^\circ) = \bar{e}_{U_k}(h_k^{min}(\mathbf{y}_i^\circ), y_i^L, y_i^U) \quad \text{and} \quad \tilde{E}_{U_k}(\mathbf{y}_i^\circ) = \bar{E}_{U_k}(h_k^{max}(\mathbf{y}_i^\circ), y_i^L, y_i^U),$$

where $\bar{e}_{U_k}(\cdot, y_i^L, y_i^U)$ and $\bar{E}_{U_k}(\cdot, y_i^L, y_i^U)$ denote the relaxations e_{U_k} and E_{U_k} constructed on the interval $[y_i^L, y_i^U]$, and

$$h_k^{min/max}(\mathbf{y}_i^\circ) = \text{mid}\left(y_i^c, y_i^C, z_k^{min/max}(\mathbf{y}_i^\circ)\right)$$

with $z_k^{min}(\mathbf{y}_i^\circ)$ and $z_k^{max}(\mathbf{y}_i^\circ)$ being, respectively, a minimum of $\bar{e}_{U_k}(\cdot, y_i^L, y_i^U)$ and a maximum of $\bar{E}_{U_k}(\cdot, y_i^L, y_i^U)$ on $[y_i^L, y_i^U]$.

As mentioned previously, it is not sensible to discuss the validity of the generalized relaxations since no significance has been attached to the collection of factors $\mathscr{V}$, the set Φ or the value of $\mathbf{y}^\circ$. However, the idea of composition is central. Accordingly, it is helpful to rephrase Proposition 2 to deal directly with compositions in the language of the generalized relaxations. Proposition 2 is of course still valid because each $v_k^{c/C}$ with $n < k \leq m$ is defined in exactly the same way for the standard and generalized McCormick relaxations.

Proposition 3 *Consider* $S_P \subset \mathbb{R}^{n_p}$*, an interval* $P \subset S_P$*, and an* n*-dimensional vector function* $\mathbf{x} : S_P \to \Phi$*. Suppose that* $\mathcal{G} : \Phi \to \mathbb{R}$ *is defined by the factors in* $\mathscr{V}$*, and let* $\mathscr{F}(\mathbf{p}) = \mathcal{G}(\mathbf{x}(\mathbf{p}))$ *for all* $\mathbf{p} \in P$*. Suppose further that real numbers* x_i^L *and* x_i^U *are available for each* $i = 1, \ldots, n$*, which bound the image of* P *under* x_i*. For any two vector functions,* $\mathbf{x}^c, \mathbf{x}^C : P \to \Phi$*, such that* $(x_1^L, x_1^U, x_1^c(\mathbf{p}), x_1^C(\mathbf{p}), \ldots, x_n^L, x_n^U, x_n^c(\mathbf{p}), x_n^C(\mathbf{p})) \in \tilde{\Phi}$ *for all* $\mathbf{p} \in P$*, if* $\mathbf{x}^c$ *and* $\mathbf{x}^C$ *are, respectively, convex and concave relaxations of* $\mathbf{x}$ *on* P*, then the functions* $\mathscr{U}, \mathscr{O} : P \to \mathbb{R}$ *defined by*

$$\mathscr{U}(\mathbf{p}) \equiv \tilde{\mathscr{U}}(x_1^L, x_1^U, x_1^c(\mathbf{p}), x_1^C(\mathbf{p}), \ldots, x_n^L, x_n^U, x_n^c(\mathbf{p}), x_n^C(\mathbf{p})) \quad \textit{and}$$
$$\mathscr{O}(\mathbf{p}) \equiv \tilde{\mathscr{O}}(x_1^L, x_1^U, x_1^c(\mathbf{p}), x_1^C(\mathbf{p}), \ldots, x_n^L, x_n^U, x_n^c(\mathbf{p}), x_n^C(\mathbf{p}))$$

are, respectively, convex and concave relaxations of $\mathscr{F}$ *on* P*.*

Proof From the definition of the function $\mathcal{G}$ and the definition of the generalized McCormick relaxations, the first n factors are assigned for any $\mathbf{p} \in P$ and for each $i = 1, \ldots, n$ as $v_i(\mathbf{p}) = x_i(\mathbf{p})$, $v_i^L = x_i^L$, $v_i^U = x_i^U$, $v_i^c(\mathbf{p}) = x_i^c(\mathbf{p})$, $v_i^C(\mathbf{p}) = x_i^C(\mathbf{p})$. Now, the procedure for computing v_k and $v_k^{L/U/c/C}$ for $n < k \leq m$ is identical to that for the standard McCormick relaxations. Therefore, it is sensible to refer to the cumulative mappings v_k and $v_k^{c/C}$ on P (note that these are not the *generalized cumulative mappings*, which are defined on $\tilde{\Phi}$). Then, by the hypothesis on $x_i^{L/U/c/C}$, Proposition 2 may be applied to conclude that $v_{n+1}^{L/U}$ are valid bounds on the image of P under the cumulative mapping v_{n+1}, and that the cumulative mappings $v_{n+1}^{c/C}$ are valid convex and concave relaxations of the cumulative mapping v_{n+1} on P. Now Assumption 6 and induction on Proposition 2 complete the proof. □

4.1 Assumptions on $U_k^{L/U}$, $\tilde{e}_{U_k}$ and $\tilde{E}_{U_k}$

As was the case with the standard relaxations, the properties of the generalized relaxations are in large part determined by the properties of the bounding operations and relaxations associated with the univariate functions U_k. The assumptions made on these functions are similar in character to the assumptions made in Sect. 3.1. However, they are strengthened to include dependence on the bounds and modified to reflect the current notation.

Assumption 7 For each $v_k \in \mathcal{V}$ defined by Definition 8(c), $\tilde{e}_{U_k}$ and $\tilde{E}_{U_k}$ are continuous functions on $\tilde{B}_k$.

Assumption 8 For each $v_k \in \mathcal{V}$ defined by Definition 8(c), $U_k^{L/U}$ are continuous on $\{y, z \in B_k : [y, z] \subset B_k\}$.

The next two assumptions address Lipschitz properties of U_k^L, U_k^U, $\tilde{e}_{U_k}$ and $\tilde{E}_{U_k}$. Though Assumption 6 ensures that assuming these properties on $\tilde{B}_k$ is sufficient, it may be overly restrictive. Consider the following subsets of $\tilde{B}_k$. For any interval $\beta_k \subset B_k$ (note that B_k is not necessarily an interval), let

$$\tilde{\beta}_k = \left\{\mathbf{y}_i^\circ(, \mathbf{y}_j^\circ) \in \mathbb{R}^4 : y_i^{c/C} \in [y_i^L, y_i^U],\ (y_j^{c/C} \in [y_j^L, y_j^U],)\ [y_i^L, y_i^U](\times[y_j^L, y_j^U]) \subset \beta_k\right\}.$$

Note that $\tilde{\beta}_k \subset \tilde{B}_k$. For certain univariate functions, the distinction between B_k and β_k is significant. For example, $\ln(z)$ is not Lipschitz on its entire domain, $(0, +\infty)$, but is Lipschitz on any interval subset. For such functions, there exist $\tilde{e}_{U_k}$ and $\tilde{E}_{U_k}$ which are Lipschitz on any $\tilde{\beta}_k$, yet no such relaxations exist on $\tilde{B}_k$ (see Sect. III of Online Resource 1). It will be shown in the course of proving that $\tilde{\mathcal{U}}$ and $\tilde{\mathcal{O}}$ are Lipschitz in the next section that the following assumptions need only hold on a particular $\tilde{\beta}_k \subset \tilde{B}_k$. These assumptions are only required for certain results and will be asserted directly wherever they required.

Assumption 9 For each $v_k \in \mathcal{V}$ defined by Definition 8(c) and any interval $\beta_k \subset B_k$, $\tilde{e}_{U_k}$ and $\tilde{E}_{U_k}$ are Lipschitz on $\tilde{\beta}_k$.

Assumption 10 For each $v_k \in \mathcal{V}$ defined by Definition 8(c), define the interval-valued function H_k by

$$H_k([y_i^L, y_i^U]) \equiv [U_k^L(y_i^L, y_i^U), U_k^U(y_i^L, y_i^U)].$$

For any interval $\beta_k \subset B_k$, $\exists L \in \mathbb{R}_+$ such that $d_H(H_k(Y_i), H_k(\hat{Y}_i)) \leq L d_H(Y_i, \hat{Y}_i)$ for any two intervals $Y_i, \hat{Y}_i \subset \beta_k$.

The Lipschitz condition in Assumption 10 implies the Lipschitz condition in Assumption 4 of Sect. 3.1 [22, Corollary 2.1.2]. Moreover, it is not hard to show that this condition is tantamount to asserting that the generalized step mappings $v_k^{L/U}$ are Lipschitz (in the real-valued sense) on any $\tilde{\beta}_k \subset \tilde{B}_k$.

Assumptions 7–10 are all true for every $U_k^{L/U}$, $\tilde{e}_{U_k}$ and $\tilde{E}_{U_k}$ defined in Sect. II of Online Resource 1. For Assumption 8, this is obvious by inspection. In general, Assumption 10 is true whenever U_k is itself Lipschitz on any interval subset of B_k, and $U_k^{L/U}$ return the exact bounds of U_k on any interval subset of B_k (see [22] Theorem 2.1.1). Similarly, Assumption 9 is true whenever U_k is Lipschitz on any interval subset of B_k and $\tilde{e}_{U_k}$ and $\tilde{E}_{U_k}$ are the generalized versions of the convex and concave envelopes of U_k, and Assumption 7 is implied by Assumption 9 whenever B_k is open (See Sect. III of Online Resource 1).

4.2 Properties of generalized McCormick relaxations

In Sects. 5, 6 and 7, the properties of the generalized McCormick's relaxations are discussed in the context of several applications. Here, some basic properties are established that hold regardless of the application. In contrast to many of the results in Sect. 3, all of the properties established in the following sections are novel. Though the proofs are quite direct in the generalized framework, the conclusions drawn here are powerful and highly non-intuitive.

Lemma 7 *For any $v_k \in \mathscr{V}$ defined by Definition 8(a), (b) or (c), suppose that the generalized cumulative mappings $v_i^{L/U/c/C}$ ($v_j^{L/U/c/C}$) are continuous on $\tilde{\Phi}$. Then the generalized cumulative mappings $v_k^{L/U/c/C}$ are continuous on $\tilde{\Phi}$.*

Proof If $v_k^{L/U/c/C}$ are defined by 4a, 5a and 6 in Definition 9, or by 4b, 5b and 6 in the same definition, then $B_k = \mathbb{R}^2$ and the generalized step mappings $v_k^{L/U/c/C}$ are clearly continuous on all of $\tilde{B}_k$. Suppose instead that $v_k^{L/U/c/C}$ are defined by Steps 4c, 5c and 6 in Definition 9. Then the generalized step mappings $v_k^{L/U/c/C}$ are continuous on $\tilde{B}_k$ by Assumptions 7 and 8.

Then, by hypothesis, the generalized cumulative mappings $v_k^{L/U/c/C}$ are compositions of continuous functions. Further, the generalized cumulative mappings $v_i^{L/U/c/C}$ ($v_j^{L/U/c/C}$) map any point in $\tilde{\Phi}$ into $\tilde{B}_k$ by Assumption 6 and Lemma 6. Therefore, the generalized cumulative mappings $v_k^{L/U/c/C}$ are continuous functions on $\tilde{\Phi}$.

Lemma 8 *For any $v_k \in \mathscr{V}$ defined by Definition 8(a), (b) or (c), if Assumptions 9 and 10 hold and the generalized cumulative mappings $v_i^{L/U/c/C}$ (and $v_j^{L/U/c/C}$) are Lipschitz on some compact, connected subset $\tilde{\Phi}' \subset \tilde{\Phi}$, then the generalized cumulative mappings $v_k^{L/U/c/C}$ are Lipschitz on $\tilde{\Phi}'$.*

Proof By the hypotheses, $\tilde{\Phi}'$ is compact and connected and the generalized cumulative mappings $v_i^{L/U/c/C}$ ($v_j^{L/U/c/C}$) are continuous on $\tilde{\Phi}'$. Then the images of $\tilde{\Phi}'$ under the generalized cumulative mappings $v_i^L, v_i^U, v_j^L, v_j^U$ are all also compact and connected [25, Theorems 4.14 and 4.22]. Accordingly, each has a maximum and minimum element, so that the values $v_i^{L,\min}, v_i^{U,\max}, v_j^{L,\min}, v_j^{U,\max}$ can be defined in the obvious manner.

Now suppose that $v_k^{L/U/c/C}$ are defined by 4c, 5c and 6 in Definition 9. It will be shown that $[v_i^{L,\min}, v_i^{U,\max}]$ must be a subset of B_k. Because $v_i^L(\mathbf{y}^\circ), v_i^U(\mathbf{y}^\circ) \in B_k$ for every $\mathbf{y}^\circ \in \tilde{\Phi}'$

by Assumption 6, the images of $\tilde{\Phi}'$ under the cumulative mappings $v_i^{L/U}$ are connected, and $v_i^L(\mathbf{y}^\circ) \leq v_i^U(\mathbf{y}^\circ)$ for every $\mathbf{y}^\circ \in \tilde{\Phi}'$, it is concluded that if any point in $[v_i^{L,\min}, v_i^{U,\max}]$ is not in B_k, it must be in the interior of every $[v_i^L(\mathbf{y}^\circ), v_i^U(\mathbf{y}^\circ)]$ with $\mathbf{y}^\circ \in \tilde{\Phi}'$. Clearly this violates Assumption 6, so $[v_i^{L,\min}, v_i^{U,\max}] \subset B_k$. Now, setting $\beta_k = [v_i^{L,\min}, v_i^{U,\max}]$ and applying Assumptions 9 and 10 shows that the generalized step mappings $v_k^{L/U/c/C}$ are Lipschitz on $\tilde{\beta}_k$ (composition with the mid function in Step 6 preserves the Lipschitz condition), so the generalized cumulative mappings $v_k^{L/U/c/C}$ are compositions of Lipschitz functions. Further, the generalized cumulative mappings $v_i^{L/U/c/C}$ map any point in $\tilde{\Phi}'$ to $\tilde{\beta}_k$ by Lemma 6 and the definition of β_k. Therefore, the generalized cumulative mappings $v_k^{L/U/c/C}$ are Lipschitz functions on $\tilde{\Phi}'$.

