Bounding the solutions of parametric weakly coupled second-order semilinear parabolic partial differential equations

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SUMMARY

In this paper, two novel techniques for bounding the solutions of parametric weakly coupled second-order semilinear parabolic partial differential equations are developed. The first provides a theorem to construct interval bounds, while the second provides a theorem to construct lower bounds convex and upper bounds concave in the parameter. The convex/concave bounds can be significantly tighter than the interval bounds because of the wrapping effect suffered by interval analysis in dynamical systems. Both types of bounds are computationally cheap to construct, requiring solving auxiliary systems twice and four times larger than the original system, respectively. An illustrative numerical example of bound construction and use for deterministic global optimization within a simple serial branch-and-bound algorithm, implemented numerically using interval arithmetic and