Suppose instead that $v_k^{L/U/c/C}$ are defined by 4a, 5a and 6 in Definition 9, or by 4b, 5b and 6 in the same definition. In either case, $B_k = \mathbb{R}^2$ and we let $\beta_k \equiv [v_i^{L,\min}, v_i^{U,\max}] \times [v_j^{L,\min}, v_j^{U,\max}]$ so that $\tilde{\beta}_k$ is compact (See Lemma 9). The bilinear terms in the definitions of the generalized step mappings $v_k^{L/U/c/C}$ (4b and 5b) are each Lipschitz on any compact subset of $\mathbb{R}^2$, and hence these expressions are Lipschitz on $\tilde{\beta}_k$. The remaining functions in the definitions of $v_k^{L/U/c/C}$ are Lipschitz on all of $\mathbb{R}^2$ (addition, min, max), so that composition with these functions preserves the Lipschitz condition. It follows from Lemma 6 and the definition of $[v_i^{L,\min}, v_i^{U,\max}] \times [v_j^{L,\min}, v_j^{U,\max}]$ that the generalized cumulative mappings $v_i^{L/U/c/C}$ and $v_j^{L/U/c/C}$ map any point in $\tilde{\Phi}'$ to $\tilde{\beta}_k$. Therefore, the generalized cumulative mappings $v_k^{L/U/c/C}$ are compositions of Lipschitz functions on all of $\tilde{\Phi}'$ and so are Lipschitz there.

Theorem 6 *The generalized McCormick relaxations $\tilde{\mathscr{U}}$ and $\tilde{\mathscr{O}}$ are continuous on $\tilde{\Phi}$. Under Assumptions 9 and 10, they are Lipschitz on any compact, connected subset $\tilde{\Phi}' \subset \tilde{\Phi}$.*

Proof Clearly, the generalized cumulative mappings $v_k^{L/U/c/C}$ are Lipschitz, and hence continuous, on $\tilde{\Phi}$ for any $1 \leq k \leq n$. Since $\tilde{\mathscr{U}}$ and $\tilde{\mathscr{O}}$ are the generalized cumulative mappings v_m^c and v_m^C, respectively, induction on Lemma 7 proves continuity on $\tilde{\Phi}$. Under Assumptions 9 and 10, induction on Lemma 8 proves the Lipschitz property on $\tilde{\Phi}'$.

The following Lemma illustrates that, when Φ is an interval, the Lipschitz assertion in Theorem 6 holds on all of $\tilde{\Phi}$.

Lemma 9 *If Φ is an interval, then $\tilde{\Phi}$ is compact and connected.*

Proof Consider the following mapping:

$$\Phi^4 \ni (\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}) \longmapsto ((\min(a_1, b_1), \max(a_1, b_1), \text{mid}(c_1, a_1, b_1), \text{mid}(d_1, a_1, b_1)) , \\ \dots, (\min(a_n, b_n), \max(a_n, b_n), \text{mid}(c_n, a_n, b_n), \text{mid}(d_n, a_n, b_n))) \in \tilde{\Phi}.$$

It is not difficult to verify that this map is continuous. Furthermore,

$$[\min(a_1, b_1), \max(a_1, b_1)] \times \cdots \times [\min(a_n, b_n), \max(a_n, b_n)] \subset \Phi$$

by the hypothesis that Φ is an interval, so the image of Φ^4 under this mapping is indeed contained in $\tilde{\Phi}$. Now, given any $\mathbf{y}^\circ \in \tilde{\Phi}$, the point

$$\left((y_1^L, \dots, y_n^L), (y_1^U, \dots, y_n^U), (y_1^c, \dots, y_n^c), (y_1^C, \dots, y_n^C)\right) \in \Phi^4$$

clearly maps to $\mathbf{y}^\circ$. Thus, this mapping is onto, so that the image of Φ^4 under this mapping is exactly $\tilde{\Phi}$. But Φ is compact and connected by hypothesis, which implies that Φ^4 is compact and connected. Therefore, $\tilde{\Phi}$ must be compact and connected because it is the image of a compact, connected set under a continuous mapping [25, Theorems 4.14 and 4.22]. □

5 Basic applications of generalized McCormick relaxations

This section treats some fairly straightforward applications of generalized McCormick relaxations. First, standard McCormick relaxations are revisited and stronger convergence results are proven. Secondly, the issue of taking relaxations with respect to only a subset of a function's arguments is discussed. Finally, the issue of relaxations for compositions of functions is treated. This last topic is central to the development of relaxations for the solutions of systems of equations in Sects. 6 and 7. In each application below, the relevant relaxations are treated as special cases of the generalized McCormick relaxations and the simple properties established in Sect. 4.2 are found to have powerful consequences for the application at hand.

5.1 Standard McCormick relaxations revisited

The standard McCormick relaxations can be recovered from the general simply by letting $\mathscr{V}$ be the factors defining $\mathscr{F}$, letting $n = n_p$ and $\Phi = P$, and for every $\mathbf{p} \in P = \Phi$, considering only those $\mathbf{y}^\circ \in \tilde{\Phi}$ such that $y_i^c = y_i^C = p_i$, $y_i^L = p_i^L$, and $y_i^U = p_i^U$, $i = 1, \ldots, n_p$. For any such $\mathbf{p}$ and $\mathbf{y}^\circ$, $\tilde{\mathscr{U}}(\mathbf{y}^\circ) = \mathscr{U}(\mathbf{p})$ and $\tilde{\mathscr{O}}(\mathbf{y}^\circ) = \mathscr{O}(\mathbf{p})$. Here, the issue of standard McCormick relaxations on nested sequences of subintervals is revisited using this generalized framework. Of course, given any subset $P^\ell \subset P$, if $\mathbf{p} \in P^\ell$ and $\mathbf{y}^\circ \in \tilde{\Phi}$ are chosen such that $y_i^c = y_i^C = p_i$, $y_i^L = p_i^{L,\ell}$, and $y_i^U = p_i^{U,\ell}$ for all $i = 1, \ldots, n_p$, then $\tilde{\mathscr{U}}(\mathbf{y}^\circ) = \mathscr{U}^\ell(\mathbf{p})$ and $\tilde{\mathscr{O}}(\mathbf{y}^\circ) = \mathscr{O}^\ell(\mathbf{p})$. Thus, the standard relaxations generated over a sequence of subintervals of P, $\{P^\ell\}$, can be represented simply by the generalized relaxations evaluated at a sequence of points in $\tilde{\Phi}$, $\{\mathbf{y}^{\circ,\ell}\}$. By Lemma 9, $\tilde{\Phi}$ is compact and connected, so $\tilde{\mathscr{U}}$ and $\tilde{\mathscr{O}}$ are continuous on $\tilde{\Phi}$ (uniformly so since $\tilde{\Phi}$ is compact). The immediate consequence of this fact is that $\mathscr{U}^\ell$ and $\mathscr{O}^\ell$ must vary continuously with respect to the bounds $\mathbf{p}^{L,\ell}$ and $\mathbf{p}^{U,\ell}$. This notion is formalized in the following Lemma.

Lemma 10 *Choose any two subintervals of P with nonempty intersection, P^1 and P^2. Given any $\epsilon > 0$, there exists δ independent of $\mathbf{p}$ such that $|\mathscr{U}^1(\mathbf{p}) - \mathscr{U}^2(\mathbf{p})| \leq \epsilon$ and $|\mathscr{O}^1(\mathbf{p}) - \mathscr{O}^2(\mathbf{p})| \leq \epsilon$, for all $\mathbf{p} \in P^1 \cap P^2$, provided that $||\mathbf{p}^{L,1} - \mathbf{p}^{L,2}||_2 + ||\mathbf{p}^{U,1} - \mathbf{p}^{U,2}||_2 \leq \delta$.*

Proof The result is a direct consequence of Theorem 6 and the discussion above. By the uniform continuity of $\tilde{\mathscr{U}}$ and $\tilde{\mathscr{O}}$ on $\tilde{\Phi}$, for any $\mathbf{y}^{\circ,1}, \mathbf{y}^{\circ,2} \in \tilde{\Phi}$ and any $\epsilon > 0$, there exists $\delta > 0$ such that $|\tilde{\mathscr{U}}(\mathbf{y}^{\circ,1}) - \tilde{\mathscr{U}}(\mathbf{y}^{\circ,2})| \leq \epsilon$ and $|\tilde{\mathscr{O}}(\mathbf{y}^{\circ,1}) - \tilde{\mathscr{O}}(\mathbf{y}^{\circ,2})| \leq \epsilon$ provided that $||\mathbf{y}^{\circ,1} - \mathbf{y}^{\circ,2}||_2 \leq \delta$. Letting $y_i^{L,\ell} = p_i^{L,\ell}$, $y_i^{U,\ell} = p_i^{U,\ell}$ and $y_i^{c,\ell} = y_i^{C,\ell} = p_i$, for all $i = 1, \ldots, n_p$ and $\ell = 1, 2$, this gives $|\mathscr{U}^1(\mathbf{p}) - \mathscr{U}^2(\mathbf{p})| \leq \epsilon$ and $|\mathscr{O}^1(\mathbf{p}) - \mathscr{O}^2(\mathbf{p})| \leq \epsilon$, for all $\mathbf{p} \in P^1 \cap P^2$, provided that $||\mathbf{p}^{L,1} - \mathbf{p}^{L,2}||_2 + ||\mathbf{p}^{U,1} - \mathbf{p}^{U,2}||_2 \leq \delta$. □

From this Lemma, convergence results can be shown much more simply. For example, the convergence result in Theorem 5 is an immediate consequence. The following theorem addresses the behavior of relaxations on a convergent sequence of intervals which do not necessarily converge to a degenerate interval. This is stronger than the convergence result presented in Sect. 3.3 and was not addressed in [17]. In fact, this result is not necessary to ensure the convergence of branch-and-bound algorithms using standard McCormick relaxations [11]. However, it will be required when relaxations of the solutions of ODEs are considered in Sect. 7.3.

Theorem 7 *McCormick's relaxations are partition convergent.*

Proof Choose any nested and convergent sequence of subintervals of P, $\{P^\ell\} \to P^*$. Given any $\epsilon > 0$, Lemma 10 provides δ such that $|\mathscr{U}^\ell(\mathbf{p}) - \mathscr{U}^*(\mathbf{p})| \leq \epsilon$ for all $\mathbf{p} \in P^*$, provided that $||\mathbf{p}^{L,\ell} - \mathbf{p}^{L,*}||_2 + ||\mathbf{p}^{U,\ell} - \mathbf{p}^{U,*}||_2 \leq \delta$. By the convergence of $\{P^\ell\}$, this condition must be satisfied for every ℓ greater than some N, which implies that $\{\mathscr{U}^\ell\} \to \mathscr{U}^*$ uniformly on P^*. The exact same proof applies to $\{\mathscr{O}^\ell\}$. □

5.2 Partial relaxations

Suppose for the following discussion that $\mathscr{F} : I \times P \to \mathbb{R}$, where $I \subset \mathbb{R}$ is a closed, bounded interval, and it is desirable to compute relaxations of $\mathscr{F}$ on P for each fixed $t \in I$. The assumption that t is scalar is unnecessary, but simplifies matters. Such a relaxation can be constructed, for any $t \in I$, by choosing the degenerate interval $[t, t]$ and constructing the $n_p + 1$ - dimensional standard McCormick relaxations of $\mathscr{F}$ on the interval $[t, t] \times P$. In the language of generalized McCormick relaxations, this task is accomplished by letting $n = n_p + 1$, defining $\Phi = I \times P$, letting $\mathscr{V}$ be the collection of factors defining $\mathscr{F}$ with variables t and $\mathbf{p}$ and considering, for each $(t, \mathbf{p}) \in I \times P$, those $\mathbf{y}^\circ \in \tilde{\Phi}$ for which $y_1^L = y_1^U = y_1^c = y_1^C = t$, $y_i^c = y_i^C = p_{i-1}$, $y_i^L = p_{i-1}^L$ and $y_i^U = p_{i-1}^U$ for all $i = 2, \ldots, n_p + 1$. Thus, for any $t \in I$, the desired relaxations can be interpreted as the generalized relaxations evaluated at certain appropriate points in $\tilde{\Phi}$. As was the case for relaxations on sequences of intervals, the properties of generalized relaxations have important implications for partial relaxations, when viewed as a special case of the generalized formulation.

Corollary 1 *Define the mapping* $\hat{\mathscr{U}} : I \times P \to \mathbb{R}$ *for any* $(t, \mathbf{p}) \in I \times P$ *by* $\hat{\mathscr{U}}(t, \mathbf{p}) = \mathscr{U}(t, \mathbf{p})$ *where* $\mathscr{U}$ *is the standard McCormick convex relaxation of* $\mathscr{F}$ *on* $[t, t] \times P$, *and define* $\hat{\mathscr{O}}$ *in an analogous manner. Then* $\hat{\mathscr{U}}$ *and* $\hat{\mathscr{O}}$ *are continuous on* $I \times P$. *Under Assumptions 9 and 10,* $\hat{\mathscr{U}}$ *and* $\hat{\mathscr{O}}$ *are Lipschitz on* $I \times P$.

Proof The result is a direct application of Theorem 6, Lemma 9 and the discussion above. □

The key result above is continuity and the Lipschitz condition on I. Since changing t requires changing the values $v_1^{L/U/c/C}$ in the standard relaxation, this result cannot be proven directly by the continuity result in the standard framework.

5.3 Compositions

Consider the function $\mathscr{F} : P \to \mathbb{R}$ defined for each $\mathbf{p} \in P$ by $\mathscr{F}(\mathbf{p}) = \mathcal{G}(\mathbf{p}, \mathbf{x}(\mathbf{p}))$, where $\mathcal{G} : P \times D \to \mathbb{R}$ is defined by the collection of factors $\mathscr{V}$, $D \subset \mathbb{R}^{n_x}$ and $\mathbf{x} : P \to D$. The functions x_i may not be factorable, but suppose that valid bounds $X \equiv [\mathbf{x}^L, \mathbf{x}^U] \subset D$

and relaxations $\mathbf{x}^{c/C}$ are available on P by some other means. Similar to the construction in Proposition 3, valid relaxations of $\mathscr{F}$ on P, $\mathscr{U}$ and $\mathscr{O}$, can be derived from the generalized relaxations $\mathscr{F}$, $\tilde{\mathscr{U}}$ and $\tilde{\mathscr{O}}$. In particular, let Φ be the $n_p + n_x$-dimensional interval $P \times X$ and define $\mathscr{U}$ and $\mathscr{O}$ for all $\mathbf{p} \in P$ by

$$\mathscr{U}(\mathbf{p}) \equiv \tilde{\mathscr{U}}\Big(p_1^L, p_1^U, p_1, p_1, \ldots, p_{n_p}^L, p_{n_p}^U, p_{n_p}, p_{n_p}, x_1^L, x_1^U, \text{mid}\left(x_1^L, x_1^U, x_1^c(\mathbf{p})\right), \text{mid}\left(x_1^L, x_1^U, x_1^C(\mathbf{p})\right), \ldots, x_{n_x}^L, x_{n_x}^U, \text{mid}\left(x_{n_x}^L, x_{n_x}^U, x_{n_x}^c(\mathbf{p})\right), \text{mid}\left(x_{n_x}^L, x_{n_x}^U, x_{n_x}^C(\mathbf{p})\right)\Big), \tag{4}$$

$$\mathscr{O}(\mathbf{p}) \equiv \tilde{\mathscr{O}}\Big(p_1^L, p_1^U, p_1, p_1, \ldots, p_{n_p}^L, p_{n_p}^U, p_{n_p}, p_{n_p}, x_1^L, x_1^U, \text{mid}\left(x_1^L, x_1^U, x_1^c(\mathbf{p})\right), \text{mid}\left(x_1^L, x_1^U, x_1^C(\mathbf{p})\right), \ldots, x_{n_x}^L, x_{n_x}^U, \text{mid}\left(x_{n_x}^L, x_{n_x}^U, x_{n_x}^c(\mathbf{p})\right), \text{mid}\left(x_{n_x}^L, x_{n_x}^U, x_{n_x}^C(\mathbf{p})\right)\Big). \tag{5}$$

Theorem 8 *If $\mathbf{x}(\mathbf{p}) \in [\mathbf{x}^L, \mathbf{x}^U]$ for all $\mathbf{p} \in P$ and $\mathbf{x}^c$ and $\mathbf{x}^C$ are, respectively, convex and concave relaxations of $\mathbf{x}$ on P, then $\mathscr{U}$ and $\mathscr{O}$ are, respectively, convex and concave relaxations of $\mathscr{F}$ on P.*

Proof By hypothesis, $\mathbf{x}^c$ and $\mathbf{x}^C$ are, respectively, convex and concave relaxations of $\mathbf{x}$ on P. Since $\mathbf{x}(\mathbf{p}) \in [\mathbf{x}^L, \mathbf{x}^U]$ for all $\mathbf{p} \in P$, this implies that $\mathbf{x}^c(\mathbf{p}) \le \mathbf{x}^U$ and $\mathbf{x}^C(\mathbf{p}) \ge \mathbf{x}^L$ for all $\mathbf{p} \in P$. Then $\text{mid}\left(\mathbf{x}^L, \mathbf{x}^U, \mathbf{x}^c(\cdot)\right)$ and $\text{mid}\left(\mathbf{x}^L, \mathbf{x}^U, \mathbf{x}^C(\cdot)\right)$ are, respectively, convex and concave relaxations of $\mathbf{x}$ on P. Proposition 3 and the definitions (4) and (5) now show that $\mathscr{U}$ and $\mathscr{O}$ are, respectively, convex and concave relaxations of $\mathscr{F}$ on P.

For this application, Φ is an interval, so $\tilde{\Phi}$ is compact and connected by Lemma 9, and hence Theorem 6 applies to all of $\tilde{\Phi}$. Then, if $\mathbf{x}^{c/C}$ are continuous on P, so are $\mathscr{U}$ and $\mathscr{O}$. Further, if $\mathbf{x}^{c/C}$ are Lipschitz on P and Assumptions 9 and 10 hold, then Theorem 6 implies that $\mathscr{U}$ and $\mathscr{O}$ are Lipschitz on P as well.

It is also possible to show that if the relaxations $\mathbf{x}^c$ and $\mathbf{x}^C$ are generated by a procedure which is partition monotonic, partition convergent and degenerate perfect, then generating relaxations of $\mathscr{F}$ through (4) and (5) is a partition monotonic, partition convergent and degenerate perfect procedure. The following assumption is required.

Assumption 11 For any subinterval $P^\ell \subset P$, valid bounds for $\mathbf{x}$ on P^ℓ, $X^\ell = [\mathbf{x}^{L,\ell}, \mathbf{x}^{U,\ell}]$, are available. Moreover, for any nested and convergent sequence of subintervals of P, $\{P^\ell\} \to P^*$,

1. $X^{\ell+1} \subset X^\ell \subset X$, for any $\ell \in \mathbb{N}$,
2. $\{X^\ell\} \to X^*$, and
3. $P^* = [\mathbf{p}, \mathbf{p}]$ for some $\mathbf{p} \in P$ implies that $X^* = [\mathbf{x}(\mathbf{p}), \mathbf{x}(\mathbf{p})]$.

For any $P^\ell(P^*)$, it is now sensible to define the functions $\mathscr{U}^\ell$ and $\mathscr{O}^\ell$ ($\mathscr{U}^*$ and $\mathscr{O}^*$) as in (4) and (5) with P^ℓ and $X^\ell(P^*$ and $X^*)$ in place of P and X.

Theorem 9 *Suppose that, given any interval $P^\ell \subset P$, convex and concave relaxations of $\mathbf{x}$ on P^ℓ, $\mathbf{x}^{c,\ell}$ and $\mathbf{x}^{C,\ell}$, respectively, are available through a procedure which is partition monotonic. Then generating convex and concave relaxations of $\mathscr{F}$ on P^ℓ by (4) and (5), respectively, is a partition monotonic procedure.*

Proof Choose any subintervals $P^2 \subset P^1 \subset P$. Now, by (4), (5) and Definition 15, for any $\mathbf{p} \in P^2$, the first $n_p + n_x$ factors in the construction of $\mathscr{U}^{\ell}$ are assigned as follows:

$$v_i^{L,\ell} = p_i^{L,\ell},\ v_i^{U,\ell} = p_i^{U,\ell},\ v_i^{c,\ell} = v_i^{C,\ell} = p_i, \quad \forall i = 1,\ldots,n_p,$$
$$\left.\begin{array}{c} v_{i+n_p}^{L,\ell} = x_i^{L,\ell},\ v_{i+n_p}^{U,\ell} = x_i^{U,\ell},\ v_{i+n_p}^{c,\ell} = \mathrm{mid}(x_i^{L,\ell}, x_i^{U,\ell}, x_i^{c,\ell}(\mathbf{p})), \\ v_{i+n_p}^{C,\ell} = \mathrm{mid}(x_i^{L,\ell}, x_i^{U,\ell}, x_i^{C,\ell}(\mathbf{p})) \end{array}\right\} \quad \forall i = 1,\ldots,n_x.$$

By hypothesis, the inequalities $\mathbf{x}^{c,2}(\mathbf{p}) \geq \mathbf{x}^{c,1}(\mathbf{p})$, $\mathbf{x}^{C,2}(\mathbf{p}) \leq \mathbf{x}^{C,1}(\mathbf{p})$, $\mathbf{x}^{c,2}(\mathbf{p}) \leq \mathbf{x}^{U,2}$ and $\mathbf{x}^{C,2}(\mathbf{p}) \geq \mathbf{x}^{L,2}$ all hold for all $\mathbf{p} \in P^2$. Then it is clear from the action of the mid function and Condition 1 in Assumption 11 that, for any $i \leq n_p + n_x$ and any $\mathbf{p} \in P^2$, $V_i^2 \subset V_i^1$, $v_i^{c/C,1}(\mathbf{p}) \in V_i^1$, $v_i^{c/C,2}(\mathbf{p}) \in V_i^2$, and $v_i^{c,1}(\mathbf{p}) \leq v_i^{c,2}(\mathbf{p}) \leq v_i^{C,2}(\mathbf{p}) \leq v_i^{C,1}(\mathbf{p})$. Choose any $n_p + n_x + 1 \leq k \leq m$ and suppose that these conditions hold for all $i < k$. Then the hypotheses of Lemma 5 are satisfied, so that $\bar{v}_k^{c,2}(\mathbf{p}) \geq \bar{v}_k^{c,1}(\mathbf{p})$ and $\bar{v}_k^{C,2}(\mathbf{p}) \leq \bar{v}_k^{C,1}(\mathbf{p})$, $\forall \mathbf{p} \in P^2$. Then, the inductive step is completed exactly as in the proof of Theorem 4, so that repeated application of Lemma 5 shows that $\mathscr{U}^2(\mathbf{p}) \geq \mathscr{U}^1(\mathbf{p})$ and $\mathscr{O}^2(\mathbf{p}) \leq \mathscr{O}^1(\mathbf{p})$, $\forall \mathbf{p} \in P^2$. □

Theorem 10 *Suppose that, given any interval $P^{\ell} \subset P$, convex and concave relaxations of $\mathbf{x}$ on P^{ℓ}, $\mathbf{x}^{c,\ell}$ and $\mathbf{x}^{C,\ell}$, respectively, are available through a procedure which is partition convergent and degenerate perfect. Then generating convex and concave relaxations of $\mathscr{F}$ on P^{ℓ} by (4) and (5), respectively, is a partition convergent and degenerate perfect procedure.*

Proof Consider any nested and convergent sequence of subintervals of P, $\{P^{\ell}\} \to P^*$. For each $\mathbf{p} \in P^*$ and each $\ell \in \mathbb{N}$ (and $\ell = *$), the point

$$\begin{aligned}\mathbf{y}^{\circ,\ell} = (&p_1^{L,\ell}, p_1^{U,\ell}, p_1, p_1, \ldots, p_{n_p}^{L,\ell}, p_{n_p}^{U,\ell}, p_{n_p}, p_{n_p},\\ &x_1^{L,\ell}, x_1^{U,\ell}, \mathrm{mid}(x_1^{L,\ell}, x_1^{U,\ell}, x_1^{c,\ell}(\mathbf{p})), \mathrm{mid}(x_1^{L,\ell}, x_1^{U,\ell}, x_1^{C,\ell}(\mathbf{p})),\\ &\ldots, x_{n_x}^{L,\ell}, x_{n_x}^{U,\ell}, \mathrm{mid}(x_{n_x}^{L,\ell}, x_{n_x}^{U,\ell}, x_{n_x}^{c,\ell}(\mathbf{p})), \mathrm{mid}(x_{n_x}^{L,\ell}, x_{n_x}^{U,\ell}, x_{n_x}^{C,\ell}(\mathbf{p})))\end{aligned}$$

is in $\tilde{\Phi}$. Now, for each $\mathbf{p} \in P^*$, the sequence $\{\mathbf{y}^{\circ,\ell}\}$ must converge to $\mathbf{y}^{\circ,*}$ by the convergence of the sequences $\{P^{\ell}\}$, $\{X^{\ell}\}$, $\{\mathbf{x}^{c,\ell}\}$ and $\{\mathbf{x}^{C,\ell}\}$. Given any $\delta > 0$, each of these sequences has some integer N above which every element deviates from its limit by less than δ in the appropriate norm. Further, these integers can be chosen independently of the point $\mathbf{p} \in P^*$ because $\{\mathbf{x}^{c,\ell}\}$ and $\{\mathbf{x}^{C,\ell}\}$ are assumed to converge uniformly on P^*. Taking the largest of these integers, this implies that, given any $\delta > 0$, it is possible to find an integer N for which $||\mathbf{y}^{\circ,\ell} - \mathbf{y}^{\circ,*}||_2 \leq \delta$ for all $\ell \geq N$ and all $\mathbf{p} \in P^*$. Now by the definition of $\mathscr{U}^{\ell}$ and $\mathscr{O}^{\ell}$ and the uniform continuity of $\tilde{\mathscr{U}}$ and $\tilde{\mathscr{O}}$ on $\tilde{\Phi}$, this implies the uniform convergence of $\{\mathscr{U}^{\ell}\}$ and $\{\mathscr{O}^{\ell}\}$ on P^*. Indeed, given any $\epsilon > 0$, uniform continuity ensures that there exists δ such that $|\tilde{\mathscr{U}}(\mathbf{y}^{\circ,\ell}) - \tilde{\mathscr{U}}(\mathbf{y}^{\circ,*})| \leq \epsilon$ if $||\mathbf{y}^{\circ,\ell} - \mathbf{y}^{\circ,*}||_2 \leq \delta$, which is true for every $\ell \geq N$, regardless of $\mathbf{p} \in P^*$. Of course, an analogous argument applies for $\{\mathscr{O}^{\ell}\}$.

Now, if $P^* = [\mathbf{p}, \mathbf{p}]$ for some $\mathbf{p} \in P$, Condition 3 of Assumption 11 ensures that $X^* = [\mathbf{x}(\mathbf{p}), \mathbf{x}(\mathbf{p})]$. Then $\mathscr{U}^*$ and $\mathscr{O}^*$ are nothing more than the standard McCormick relaxations of $\mathcal{G}$ constructed on the degenerate interval $P^* \times X^*$. Therefore, $\mathscr{U}^*(\mathbf{p}) = \mathscr{O}^*(\mathbf{p}) = \mathcal{G}(\mathbf{p}, \mathbf{x}(\mathbf{p})) = \mathscr{F}(\mathbf{p})$ by Theorem 5. □

6 Relaxations of the parametric solutions of algebraic systems

In this section, relaxations for the parametric solutions of algebraic systems are discussed. In particular, the system of equations

$$\mathbf{x}(\mathbf{p}) = \mathbf{h}(\mathbf{p}, \mathbf{x}(\mathbf{p})), \tag{6}$$

is considered, where $\mathbf{h} : P \times D \to \mathbb{R}^{n_x}$ is continuous and $D \subset \mathbb{R}^{n_x}$ is an open connected set. The objective is to construct convex and concave relaxations of the parametric solution $\mathbf{x}$ on P. This is the first application where the aim is to construct relaxations for a function which is not factorable and in fact not even known explicitly. Our approach is to construct a convergent sequence of iterates, which are in fact factorable functions, and to construct corresponding sequences of convex and concave relaxations.

6.1 Algebraic systems background

Definition 18 ($\mathscr{C}^0(P), Z_\infty, \mathscr{H}$) Let $\mathscr{C}^0(P)$ denote the space of continuous functions from P to $\mathbb{R}^{n_x}$ with norm $\|\mathbf{z}\|_\infty \equiv \max_{\mathbf{p}\in P} \|\mathbf{z}(\mathbf{p})\|_1$. For any $Z \subset D$, let $Z_\infty \equiv \{\mathbf{z} \in \mathscr{C}^0(P) : \mathbf{z}(\mathbf{p}) \in Z,\ \forall \mathbf{p} \in P\}$. Finally, define $\mathscr{H} : \mathscr{C}^0(P) \to \mathscr{C}^0(P)$ by $(\mathscr{H}\mathbf{z})(\mathbf{p}) \equiv \mathbf{h}(\mathbf{p}, \mathbf{z}(\mathbf{p}))$, for every $\mathbf{p} \in P$.

Definition 19 (Contraction) For any $Z \subset D$, an operator $\mathscr{L} : \mathscr{C}^0(P) \to \mathscr{C}^0(P)$ is a contraction of Z_∞ into itself if $\mathscr{L} : Z_\infty \to Z_\infty$ and $\exists \gamma \in [0, 1)$ such that $\|\mathscr{L}\mathbf{z} - \mathscr{L}\mathbf{y}\|_\infty \leq \gamma\|\mathbf{z} - \mathbf{y}\|_\infty, \forall \mathbf{z}, \mathbf{y} \in Z_\infty$.

Assumption 12 There exists some $X \equiv [\mathbf{x}^L, \mathbf{x}^U] \subset D$ such that $\mathscr{H}$ is a contraction of X_∞ into itself.

Remark 3 Numerical methods for computing an appropriate interval X by extension of the non-parametric interval methods in [20] are briefly discussed in [9]. Furthermore, the parametric case is treated in detail in an article in preparation by the authors [31].

$\mathscr{C}^0(P)$ is a Banach space under the given norm. Furthermore, X_∞ is itself a complete metric space because it is a closed subset of $\mathscr{C}^0(P)$. Thus, under Assumption 12, the contraction mapping theorem [25, Theorem 9.23] may be applied to show that (6) has a unique solution in X_∞, denoted $\mathbf{x}$, and the sequence $\{\mathbf{x}^k\}$ defined by $\mathbf{x}^{k+1} = \mathscr{H}\mathbf{x}^k$, with any $\mathbf{x}^0 \in X_\infty$, converges to $\mathbf{x}$ uniformly on P.

6.2 Constructing relaxations of the solutions of algebraic systems

Here, it is shown that generalized McCormick relaxations of $\mathbf{h}$ can be used to generate convex and concave relaxations of each $\mathbf{x}^k$. Since $\{\mathbf{x}^k\} \to \mathbf{x}$ uniformly on P for any $\mathbf{x}^0 \in X_\infty$, this implies that convex and concave relaxations of arbitrarily good approximations of $\mathbf{x}$ can be constructed by this method.

For the following discussion, assume that h_i is factorable for all $i = 1, \ldots, n_x$ and let $\mathscr{V}_i$ denote the corresponding collection of factors. Let $\Phi = P \times X$, let $\tilde{\mathscr{U}}_{h_i}$ and $\tilde{\mathscr{O}}_{h_i}$ denote the generalized McCormick relaxations of h_i, and let $\tilde{\mathscr{U}}_{\mathbf{h}}$ and $\tilde{\mathscr{O}}_{\mathbf{h}}$ be vector functions with elements $\tilde{\mathscr{U}}_{h_i}$ and $\tilde{\mathscr{O}}_{h_i}$. Finally, assume that $\mathscr{V}_i$ and the univariate relaxations and bounding operations defining $\tilde{\mathscr{U}}_{h_i}$ and $\tilde{\mathscr{O}}_{h_i}$ satisfy Assumptions 6, 7 and 8 in Sect. 4, for each

$i = 1, \ldots, n_x$. Now define the functions $\mathbf{u_h}, \mathbf{o_h} : P \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_x}$ by

$$\begin{aligned} \mathbf{u_h}(\mathbf{p}, \mathbf{z}, \mathbf{y}) = \tilde{\mathscr{U}}_{\mathbf{h}}(&p_1^L, p_1^U, p_1, p_1, \ldots, p_{n_p}^L, p_{n_p}^U, p_{n_p}, p_{n_p}, \\ &x_1^L, x_1^U, \text{mid}\left(x_1^L, x_1^U, z_1\right), \text{mid}\left(x_1^L, x_1^U, y_1\right), \ldots, \\ &x_{n_x}^L, x_{n_x}^U, \text{mid}\left(x_{n_x}^L, x_{n_x}^U, z_{n_x}\right), \text{mid}\left(x_{n_x}^L, x_{n_x}^U, y_{n_x}\right)), \end{aligned} \tag{7}$$

$$\begin{aligned} \mathbf{o_h}(\mathbf{p}, \mathbf{z}, \mathbf{y}) = \tilde{\mathscr{O}}_{\mathbf{h}}(&p_1^L, p_1^U, p_1, p_1, \ldots, p_{n_p}^L, p_{n_p}^U, p_{n_p}, p_{n_p}, \\ &x_1^L, x_1^U, \text{mid}\left(x_1^L, x_1^U, z_1\right), \text{mid}\left(x_1^L, x_1^U, y_1\right), \ldots, \\ &x_{n_x}^L, x_{n_x}^U, \text{mid}\left(x_{n_x}^L, x_{n_x}^U, z_{n_x}\right), \text{mid}\left(x_{n_x}^L, x_{n_x}^U, y_{n_x}\right)). \end{aligned} \tag{8}$$

It is clear from Theorem 6 that $\mathbf{u_h}$ and $\mathbf{o_h}$ are continuous on $P \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$. Further, under Assumptions 9 and 10, they are Lipschitz there.

Consider the sequences $\{\mathbf{c}^k\}$ and $\{\mathbf{C}^k\}$ defined by

$$\begin{aligned} \mathbf{c}^{k+1}(\mathbf{p}) &= \mathbf{u_h}(\mathbf{p}, \mathbf{c}^k(\mathbf{p}), \mathbf{C}^k(\mathbf{p})), \\ \mathbf{C}^{k+1}(\mathbf{p}) &= \mathbf{o_h}(\mathbf{p}, \mathbf{c}^k(\mathbf{p}), \mathbf{C}^k(\mathbf{p})), \end{aligned} \tag{9}$$

for all $\mathbf{p} \in P$, with any continuous $\mathbf{c}^0, \mathbf{C}^0 : P \to \mathbb{R}^{n_x}$. It is clear from the continuity of $\mathbf{u_h}, \mathbf{o_h}, \mathbf{c}^0$ and $\mathbf{C}^0$ that $\mathbf{c}^k$ and $\mathbf{C}^k$ are continuous for every $k \in \mathbb{N}$. In addition, the following relaxation properties hold.

Theorem 11 *Let $\mathbf{x}^0 \in X_\infty$. If $\mathbf{c}^0$ and $\mathbf{C}^0$ are, respectively, convex and concave relaxations of $\mathbf{x}^0$ on P, then $\mathbf{c}^k$ and $\mathbf{C}^k$ are, respectively, convex and concave relaxations of $\mathbf{x}^k$ on P, for every $k \in \mathbb{N}$.*

Proof By hypothesis, $\mathbf{c}^0$ and $\mathbf{C}^0$ are, respectively, convex and concave relaxations of $\mathbf{x}^0$ on P and $\mathbf{x}^0 \in X_\infty$. Suppose that this is true of $\mathbf{c}^k$, $\mathbf{C}^k$ and $\mathbf{x}^k$, for some $k \in \mathbb{N}$. Then, by Theorem 8, definitions (7) and (8), and the fact that $\mathscr{H} : X_\infty \to X_\infty$, it is also true of $\mathbf{c}^{k+1}$, $\mathbf{C}^{k+1}$ and $\mathbf{x}^{k+1}$. Now induction completes the proof. □

Theorem 11 only provides a means for generating relaxations of the iterates $\mathbf{x}^k$, not the solution $\mathbf{x}$, and there is no guarantee that the iterates generated through (9) converge. It is certainly true that any computational procedure for evaluating the function $\mathbf{x}$ is in fact only evaluating some iterate $\mathbf{x}^k$, and convex and concave relaxations for this approximate function evaluation are given by Theorem 11. Even so, the theory presented here is somewhat unsatisfactory since it cannot rigorously provide relaxations for the true solution of a general algebraic system. Rigorous relaxation and global optimization of the solutions of algebraic systems remains an active area of research for the authors.

Note that the interval X, which can be computed by an interval Newton-type method [31], is used directly in computing $\mathbf{c}^k$ and $\mathbf{C}^k$. Thus, the method presented here is not an alternative to interval Newton-type methods, but offers a potential refinement to bounds computed through such methods by deriving parameter dependent convex and concave bounds. By Step 6 in Definition 15, $\mathbf{c}^k$ and $\mathbf{C}^k$ are always at least as tight as X. On the other hand, they are often significantly tighter (See Sect. 6.4).

6.3 Relaxations of algebraic systems on nested sequences of intervals

In this section, we consider relaxations of $\mathbf{x}^k$ on subintervals $P^\ell \subset P$. The following assumption is required.

Assumption 13 For any interval $P^\ell \subset P$, some $X^\ell \subset X$ is available such that $\mathscr{H}$ is a contraction of $X^\ell_\infty \equiv \{\mathbf{z} \in \mathscr{C}^0(P^\ell) : \mathbf{z}(\mathbf{p}) \in X^\ell,\ \forall \mathbf{p} \in P^\ell\}$ into itself. Furthermore, for any nested and convergent sequence of subintervals of P, $\{P^\ell\} \to P^*$,

1. $X^{\ell+1} \subset X^\ell$ for every $\ell \in \mathbb{N}$,
2. $\{X^\ell\} \to X^*$, and
3. $P^* = [\mathbf{p}, \mathbf{p}]$ for some $\mathbf{p} \in P$ implies that $X^* = [\mathbf{x}(\mathbf{p}), \mathbf{x}(\mathbf{p})]$.

Consider a convergent sequence of intervals $\{P^\ell\} \to P^*$ and, for each $\ell \in \mathbb{N}$ and $\ell = *$, define $\mathbf{u}^\ell_\mathbf{h}$ and $\mathbf{o}^\ell_\mathbf{h}$ as in (7) and (8) with P^ℓ and X^ℓ in place of P and X. Furthermore, define the functions $\mathbf{x}^{k,\ell}$, $\mathbf{c}^{k,\ell}$ and $\mathbf{C}^{k,\ell}$ in the obvious manner. The following result concerns the convergence of the sequences of relaxations $\{\mathbf{c}^{k,\ell}\}$ and $\{\mathbf{C}^{k,\ell}\}$, for fixed $k \in \mathbb{N}$. Note that these iterates may not converge as $k \to \infty$ for fixed ℓ. Therefore, the choice of initial guesses $\mathbf{x}^{0,\ell}$, $\mathbf{c}^{0,\ell}$ and $\mathbf{C}^{0,\ell}$ is crucial to the result.

Theorem 12 *Consider any nested and convergent sequence of subintervals of P, $\{P^\ell\} \to P^*$. For each $\ell \in \mathbb{N}$ and $\ell = *$, let $\mathbf{x}^{0,\ell} \in X^\ell$ and let $\mathbf{c}^{0,\ell}$ and $\mathbf{C}^{0,\ell}$ be, respectively, convex and concave relaxations of $\mathbf{x}^{0,\ell}$ on P^ℓ. Suppose further that $\{\mathbf{x}^{0,\ell}\} \to \mathbf{x}^{0,*}$, $\{\mathbf{c}^{0,\ell}\} \to \mathbf{c}^{0,*}$ and $\{\mathbf{C}^{0,\ell}\} \to \mathbf{C}^{0,*}$ uniformly on P^*. Then, for any fixed $k \in \mathbb{N}$, $\{\mathbf{x}^{k,\ell}\} \to \mathbf{x}^{k,*}$, $\{\mathbf{c}^{k,\ell}\} \to \mathbf{c}^{k,*}$ and $\{\mathbf{C}^{k,\ell}\} \to \mathbf{C}^{k,*}$ uniformly on P^*. Furthermore, if $P^* = [\mathbf{p}, \mathbf{p}]$ for some $\mathbf{p} \in P$, then $\mathbf{c}^{k,*}(\mathbf{p}) = \mathbf{x}(\mathbf{p}) = \mathbf{C}^{k,*}(\mathbf{p})$ for every $k > 0$.*

Proof Choose any nested and convergent sequence of subintervals of P, $\{P^\ell\} \to P^*$. Since the set $P \times X$ is compact, $\mathbf{h}$ is uniformly continuous there. Then, choosing any $k \in \mathbb{N}$ and any $\epsilon > 0$, there must exist $\delta > 0$ such that $\|\mathbf{x}^{k+1,\ell}(\mathbf{p}) - \mathbf{x}^{k+1,*}(\mathbf{p})\|_1 \le \epsilon$ for all $\mathbf{p} \in P^*$ provided that $\|\mathbf{x}^{k,\ell}(\mathbf{p}) - \mathbf{x}^{k,*}(\mathbf{p})\|_1 \le \delta$ for all $\mathbf{p} \in P^*$. Note that δ is independent of k because the sequence $\{X^\ell\}$ is nested so that $X^\ell \subset X$ for every $\ell \in \mathbb{N}$. Now if $\{\mathbf{x}^{k,\ell}\} \to \mathbf{x}^{k,*}$ uniformly on P^* for some fixed $k \in \mathbb{N}$, then there exists ℓ large enough that $\|\mathbf{x}^{k,\ell}(\mathbf{p}) - \mathbf{x}^{k,*}(\mathbf{p})\|_1 \le \delta$ for all $\mathbf{p} \in P^*$. But this implies that there exists ℓ large enough that $\|\mathbf{x}^{k+1,\ell}(\mathbf{p}) - \mathbf{x}^{k+1,*}(\mathbf{p})\|_1 \le \epsilon$ for all $\mathbf{p} \in P^*$. Thus, $\{\mathbf{x}^{k+1,\ell}\} \to \mathbf{x}^{k+1,*}$ uniformly on P^* as $\ell \to \infty$. Now by the hypothesis that $\{\mathbf{x}^{0,\ell}\} \to \mathbf{x}^{0,*}$ uniformly on P^*, induction shows that $\{\mathbf{x}^{k,\ell}\} \to \mathbf{x}^{k,*}$ uniformly on P^*, for every $k \in \mathbb{N}$.

Suppose that, for some $k \in \mathbb{N}$, $\{\mathbf{c}^{k,\ell}\} \to \mathbf{c}^{k,*}$ and $\{\mathbf{C}^{k,\ell}\} \to \mathbf{C}^{k,*}$ uniformly on P^*. By hypothesis, this is true for $k = 0$. An argument identical to the proof of Theorem 10 shows that $\{\mathbf{c}^{k+1,\ell}\} \to \mathbf{c}^{k+1,*}$ and $\{\mathbf{C}^{k+1,\ell}\} \to \mathbf{C}^{k+1,*}$ uniformly on P^*, and induction proves that this is true for all $k \in \mathbb{N}$.

Finally, $P^* = [\mathbf{p}, \mathbf{p}]$ for some $\mathbf{p} \in P$ directly implies that $\mathbf{c}^{k,*}(\mathbf{p}) = \mathbf{x}(\mathbf{p}) = \mathbf{C}^{k,*}(\mathbf{p})$ for every $k > 0$ by Assumption 13 and induction on Theorem 10. □

Under the assumptions of the previous theorem, it is not sensible to consider partition monotonicity or partition convergence. This is simply because the function being relaxed, $\mathbf{x}^{k,\ell}$, varies with ℓ. However, if $\mathbf{x}^0$ is fixed (i.e., each $\mathbf{x}^{0,\ell}$ is simply the restriction of $\mathbf{x}^0$ to P^ℓ), then it is clear that each $\mathbf{x}^k$ is also fixed and Theorem 12 clearly implies that the procedure for generating $\mathbf{c}^{k,\ell}$ and $\mathbf{C}^{k,\ell}$ is partition convergent for each fixed $k \in \mathbb{N}$. Moreover, in this case it follows easily from Theorem 9 that the procedure for generating $\mathbf{c}^{k,\ell}$ and $\mathbf{C}^{k,\ell}$, for any $k \in \mathbb{N}$, is partition monotonic provided that the procedure for generating $\mathbf{c}^{0,\ell}$ and $\mathbf{C}^{0,\ell}$ is partition monotonic.

6.4 Example problem

Consider the nonlinear equation

$$f(p,x) = x - \left(p - \frac{p^3}{6} + \frac{p^5}{120}\right)x^{-1/2} - 100 = 0, \tag{10}$$

with $p \in P \equiv [0.5, 5.0]$. It is desired to solve (10) for the implicit function $x : P \to \mathbb{R}$ and to calculate convex and concave relaxations of x which are valid on P. The Eq. (10) is easily rearranged to the form of (6) with

$$h(p,x) = \left(p - \frac{p^3}{6} + \frac{p^5}{120}\right)x^{-1/2} + 100. \tag{11}$$

An interval X satisfying Assumptions 12 and 13 can be computed using the parametric interval successive substitution algorithm, described in an article in preparation by the authors (see Remark 3), which results in $X = [x^L, x^U] = [97.9, 103.1]$. Now, it is guaranteed that the iterates x^k defined by

$$x^{k+1} := \left(p - \frac{p^3}{6} + \frac{p^5}{120}\right)(x^k)^{-1/2} + 100 \tag{12}$$

will converge for any $p \in P$, beginning from any $x_0 \in X$.

In order to construct convex and concave relaxations for the iterates x^k, we need to construct functions u_h and o_h through (7), (8) and Definition 15. These functions are given explicitly by the factorization in Table 1. Note that the table omits the simple calculation of $v_k^{c/C}$ from $\bar{v}_k^{c/C}$ as per Step 6 in Definition 15. Using the relaxations and bounding operations for univariate functions described in Sect. II of Online Resource 1, the quantities and functions in Table 1 are specified as follows.

First, consider factors 3 and 6, which both involve raising a previous factor to an odd integer power. The convex and concave envelopes of odd powers are described in detail in [13]. Accordingly, the functions e_{U_3}, E_{U_3}, e_{U_6} and E_{U_6} are all defined by the procedure below, where $q = 3$ in the definition of e_{U_3} and E_{U_3}, and $q = 5$ in the definition of e_{U_6} and E_{U_6}. Let p' and p'' be, respectively, the solutions of

$$(q-1)(p')^q - qp^L(p')^{q-1} + (p^L)^q = 0 \quad \text{and} \quad (q-1)(p'')^q - qp^U(p'')^{q-1} + (p^U)^q = 0.$$

Next, define

$$p^* = \begin{cases} p^U & \text{if } \ p^U \le 0 \\ p^L & \text{if } \ p^L \ge 0 \\ p' & \text{otherwise} \end{cases}, \quad p^{**} = \begin{cases} p^U & \text{if } \ p^U \le 0 \\ p^L & \text{if } \ p^L \ge 0 \\ p'' & \text{otherwise} \end{cases}.$$

Now, let

$$\omega(s) = \begin{cases} s^q & \text{if } \ s \in [p^*, p^U] \\ (p^L)^q + \frac{(p^*)^q - (p^L)^q}{p^* - p^L}(s - p^L) & \text{otherwise} \end{cases}$$

and

$$\Omega(s) = \begin{cases} s^q & \text{if } \ s \in [p^L, p^{**}] \\ (p^{**})^q + \frac{(p^U)^q - (p^{**})^q}{p^U - p^{**}}(s - p^{**}) & \text{otherwise} \end{cases}.$$

Table 1 Factorization of h, evaluated at (p, x), and the relaxations u_h and o_h, evaluated at (p, z, y)

i	v_i	v_i^L	v_i^U	$\bar{v}_i^c$	$\bar{v}_i^C$
1	p	p^L	p^U	p	p
2	x	x^L	x^U	$\text{mid}(x^L, x^U, z)$	$\text{mid}(x^L, x^U, y)$
3	v_1^3	$(v_1^L)^3$	$(v_1^U)^3$	$e_{U_3}(\text{mid}(v_1^c, v_1^C, v_1^L))$	$E_{U_3}(\text{mid}(v_1^c, v_1^C, v_1^U))$
4	$(1/6)v_3$	$(1/6)v_3^L$	$(1/6)v_3^U$	$(1/6)v_3^c$	$(1/6)v_3^C$
5	$-v_4$	$-v_4^U$	$-v_4^L$	$-\text{mid}(v_4^c, v_4^C, v_4^U)$	$-\text{mid}(v_4^c, v_4^C, v_4^L)$
6	v_1^5	$(v_1^L)^5$	$(v_1^U)^5$	$e_{U_6}(\text{mid}(v_1^c, v_1^C, v_1^L))$	$E_{U_6}(\text{mid}(v_1^c, v_1^C, v_1^U))$
7	$(1/120)v_6$	$(1/120)v_6^L$	$(1/120)v_6^U$	$(1/120)\text{mid}(v_6^c, v_6^C, v_6^L)$	$(1/120)\text{mid}(v_6^c, v_6^C, v_6^U)$
8	$v_1 + v_5$	$v_1^L + v_5^L$	$v_1^U + v_5^U$	$v_1^c + v_5^c$	$v_1^C + v_5^C$
9	$v_7 + v_8$	$v_7^L + v_8^L$	$v_7^U + v_8^U$	$v_7^c + v_8^c$	$v_7^C + v_8^C$
10	$\sqrt{v_2}$	$\sqrt{v_2^L}$	$\sqrt{v_2^U}$	$e_{U_{10}}(\text{mid}(v_2^c, v_2^C, v_2^L))$	$E_{U_{10}}(\text{mid}(v_2^c, v_2^C, v_2^U))$
11	$1/v_{10}$	$1/v_{10}^U$	$1/v_{10}^L$	$e_{U_{11}}(\text{mid}(v_{10}^c, v_{10}^C, v_{10}^U))$	$E_{U_{11}}(\text{mid}(v_{10}^c, v_{10}^C, v_{10}^L))$
12	$v_9 v_{11}$	min	max	max	min
		$(v_9^L v_{11}^L, v_9^U v_{11}^U,$	$(v_9^L v_{11}^L, v_9^U v_{11}^U,$	$(\alpha_9 + \alpha_{11} - v_{11}^L v_9^L,$	$(\gamma_9 + \gamma_{11} - v_{11}^L v_9^U,$
		$v_9^L v_{11}^U, v_9^U v_{11}^L)$	$v_9^L v_{11}^U, v_9^U v_{11}^L)$	$\beta_9 + \beta_{11} - v_{11}^U v_9^U)$	$\delta_9 + \delta_{11} - v_{11}^U v_9^L)$
13	$v_{12} + 100$	$v_{12}^L + 100$	$v_{12}^U + 100$	$\text{mid}(v_{12}^c, v_{12}^C, v_{12}^L) + 100$	$\text{mid}(v_{12}^c, v_{12}^C, v_{12}^U) + 100$

Finally, if $q = 3$, then $e_{U_3}(s) = \omega(s)$ and $E_{U_3}(s) = \Omega(s)$, and if $q = 5$, then $e_{U_6}(s) = \omega(s)$ and $E_{U_6}(s) = \Omega(s)$.

The convex and concave relaxations for the square root in factor 10 are defined by

$$e_{U_{10}}(s) = \sqrt{v_2^L} + \frac{\sqrt{v_2^U} - \sqrt{v_2^L}}{v_2^U - v_2^L}(s - v_2^L), \quad \text{and} \quad E_{U_{10}}(s) = \sqrt{s}.$$

Next, the convex and concave relaxations for the reciprocal in factor 11 are defined by

$$e_{U_{11}}(s) = \begin{cases} 1/s & \text{if } v_{10}^L > 0 \\ \frac{1}{v_{10}^L} + \frac{1/v_{10}^U - 1/v_{10}^L}{v_{10}^U - v_{10}^L}(s - v_{10}^L) & \text{if } v_{10}^U < 0 \end{cases}$$

and

$$E_{U_{11}}(s) = \begin{cases} 1/s & \text{if } v_{10}^U < 0 \\ \frac{1}{v_{10}^L} + \frac{1/v_{10}^U - 1/v_{10}^L}{v_{10}^U - v_{10}^L}(s - v_{10}^L) & \text{if } v_{10}^L > 0 \end{cases}.$$

Finally, the quantities α, β, δ and γ are defined as

$$\begin{aligned} \alpha_9 &= \min(v_{11}^L v_9^c, v_{11}^L v_9^C), & \alpha_{11} &= \min(v_9^L v_{11}^c, v_9^L v_{11}^C), \\ \beta_9 &= \min(v_{11}^U v_9^c, v_{11}^U v_9^C), & \beta_{11} &= \min(v_9^U v_{11}^c, v_9^U v_{11}^C), \\ \gamma_9 &= \max(v_{11}^L v_9^c, v_{11}^L v_9^C), & \gamma_{11} &= \max(v_9^U v_{11}^c, v_9^U v_{11}^C), \\ \delta_9 &= \max(v_{11}^U v_9^c, v_{11}^U v_9^C), & \delta_{11} &= \max(v_9^L v_{11}^c, v_9^L v_{11}^C). \end{aligned}$$

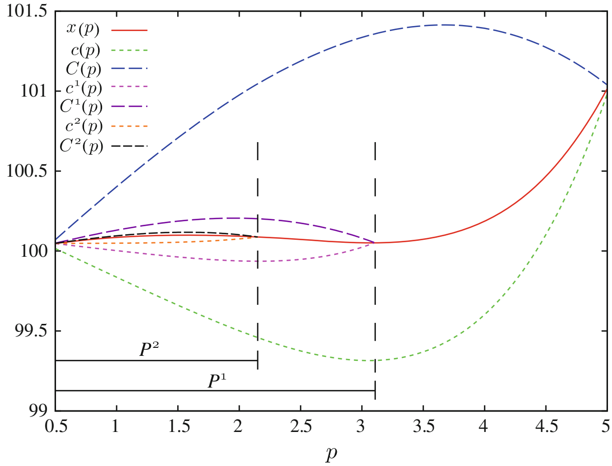

Fig. 1 The implicit function x on the interval $P = [0.5, 5]$, along with convex and concave relaxations c and C valid on P. The functions c^ℓ and C^ℓ, $\ell = 1, 2$, are convex and concave relaxations of x, respectively, valid on the nested subintervals $P^2 \subset P^1 \subset P$

Now $u_h(p, z, y)$ and $o_h(p, z, y)$ evaluate to v_{13}^c and v_{13}^C in Table 1, respectively.

Using u_h and o_h as defined above, convex and concave relaxations of each x^k, c^k and C^k, were generated by application of Theorem 11 with constant initial guesses $x^0(p) = x^U$, $c^0(p) = x^L$ and $C^0(p) = x^U$, $\forall p \in P$. Computation of the generalized McCormick relaxations (7) and (8) was performed automatically using the open source C++ library libMC [18,3]. Figure 1 shows the parametric solution x on P (the final iterate of the successive substitution scheme (12), x^4, converged to within a 10^{-10} relative tolerance), as well as convex and concave relaxations of x on P (the iterates c^4 and C^4 corresponding to x^4). Note that the relaxations c^4 and C^4 provide significantly refined bounding information as compared to the initial interval calculated by the parametric successive substitution method, $X = [97.9, 103.1]$. Finally, the figure shows convex and concave relaxations constructed in the same way over the subintervals $P^2 \subset P^1 \subset P$, where $X^2 \subset X^1 \subset X$ have been generated as described above and the initial guesses are $x^{0,\ell}(p) = x^{U,\ell}$, $c^{0,\ell}(p) = x^{L,\ell}$ and $C^{0,\ell}(p) = x^{U,\ell}$, $\ell = 1, 2$, $\forall p \in P$.

7 Relaxations of the solutions of ODEs

In this section, relaxations are presented for the solutions of parametric ODEs of the form

$$\dot{\mathbf{x}}(t, \mathbf{p}) = \mathbf{f}\,(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}))\,, \quad \mathbf{x}\,(t_0, \mathbf{p}) = \mathbf{x}_0\,(\mathbf{p})\,, \tag{13}$$

where $I = [t_0, t_f] \subset \mathbb{R}$, $D \subset \mathbb{R}^{n_x}$ is an open connected set, $\mathbf{f} : I \times P \times D \to \mathbb{R}^{n_x}$ and $\mathbf{x}_0 : P \to D$. In addition, the following assumptions on (13) are required.

Assumption 14 The ODEs (13) satisfy the following conditions:

1. $\mathbf{x}_0$ is continuous on P,
2. $\mathbf{f}$ is continuous on $I \times P \times D$,
3. for any compact $K \subset D$, $\exists L_K \in \mathbb{R}_+$ such that $\|\mathbf{f}(t, \mathbf{p}, \mathbf{z}) - \mathbf{f}(t, \mathbf{p}, \hat{\mathbf{z}})\|_1 \le L_K \|\mathbf{z} - \hat{\mathbf{z}}\|_1$, for all $(t, \mathbf{p}, \mathbf{z}, \hat{\mathbf{z}}) \in I \times P \times K \times K$.

Under these assumptions, (13) is guaranteed to have a unique, continuous solution on some $I' \times P$, $I' \subset I$. It is assumed in the remainder of this section that I and P have been chosen so that such a solution exists on all of $I \times P$. Then, the aim of this section is to construct state relaxations for the ODEs (13), as defined below.

Definition 20 (State relaxations) Two continuous functions $\mathbf{c}, \mathbf{C} : I \times P \to \mathbb{R}^{n_x}$ are *state relaxations* for (13) on P if $\mathbf{c}(t, \cdot)$ and $\mathbf{C}(t, \cdot)$ are, respectively, convex and concave relaxations of $\mathbf{x}(t, \cdot)$ on P, for every fixed $t \in I$.

The function $\mathbf{x}$ is not factorable or even known explicitly. Nonetheless, it is possible to construct the desired convex and concave relaxations through the use of generalized McCormick relaxations.

Previously, a few authors have presented methods for constructing state relaxations for (13). In [7,23,24], the αBB convexification method [2] is extended to relax the solutions of ODEs, yet the resulting relaxations are typically very weak, as is the case with standard αBB relaxations. In [30], a method is developed for generating under/overestimators for the solutions of (13) which are affine with respect to $\mathbf{p}$, and thus trivially convex and concave. These relaxations are significantly tighter than those in [23], yet have the disadvantage of being affine, and so cannot tightly approximate sufficiently nonlinear functions. More recently, an article in review by the authors has demonstrated a set of sufficient conditions for an auxiliary system of ODEs to have solutions which are non-affine state relaxations for (13). The main developments of that article are summarized in the following section. In Sect. 7.2, it is shown that appropriate right-hand sides and initial condition functions for this auxiliary system can be constructed simply from the generalized McCormick relaxations of $\mathbf{f}$ and $\mathbf{x}_0$.

7.1 ODE relaxation theory

The following development is from a separate article by the authors, currently under review [27]. All proofs are presented in full there. The first definition describes an auxiliary system of ODEs corresponding to (13), and Assumption 15 and Definition 22 together describe sufficient conditions under which the unique solutions of this auxiliary system are state relaxations for (13). Theorem 13 establishes the sufficiency of these conditions.

Definition 21 **($\mathbf{u}, \mathbf{o}, \mathbf{c}_0, \mathbf{C}_0$)** Let $\mathbf{c}_0, \mathbf{C}_0 : P \to \mathbb{R}^{n_x}$ and $\mathbf{u}, \mathbf{o} : I \times P \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_x}$, and define the auxiliary ODEs:

$$\begin{aligned} \dot{\mathbf{c}}(t, \mathbf{p}) &= \mathbf{u}(t, \mathbf{p}, \mathbf{c}(t, \mathbf{p}), \mathbf{C}(t, \mathbf{p})), \quad \mathbf{c}(t_0, \mathbf{p}) = \mathbf{c}_0(\mathbf{p}), \\ \dot{\mathbf{C}}(t, \mathbf{p}) &= \mathbf{o}(t, \mathbf{p}, \mathbf{c}(t, \mathbf{p}), \mathbf{C}(t, \mathbf{p})), \quad \mathbf{C}(t_0, \mathbf{p}) = \mathbf{C}_0(\mathbf{p}), \end{aligned} \tag{14}$$

for all $(t, \mathbf{p}) \in I \times P$.

Assumption 15 The ODEs (14) satisfy the following conditions:

1. $\mathbf{c}_0$ and $\mathbf{C}_0$ are continuous on P,
2. $\mathbf{u}$ and $\mathbf{o}$ are continuous on $I \times P \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$,
3. $\exists L_{\mathbf{uo}} \in \mathbb{R}_+$ such that

$$\begin{aligned} &\|\mathbf{u}(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) - \mathbf{u}(t, \mathbf{p}, \hat{\mathbf{z}}, \hat{\mathbf{y}})\|_1 + \|\mathbf{o}(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) - \mathbf{o}(t, \mathbf{p}, \hat{\mathbf{z}}, \hat{\mathbf{y}})\|_1 \\ &\quad \leq L_{\mathbf{uo}}(\|\mathbf{z} - \hat{\mathbf{z}}\|_1 + \|\mathbf{y} - \hat{\mathbf{y}}\|_1) \end{aligned}$$

   for all $(t, \mathbf{p}, \mathbf{z}, \mathbf{y}, \hat{\mathbf{z}}, \hat{\mathbf{y}}) \in I \times P \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$.

Definition 22 (C-system) The auxiliary system of ODEs (14) is called a *C-system* of (13) on P if, in addition to satisfying Assumption 15, the following conditions hold:

1. $\mathbf{c}_0$ and $\mathbf{C}_0$ are, respectively, convex and concave relaxations of $\mathbf{x}_0$ on P,
2. for any continuous mappings $\boldsymbol{\varphi}^c, \boldsymbol{\varphi}^C : I \times P \to \mathbb{R}^{n_x}$ and any fixed $t \in I$,

$$\mathbf{u}(t, \cdot, \boldsymbol{\varphi}^c(t, \cdot), \boldsymbol{\varphi}^C(t, \cdot)) \quad \text{and} \quad \mathbf{o}(t, \cdot, \boldsymbol{\varphi}^c(t, \cdot), \boldsymbol{\varphi}^C(t, \cdot))$$

are, respectively, convex and concave relaxations of $\mathbf{f}(t, \cdot, \mathbf{x}(t, \cdot))$ on P, provided that $\boldsymbol{\varphi}^c(t, \cdot)$ and $\boldsymbol{\varphi}^C(t, \cdot)$ are, respectively, convex and concave relaxations of $\mathbf{x}(t, \cdot)$ on P.

Theorem 13 *If the auxiliary system of ODEs* (14) *is a C-system of* (13) *on P, then* $\mathbf{c}(t, \cdot)$ *and* $\mathbf{C}(t, \cdot)$ *are, respectively, convex and concave relaxations of* $\mathbf{x}(t, \cdot)$ *on P, for each fixed* $t \in I$.

7.2 Constructing the auxiliary system via generalized McCormick relaxations

This section defines the functions $\mathbf{u}$ and $\mathbf{o}$ in terms of the generalized McCormick relaxations of $\mathbf{f}$, and demonstrates that the conditions of Assumption 15 and Definition 22 are all satisfied. This construction requires *state bounds*, defined as follows.

Definition 23 ($\mathbf{x}^L, \mathbf{x}^U, X(t)$) Two continuous functions, $\mathbf{x}^L, \mathbf{x}^U : I \to D$, are called *state bounds* for (13) if $\mathbf{x}^L(t) \leq \mathbf{x}(t, \mathbf{p}) \leq \mathbf{x}^U(t)$, for all $(t, \mathbf{p}) \in I \times P$, and $[\mathbf{x}^L(t), \mathbf{x}^U(t)] \subset D$ for all $t \in I$. The interval $[\mathbf{x}^L(t), \mathbf{x}^U(t)]$ is denoted by $X(t)$.

Remark 4 Numerical techniques for generating state bounds may be found in [10,14,15,21,26,28,29]. In general, the existence of a solution of (13) on $I \times P$ does not imply that state bounds exist on all of I; when $n_x > 1$ there may exist no interval which both encloses the image of P under $\mathbf{x}(t, \cdot)$ for some $t \in I$ and is contained in D. Nevertheless, the variety of interval methods for ODEs cited above demonstrates that the existence and generation of state bounds is rarely an issue in practical applications. Therefore, it will be assumed in the remainder of this work that state bounds are available over all of I, as stated formally below.

Assumption 16 State bounds for (13) are known on all of I.

For the following discussion, we assume that f_i is factorable for all $i = 1, \ldots, n_x$ and let $\mathscr{V}_i$ denote the corresponding collection of factors. Define

$$\Phi = \{(t, \mathbf{p}, \mathbf{z}) : t \in I, \ \mathbf{p} \in P, \ \mathbf{z} \in X(t)\}.$$

Let $\tilde{\mathscr{U}}_{f_i}$ and $\tilde{\mathscr{O}}_{f_i}$ denote the generalized McCormick relaxations of f_i, and let $\tilde{\mathscr{U}}_{\mathbf{f}}$ and $\tilde{\mathscr{O}}_{\mathbf{f}}$ be vector functions with elements $\tilde{\mathscr{U}}_{f_i}$ and $\tilde{\mathscr{O}}_{f_i}$. Finally, assume that $\mathscr{V}_i$ and the univariate relaxations and bounding operations defining $\tilde{\mathscr{U}}_{f_i}$ and $\tilde{\mathscr{O}}_{f_i}$ satisfy Assumptions 6–10 in Sect. 4, for each $i = 1, \ldots, n_x$.

The functions **u** and **o** can now be formulated as

$$\mathbf{u}(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) = \tilde{\mathscr{U}}_{\mathbf{f}} \Big(t, t, t, t, p_1^L, p_1^U, p_1, p_1, \ldots, p_{n_p}^L, p_{n_p}^U, p_{n_p}, p_{n_p}, \\ x_1^L(t), x_1^U(t), \mathrm{mid}\left(x_1^L(t), x_1^U(t), z_1\right), \mathrm{mid}\left(x_1^L(t), x_1^U(t), y_1\right), \\ \ldots, x_{n_x}^L(t), x_{n_x}^U(t), \mathrm{mid}\left(x_{n_x}^L(t), x_{n_x}^U(t), z_{n_x}\right), \mathrm{mid}\left(x_{n_x}^L(t), x_{n_x}^U(t), y_{n_x}\right)\Big), \tag{15}$$

$$\mathbf{o}(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) = \tilde{\mathscr{O}}_{\mathbf{f}} \Big(t, t, t, t, p_1^L, p_1^U, p_1, p_1, \ldots, p_{n_p}^L, p_{n_p}^U, p_{n_p}, p_{n_p}, \\ x_1^L(t), x_1^U(t), \mathrm{mid}\left(x_1^L(t), x_1^U(t), z_1\right), \mathrm{mid}\left(x_1^L(t), x_1^U(t), y_1\right), \\ \ldots, x_{n_x}^L(t), x_{n_x}^U(t), \mathrm{mid}\left(x_{n_x}^L(t), x_{n_x}^U(t), z_{n_x}\right), \mathrm{mid}\left(x_{n_x}^L(t), x_{n_x}^U(t), y_{n_x}\right)\Big), \tag{16}$$

for any $(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) \in I \times P \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$. In addition, define the functions $\mathbf{c}_0$ and $\mathbf{C}_0$ as the standard McCormick relaxations of $\mathbf{x}_0$ on P.

The properties of generalized McCormick relaxations will be used to prove that **u** and **o** defined in this way satisfy all of the properties required in Sect. 7.1. Note, however, that Φ is not an interval for this application. Accordingly, Lemma 9 does not apply and Theorem 6 does not ensure that $\tilde{\mathscr{U}}_{\mathbf{f}}$ and $\tilde{\mathscr{O}}_{\mathbf{f}}$ are Lipschitz on $\tilde{\Phi}$. However, Theorem 6 may be applied to the subset

$$\tilde{\Phi}' \equiv \left\{\mathbf{y}^\circ \in \tilde{\Phi} : y_1^L = y_1^U = y_1^c = y_1^C\right\},$$

as shown below.

Lemma 11 *Under Assumptions 9 and 10, $\tilde{\mathscr{U}}_{\mathbf{f}}$ and $\tilde{\mathscr{O}}_{\mathbf{f}}$ are Lipschitz on $\tilde{\Phi}'$.*

Proof By Theorem 6, it suffices to show that $\tilde{\Phi}'$ is compact and connected. Noting that $\mathbf{x}^L$ and $\mathbf{x}^U$ are continuous and I is compact, define

$$x_i^{L,\dagger} \equiv \min_{t \in I} x_i^L(t) \quad \text{and} \quad x_i^{U,\dagger} \equiv \max_{t \in I} x_i^U(t),$$

for each $i = 1, \ldots, n_x$. Now, the set $I \times P^4 \times [\mathbf{x}^{L,\dagger}, \mathbf{x}^{U,\dagger}]^4$ is clearly compact and connected (the superscript 4 here denotes the number of Cartesian products, not a subset $P^\ell \subset P$). It will be shown that $\tilde{\Phi}'$ is the image of this set under the continuous mapping

$$I \times P^4 \times [\mathbf{x}^{L,\dagger}, \mathbf{x}^{U,\dagger}]^4 \ni (t, \mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}, \mathbf{q}, \mathbf{r}, \mathbf{s}, \mathbf{t}) \\ \longmapsto \left(\left(y_1^L, y_1^U, y_1^c, y_1^C\right), \ldots, \left(y_{n_x+n_p+1}^L, y_{n_x+n_p+1}^U, y_{n_x+n_p+1}^c, y_{n_x+n_p+1}^C\right)\right) \in \tilde{\Phi},$$

where

$$
\begin{aligned}
&y_1^L = y_1^U = y_1^c = y_1^C = t,\\
&\left.\begin{aligned}
y_{i+1}^L &= \min(a_i, b_i)\\
y_{i+1}^U &= \max(a_i, b_i)\\
y_{i+1}^c &= \operatorname{mid}(c_i, y_{i+1}^L, y_{i+1}^U)\\
y_{i+1}^C &= \operatorname{mid}(d_i, y_{i+1}^L, y_{i+1}^U)
\end{aligned}\right\}, \quad \forall i = 1, \ldots, n_p,\\
&\left.\begin{aligned}
y_{i+n_p+1}^L &= \operatorname{mid}(\min(q_i, r_i), x_i^L(t), x_i^U(t))\\
y_{i+n_p+1}^U &= \operatorname{mid}(\max(q_i, r_i), x_i^L(t), x_i^U(t))\\
y_{i+n_p+1}^c &= \operatorname{mid}(s_i, y_{i+n_p+1}^L, y_{i+n_p+1}^U)\\
y_{i+n_p+1}^C &= \operatorname{mid}(t_i, y_{i+n_p+1}^L, y_{i+n_p+1}^U)
\end{aligned}\right\}, \quad \forall i = 1, \ldots, n_x.
\end{aligned}
$$

By definition, $[y_1^L, y_1^U] = [t, t] \subset I$ and $[y_2^L, y_2^U] \times \cdots \times [y_{n_x+n_p+1}^L, y_{n_x+n_p+1}^U] \subset P \times X(t)$. Furthermore, the mid functions ensure that $y_i^{c/C} \in [y_i^L, y_i^U]$ for every $i = 1, \ldots, n_x + n_p + 1$. Then the image of $I \times P^4 \times [\mathbf{x}^{L,\dagger}, \mathbf{x}^{U,\dagger}]^4$ under this mapping must be contained in $\tilde{\Phi}$. Indeed, it is also contained in $\tilde{\Phi}'$, since every point in the image has $y_1^L = y_1^U = y_1^c = y_1^C$. Now, given any $\mathbf{y}^\circ \in \tilde{\Phi}'$, it is not difficult to see that the point

$$
\begin{aligned}
&\Big(y_1^L, (y_2^L, \ldots, y_{n_p+1}^L), (y_2^U, \ldots, y_{n_p+1}^U), (y_2^c, \ldots, y_{n_p+1}^c), (y_2^C, \ldots, y_{n_p+1}^C),\\
&\quad (y_{n_p+2}^L, \ldots, y_{n_x+n_p+1}^L), (y_{n_p+2}^U, \ldots, y_{n_x+n_p+1}^U), (y_{n_p+2}^c, \ldots, y_{n_x+n_p+1}^c),\\
&\quad (y_{n_p+2}^C, \ldots, y_{n_x+n_p+1}^C)\Big)\\
&\quad \in I \times P^4 \times [\mathbf{x}^{L,\dagger}, \mathbf{x}^{U,\dagger}]^4
\end{aligned}
$$

maps to $\mathbf{y}^\circ$. Thus, this mapping is onto, so that the image of $I \times P^4 \times [\mathbf{x}^{L,\dagger}, \mathbf{x}^{U,\dagger}]^4$ under this mapping must be exactly $\tilde{\Phi}'$. Now, by Theorems 4.14 and 4.22 in [25], $\tilde{\Phi}'$ is compact and connected. □

Theorem 14 *With* $\mathbf{u}$ *and* $\mathbf{o}$ *defined as in* (15) *and* (16) *and* $\mathbf{c}_0$ *and* $\mathbf{C}_0$ *defined as the standard McCormick relaxations of* $\mathbf{x}_0$ *on* P*, the auxiliary system* (14) *is a C-system of* (13) *on* P.

Proof First it is demonstrated that Assumption 15 is satisfied. Condition 1 follows directly from Theorem 3. Noting that the arguments of $\tilde{\mathscr{U}}_{\mathbf{f}}$ and $\tilde{\mathscr{O}}_{\mathbf{f}}$ above are guaranteed to be in $\tilde{\Phi}' \subset \tilde{\Phi}$ for any $(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) \in I \times P \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$, Condition 2 follows from Lemma 11 and the facts that $\mathbf{x}^L$ and $\mathbf{x}^U$ are continuous on I and the mid function is continuous on $\mathbb{R}^{3n_x}$. For any fixed $(t, \mathbf{p}) \in I \times P$, $\operatorname{mid}(\mathbf{x}^L(t), \mathbf{x}^U(t), \cdot)$ is Lipschitz on $\mathbb{R}^{n_x}$ with constant one, so Condition 3 follows from Lemma 11.

It remains to verify the two conditions of Definition 22. The first is obviously satisfied since $\mathbf{c}_0$ and $\mathbf{C}_0$ are standard McCormick relaxations of $\mathbf{x}_0$ on P. Choose any $\varphi^c, \varphi^C : I \times P \to \mathbb{R}^{n_x}$, fix some $t \in I$ and suppose that $\varphi^c(t, \cdot)$ and $\varphi^C(t, \cdot)$ are, respectively, convex and concave relaxations of $\mathbf{x}(t, \cdot)$ on P. Then, by arguments analogous to the proof of Theorem 8, $\mathbf{u}(t, \cdot, \varphi^c(t, \cdot), \varphi^C(t, \cdot))$ and $\mathbf{o}(t, \cdot, \varphi^c(t, \cdot), \varphi^C(t, \cdot))$ are, respectively, convex and concave relaxations of $\mathbf{f}(t, \cdot, \mathbf{x}(t, \cdot))$ on P. □

This completes the necessary conditions for the ODEs in (14) to describe trajectories which are convex and concave relaxations of $\mathbf{x}(t, \cdot)$ on P for each $t \in I$. According to the previous discussion, the procedure for evaluating these relaxations is now evident. Given $\mathbf{f}$, $\mathbf{x}_0$, $X(t)$ and $\mathbf{p} \in P$, first evaluate the functions $\mathbf{c}_0$ and $\mathbf{C}_0$ at $\mathbf{p}$ according to Definition 9.

Using these as initial conditions, solve the coupled auxiliary ODE system (14) on I, where the right-hand side is evaluated according to (15), (16) and Definition 15. This procedure is stated formally in the following Corollary.

Corollary 2 *With* $\mathbf{c}_0$ *and* $\mathbf{C}_0$ *defined as the standard McCormick relaxations of* $\mathbf{x}_0$ *on* P *and* $\mathbf{u}$ *and* $\mathbf{o}$ *defined by* (15) *and* (16)*, the solutions of the auxiliary system* (14)*,* $\mathbf{c}$ *and* $\mathbf{C}$*, are state relaxations for* (13) *on* P.

7.3 State relaxations on nested sequences of intervals

In this section, the behavior of $\mathbf{c}$ and $\mathbf{C}$ on sequences of nested subintervals is examined. First, note that the results of the previous sections all remain true if some subinterval $P^\ell \subset P$ is considered in place of P. Thus, it is sensible to define the functions $\mathbf{c}^\ell$ and $\mathbf{C}^\ell$ as the relaxations of $\mathbf{x}$ constructed over some subinterval P^ℓ. Analogously, it is sensible to refer to the state bounds, X^ℓ, the initial condition functions, $\mathbf{c}_0^\ell$ and $\mathbf{C}_0^\ell$, and the right-hand sides, $\mathbf{u}^\ell$ and $\mathbf{o}^\ell$, all defined as before with P^ℓ in place of P. Using this notation, consider the auxiliary system of ODEs

$$\begin{aligned} \dot{\mathbf{c}}^\ell(t,\mathbf{p}) &= \mathbf{u}^\ell(t,\mathbf{p},\mathbf{c}^\ell(t,\mathbf{p}),\mathbf{C}^\ell(t,\mathbf{p})), \quad \mathbf{c}^\ell(t_0,\mathbf{p}) = \mathbf{c}_0^\ell(\mathbf{p}), \\ \dot{\mathbf{C}}^\ell(t,\mathbf{p}) &= \mathbf{o}^\ell(t,\mathbf{p},\mathbf{c}^\ell(t,\mathbf{p}),\mathbf{C}^\ell(t,\mathbf{p})), \quad \mathbf{C}^\ell(t_0,\mathbf{p}) = \mathbf{C}_0^\ell(\mathbf{p}), \end{aligned} \tag{17}$$

for any $P^\ell \subset P$. Fixing any $P^\ell \subset P$, it has been shown that when $\mathbf{u}^\ell$ and $\mathbf{o}^\ell$ are defined by (15) and (16), and $\mathbf{c}_0$ and $\mathbf{C}_0$ are defined as the standard McCormick relaxations of $\mathbf{x}_0$ on P^ℓ, then all of the conditions of Assumption 15 and Definition 22 are satisfied. Thus, we have a procedure which, given any $P^\ell \subset P$, generates a C-system of (13) on P^ℓ. Of course, this implies that $\mathbf{c}^\ell(t,\cdot)$ and $\mathbf{C}^\ell(t,\cdot)$ are valid convex and concave relaxations of $\mathbf{x}(t,\cdot)$ on P^ℓ for each $t \in I$. Consider any convergent sequence of subintervals $\{P^\ell\} \to P^*$ and denote the right-hand sides and solutions of (17) with P^* in place of P^ℓ by $\mathbf{u}^*$, $\mathbf{o}^*$, $\mathbf{c}^*$ and $\mathbf{C}^*$. It will be shown that generating state relaxations for (13) by the solution of (17) is a partition monotonic, partition convergent and degenerate perfect procedure, as defined below.

Definition 24 (Partition monotonic state relaxations) A procedure for generating state relaxations for (13), $\mathbf{c}^\ell$ and $\mathbf{C}^\ell$, is *partition monotonic* if, for any subintervals $P^2 \subset P^1 \subset P$, $\mathbf{c}^2(t,\mathbf{p}) \geq \mathbf{c}^1(t,\mathbf{p})$ and $\mathbf{C}^2(t,\mathbf{p}) \leq \mathbf{C}^1(t,\mathbf{p})$ for all $(t,\mathbf{p}) \in I \times P^2$.

Definition 25 (Partition convergent and degenerate perfect state relaxations) A procedure for generating state relaxations for (13), $\mathbf{c}^\ell$ and $\mathbf{C}^\ell$, is *partition convergent* if, for any nested sequence of subintervals $\{P^\ell\} \to P^*$, $\{\mathbf{c}^\ell\} \to \mathbf{c}^*$ and $\{\mathbf{C}^\ell\} \to \mathbf{C}^*$ uniformly on $I \times P^*$. Furthermore, a procedure for generating state relaxations is *degenerate perfect* if the condition $P^* = [\mathbf{p},\mathbf{p}]$ for some $\mathbf{p} \in P$ implies that $\mathbf{c}^*(\cdot,\mathbf{p}) = \mathbf{x}(\cdot,\mathbf{p}) = \mathbf{C}^*(\cdot,\mathbf{p})$.

As was the case with the validity of the relaxations themselves, the properties defined above are largely proven in [27]. The following two definitions describe properties of C-systems of (13) which are analogous to partition monotonicity, partition convergence and degenerate perfection for state relaxations. Subsequently, two Lemmata from the [27] are stated which show that, when the C-systems (17) satisfy these conditions, the resulting state relaxations are partition monotonic, partition convergent and degenerate perfect.

Definition 26 (Partition monotonic C-system) A procedure for generating C-systems of (13) of the form (17) is *partition monotonic* if, for any $P^2 \subset P^1 \subset P$, the C-systems satisfy

1. $\mathbf{c}_0^1(\mathbf{p}) \le \mathbf{c}_0^2(\mathbf{p})$ and $\mathbf{C}_0^2(\mathbf{p}) \le \mathbf{C}_0^1(\mathbf{p}), \quad \forall \mathbf{p} \in P^2$, and
2. for any $(t, \mathbf{p}, \bar{\mathbf{z}}^1, \bar{\mathbf{y}}^1, \bar{\mathbf{z}}^2, \bar{\mathbf{y}}^2) \in I \times P^2 \times \mathbb{R}^{4n_x}$, the inequalities

$$\mathbf{u}^1(t, \mathbf{p}, \bar{\mathbf{z}}^1, \bar{\mathbf{y}}^1) \le \mathbf{u}^2(t, \mathbf{p}, \bar{\mathbf{z}}^2, \bar{\mathbf{y}}^2) \quad \text{and} \quad \mathbf{o}^2(t, \mathbf{p}, \bar{\mathbf{z}}^2, \bar{\mathbf{y}}^2) \le \mathbf{o}^1(t, \mathbf{p}, \bar{\mathbf{z}}^1, \bar{\mathbf{y}}^1)$$

   hold, provided that $\bar{\mathbf{z}}^1 \le \bar{\mathbf{z}}^2 \le \mathbf{x}(t, \mathbf{p}) \le \bar{\mathbf{y}}^2 \le \bar{\mathbf{y}}^1$.

Definition 27 (Partition convergent and degenerate perfect C-system) A procedure for generating C-systems of (13) of the form (17) is *partition convergent* if, for any nested sequence of subintervals $\{P^\ell\} \to P^*$, the C-systems satisfy

1. $\{\mathbf{c}_0^\ell\} \to \mathbf{c}_0^*$ and $\{\mathbf{C}_0^\ell\} \to \mathbf{C}_0^*$ uniformly on P^*, and
2. $\{\mathbf{u}^\ell\} \to \mathbf{u}^*$ and $\{\mathbf{o}^\ell\} \to \mathbf{o}^*$ uniformly on $I \times P^* \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$.

Furthermore, a procedure for generating C-systems is *degenerate perfect* if the condition $P^* = [\mathbf{p}, \mathbf{p}]$ for some $\mathbf{p} \in P$ implies that

(i) $\mathbf{c}_0^*(\mathbf{p}) = \mathbf{x}_0(\mathbf{p}) = \mathbf{C}_0^*(\mathbf{p})$, and
(ii) $\mathbf{u}^*(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) = \mathbf{f}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p})) = \mathbf{o}^*(t, \mathbf{p}, \mathbf{z}, \mathbf{y}), \quad \forall (t, \mathbf{z}, \mathbf{y}) \in I \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$.

Lemma 12 *If the C-systems* (17) *are generated by a procedure which is partition monotonic, then generating state relaxations for* (13)*,* $\mathbf{c}^\ell$ *and* $\mathbf{C}^\ell$*, as the solutions of* (17) *is a partition monotonic procedure.*

Proof The lemma is proven in a separate article by the authors, currently in review [27]. □

Lemma 13 *If the C-systems* (17) *are generated by a procedure which is partition convergent, then generating state relaxations for* (13)*,* $\mathbf{c}^\ell$ *and* $\mathbf{C}^\ell$*, as the solutions of* (17) *is a partition convergent procedure. Furthermore, if the C-systems* (17) *are generated by a procedure which is degenerate perfect, then generating state relaxations for* (13)*,* $\mathbf{c}^\ell$ *and* $\mathbf{C}^\ell$*, as the solutions of* (17) *is a degenerate perfect procedure.*

Proof The lemma is proven in a separate article by the authors, currently in review [27]. □

Thus, to prove that the state relaxations $\mathbf{c}^\ell$ and $\mathbf{C}^\ell$ are partition monotonic, partition convergent and degenerate perfect, it is only necessary to verify that $\mathbf{u}^\ell$, $\mathbf{o}^\ell$, $\mathbf{c}_0^\ell$ and $\mathbf{C}_0^\ell$ satisfy Definitions 26 and 27. These results require some properties of the state bounds which cannot be verified without specifying the method by which they are generated. Accordingly, the following assumption is necessary.

Assumption 17 Let $\{P^\ell\}$ be any nested sequence of subintervals, $P^\ell \subset P$, and suppose that $\{P^\ell\} \to P^*$. Denote the state bounds generated on P^ℓ by $X^\ell(t) \equiv [\mathbf{x}^{L,\ell}(t), \mathbf{x}^{U,\ell}(t)]$ and those generated on P^* by $X^*(t) \equiv [\mathbf{x}^{L,*}(t), \mathbf{x}^{U,*}(t)]$. Then

1. for any $\ell \in \mathbb{N}$, $X^{\ell+1}(t) \subset X^\ell(t) \subset X(t)$ for each $t \in I$,
2. $\{\mathbf{x}^{L,\ell}\} \to \mathbf{x}^{L,*}$ and $\{\mathbf{x}^{U,\ell}\} \to \mathbf{x}^{U,*}$ uniformly on I, and
3. for any $\mathbf{p} \in P$, $P^* = [\mathbf{p}, \mathbf{p}]$ implies that $\mathbf{x}^{L,*}(t) = \mathbf{x}(t, \mathbf{p}) = \mathbf{x}^{U,*}(t), \quad \forall t \in I$.

If the state bounds are constructed using the method described in [10], then it can be shown through relatively standard results in ODE theory that Assumption 17 is satisfied. These arguments, however, are beyond the scope of this article.

Theorem 15 *For any* $P^\ell \subset P$*, let* $\mathbf{c}_0^\ell$ *and* $\mathbf{C}_0^\ell$ *be the standard McCormick relaxations of* $\mathbf{x}_0$ *on* P^ℓ*, and let* $\mathbf{u}^\ell$ *and* $\mathbf{o}^\ell$ *be defined analogously to* (15) *and* (16)*. If Assumption* 17 *holds, then constructing state relaxations for* (13)*,* $\mathbf{c}^\ell$ *and* $\mathbf{C}^\ell$*, by solving* (17) *is a partition monotonic procedure.*

Proof By Lemma 12, it is only necessary to show that the conditions of Definition 26 are satisfied. Condition 1 holds by Theorem 4. Choose any $P^2 \subset P^1 \subset P$ and any $(t, \mathbf{p}, \bar{\mathbf{z}}^1, \bar{\mathbf{y}}^1, \bar{\mathbf{z}}^2, \bar{\mathbf{y}}^2) \in I \times P^2 \times \mathbb{R}^{4n_x}$ such that $\bar{\mathbf{z}}^1 \leq \bar{\mathbf{z}}^2 \leq \mathbf{x}(t, \mathbf{p}) \leq \bar{\mathbf{y}}^2 \leq \bar{\mathbf{y}}^1$.

Choose any $1 \leq j \leq n_x$. Now, by (15), (16) and Definition 15, the first $n_p + n_x + 1$ factors in the computation of $u_j^\ell(t, \mathbf{p}, \bar{\mathbf{z}}^\ell, \bar{\mathbf{y}}^\ell)$ are assigned as follows:

$$
\begin{aligned}
&v_1^{L,\ell} = v_1^{U,\ell} = v_1^{c,\ell} = v_1^{C,\ell} = t,\\
&v_{i+1}^{L,\ell} = p_i^{L,\ell},\ v_{i+1}^{U,\ell} = p_i^{U,\ell},\ v_{i+1}^{c,\ell} = v_{i+1}^{C,\ell} = p_i, \quad \forall i = 1, \ldots, n_p,\\
&v_{i+n_p+1}^{L,\ell} = x_i^{L,\ell}(t),\ v_{i+n_p+1}^{U,\ell} = x_i^{U,\ell}(t),\\
&v_{i+n_p+1}^{c,\ell} = \mathrm{mid}(x_i^{L,\ell}(t), x_i^{U,\ell}(t), \bar{z}_i^\ell),\\
&v_{i+n_p+1}^{C,\ell} = \mathrm{mid}(x_i^{L,\ell}(t), x_i^{U,\ell}(t), \bar{y}_i^\ell), \quad \forall i = 1, \ldots, n_x.
\end{aligned}
$$

It is clear from the action of the mid function and Condition 1 in Assumption 17 that, for every $i \leq n_p + n_x + 1$, $V_i^2 \subset V_i^1$, $v_i^{c/C,\ell} \in V_i^\ell$, $\ell = 1, 2$, and $v_i^{c,1} \leq v_i^{c,2} \leq v_i^{C,2} \leq v_i^{C,1}$. Choose any $n_p + n_x + 1 \leq k \leq m$ and suppose that these conditions hold for all $i < k$. Then the hypotheses of Lemma 5 are satisfied, so that $\bar{v}_k^{c,2}(\mathbf{p}) \geq \bar{v}_k^{c,1}(\mathbf{p})$ and $\bar{v}_k^{C,2}(\mathbf{p}) \leq \bar{v}_k^{C,1}(\mathbf{p})$, $\forall \mathbf{p} \in P^2$. Then, the inductive step is completed exactly as in the proof of Theorem 4, so that repeated application of Lemma 5 shows that $u_j^1(t, \mathbf{p}, \bar{\mathbf{z}}^1, \bar{\mathbf{y}}^1) \leq u_j^2(t, \mathbf{p}, \bar{\mathbf{z}}^2, \bar{\mathbf{y}}^2)$. Of course, an identical argument proves that $o_j^1(t, \mathbf{p}, \bar{\mathbf{z}}^1, \bar{\mathbf{y}}^1) \geq o_j^2(t, \mathbf{p}, \bar{\mathbf{z}}^2, \bar{\mathbf{y}}^2)$, and that these inequalities hold for all $j = 1, \ldots, n_x$. □

Theorem 16 *For any $P^\ell \subset P$, let $\mathbf{c}_0^\ell$ and $\mathbf{C}_0^\ell$ be the standard McCormick relaxations of $\mathbf{x}_0$ on P^ℓ, and let $\mathbf{u}^\ell$ and $\mathbf{o}^\ell$ be defined analogously to (15) and (16). If Assumption 17 holds, then constructing state relaxations for (13), $\mathbf{c}^\ell$ and $\mathbf{C}^\ell$, by solving (17) is a partition convergent and degenerate perfect procedure.*

Proof Choose any nested sequence of subintervals of P, $\{P^\ell\}$, such that $\{P^\ell\} \to P^*$. By Lemma 13, it suffices to show that the conditions of Definition 27 hold. Since $\mathbf{c}_0^\ell$ and $\mathbf{C}_0^\ell$ are standard McCormick relaxations of $\mathbf{x}_0$ on P^ℓ, Conditions 1 and (i) are true by Theorems 7 and 5.

Consider Condition 2. From the definition of $\mathbf{u}^\ell$, given any $(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) \in I \times P^* \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$ and any $\ell \in \mathbb{N}$, $\mathbf{u}^\ell$ is given by evaluating $\tilde{\mathscr{U}}_{\mathbf{f}}$ at the point

$$
\begin{aligned}
\Big(&t, t, t, t, p_1^{L,\ell}, p_1^{U,\ell}, p_1, p_1, \ldots, p_{n_p}^{L,\ell}, p_{n_p}^{U,\ell}, p_{n_p}, p_{n_p},\\
&x_1^{L,\ell}(t), x_1^{U,\ell}(t), \mathrm{mid}\left(x_1^{L,\ell}(t), x_1^{U,\ell}(t), z_1\right), \mathrm{mid}\left(x_1^{L,\ell}(t), x_1^{U,\ell}(t), y_1\right), \ldots,\\
&x_{n_x}^{L,\ell}(t), x_{n_x}^{U,\ell}(t), \mathrm{mid}\left(x_{n_x}^{L,\ell}(t), x_{n_x}^{U,\ell}(t), z_{n_x}\right), \mathrm{mid}\left(x_{n_x}^{L,\ell}(t), x_{n_x}^{U,\ell}(t), y_{n_x}\right)\Big). \qquad (18)
\end{aligned}
$$

It is not difficult to verify that this point is in $\tilde{\Phi}'$ for any ℓ (this requires that the sequence $\{X^\ell(t)\}$ is nested for each $t \in I$, so that $X^\ell(t) \subset X(t)$). Furthermore, if

$$
\begin{aligned}
\delta_\ell = \max\Big(&|p_1^{L,\ell} - p_1^{L,*}|, |p_1^{U,\ell} - p_1^{U,*}|, \ldots, |p_{n_p}^{L,\ell} - p_{n_p}^{L,*}|, |p_{n_p}^{U,\ell} - p_{n_p}^{U,*}|,\\
&\max_{t\in I} |x_1^{L,\ell}(t) - x_1^{L,*}(t)|, \max_{t\in I} |x_1^{U,\ell}(t) - x_1^{U,*}(t)|, \ldots,\\
&\max_{t\in I} |x_{n_x}^{L,\ell}(t) - x_{n_x}^{L,*}(t)|, \max_{t\in I} |x_{n_x}^{U,\ell}(t) - x_{n_x}^{U,*}(t)|\Big), \qquad (19)
\end{aligned}
$$

then the Euclidean distance between (18) and the point corresponding to P^* and $X^*(t)$ is less than $\sqrt{2n_p + 4n_x}\delta_\ell$, regardless of the point $(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) \in I \times P^* \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$. Then for any $(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) \in I \times P^* \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$, the sequence $\{\mathbf{u}^\ell(t, \mathbf{p}, \mathbf{z}, \mathbf{y})\}$ is nothing more than $\tilde{\mathscr{U}}_\mathbf{f}$ evaluated on a convergent sequence of points in $\tilde{\Phi}'$. Because $\tilde{\mathscr{U}}_\mathbf{f}$ is continuous on $\tilde{\Phi}'$, it is concluded that $\{\mathbf{u}^\ell(t, \mathbf{p}, \mathbf{z}, \mathbf{y})\} \to \mathbf{u}^*(t, \mathbf{p}, \mathbf{z}, \mathbf{y})$. Furthermore, $\tilde{\Phi}'$ is compact, so $\tilde{\mathscr{U}}_\mathbf{f}$ is uniformly continuous on $\tilde{\Phi}'$. Combining this with the fact that the deviation of (18) from its limit as $\ell \to \infty$ is bounded by $\sqrt{2n_p + 4n_x}\delta_\ell$, regardless of the point $(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) \in I \times P^* \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$, this implies that $\{\mathbf{u}^\ell\}$ must converge to $\mathbf{u}^*$ uniformly on $I \times P^* \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$. Of course, by identical arguments, $\{\mathbf{o}^\ell\} \to \mathbf{o}^*$ uniformly on $I \times P^* \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$. Thus, Condition 2 holds.

With $P^* = [\mathbf{p}, \mathbf{p}]$, Assumption 17 guarantees that $\mathbf{x}^{L,\ell}(t) = \mathbf{x}(t, \mathbf{p}) = \mathbf{x}^{U,\ell}(t)$ for all $t \in I$. Then

$$\begin{aligned}
\mathbf{u}^*(t, \mathbf{p}, \mathbf{z}, \mathbf{y}) = \tilde{\mathscr{U}}_\mathbf{f}(&t, t, t, t, p_1, p_1, p_1, p_1, \ldots, p_{n_p}, p_{n_p}, p_{n_p}, p_{n_p},\\
&x_1(t, \mathbf{p}), x_1(t, \mathbf{p}), x_1(t, \mathbf{p}), x_1(t, \mathbf{p}),\\
&\ldots, x_{n_x}(t, \mathbf{p}), x_{n_x}(t, \mathbf{p}), x_{n_x}(t, \mathbf{p}), x_{n_x}(t, \mathbf{p}))\\
= \mathbf{f}(&t, \mathbf{p}, \mathbf{x}(t, \mathbf{p})), \quad \forall (t, \mathbf{z}, \mathbf{y}) \in I \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x},
\end{aligned}$$

where the second equality comes from the fact that evaluating $\tilde{\mathscr{U}}_\mathbf{f}$ at such points is exactly the special case of standard relaxations (see Sect. 5.1) on a degenerate interval. Then Theorem 5 gives the equality. Since an analogous argument holds for $\mathbf{o}^*$, this establishes Condition (ii) in Definition 27, which completes the proof. □

The previous theorem is a very strong result. It demonstrates that even the most demanding convergence result for the standard McCormick relaxations remains true for the relaxations **c** and **C**. Accordingly, **c** and **C** may be further composed with other generalized relaxations and every convergence property proven for standard relaxations will be satisfied by the result of those compositions (see Sect. 5.3). Thus, relaxations for very general optimal control problems can be generated by the procedure described here and implemented in branch-and-bound global optimization algorithms.

7.4 Example problem

Consider the initial value problem in ODEs

$$\begin{aligned}
\dot{x}_1(t, \mathbf{p}) &= \left(p_1 - \frac{p_1^3}{3}\right) x_1(t, \mathbf{p}) x_2(t, \mathbf{p}), \quad x_{0,1}(\mathbf{p}) = 1,\\
\dot{x}_2(t, \mathbf{p}) &= (x_1(t, \mathbf{p}))^3 - p_2, \quad x_{0,2}(\mathbf{p}) = 0,
\end{aligned} \tag{20}$$

with $(p_1, p_2) \equiv \mathbf{p} \in P \equiv [-6.5, 6.5] \times [0.01, 0.5]$ and $[t_0, t_f] = [0, 0.1]$. The parametric solution $x_1(t_f, \cdot)$, shown in Fig. 2, is clearly nonconvex. Convex and concave relaxations, also shown in Fig. 2, were generated by application of Corollary 2. For brevity, **u** and **o** are not shown explicitly here. These functions are completely specified by (15), (16), Definition 15, and the relaxations and bounding operations for univariate functions given in Sect. II of Online Resource 1 (See also Sect. 6.4 for details). The computation of the generalized McCormick relaxations (15) and (16), via Definition 15, was performed automatically using the open source `C++` library `libMC` [3,18]. State bounds were computed using the method described in [10] and all numerical integration was carried out with the software `CVODE` [5].

The relaxations in Fig. 2 are clearly very tight. They are also nonlinear, which represents a significant improvement over previous efforts. It is easy to visualize, for example, that an

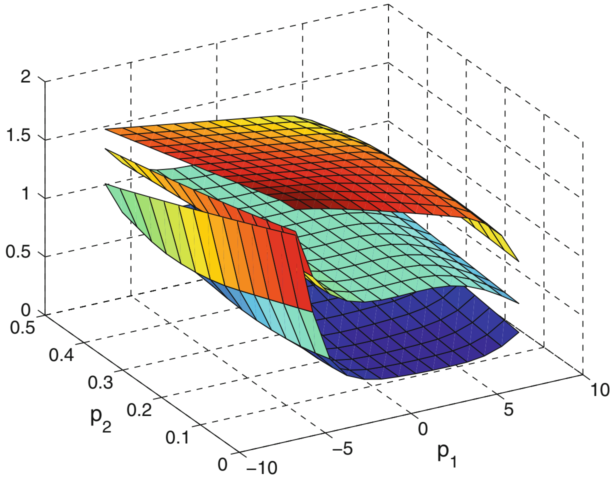

Fig. 2 The parametric fixed-time solution of (20), $x_1(t_f, \cdot)$, on the interval $P = [-6.5, 6.5] \times [0.01, 0.5]$ (*middle surface*), along with convex and concave relaxations $c_1(t_f, \cdot)$ and $C_1(t_f, \cdot)$ valid on P (*lower* and *upper surfaces*, respectively)

affine underestimator [30] for $x_1(t_f, \cdot)$ could not possibly be as tight as $c_1(t_f, \cdot)$ everywhere on P.

8 Conclusion

A generalized form of McCormick's relaxation technique has been introduced which extends the applicability of McCormick-type relaxations greatly. The primary goal of this extension is to address the problem of relaxing functions which are defined implicitly as the parametric solution of a system of equations. Optimizing functions of this type is extremely common in applications where physical systems are described by the dynamic or steady-state solutions of conservation equations such as mass, energy and momentum balances. Relaxations for the solutions of parameter dependent nonlinear algebraic systems were discussed and a method for generating relaxations of approximate solutions was described (Theorem 11). At present, rigorous convex and concave relaxations for the true solutions require assumptions which are not guaranteed by the construction of the generalized relaxations, and the relaxation and global optimization of such systems remains an active area of research for the authors. Convex and concave relaxations for the parametric solutions of ODEs, on the other hand, can be readily computed using generalized McCormick relaxations, and a complete computational procedure for generating such relaxations was described (see Corollary 2, Definitions 9, 15). Taken in conjunction with the treatment of composite functions in Sect. 5.3, these relaxations may be used to construct convex underestimating programs for very general optimal control problems. Furthermore, convergence properties were proven which guarantee that using these relaxations in a spatial branch-and-bound global optimization framework results in a finite ϵ-convergent algorithm (see Theorems 15, 16).

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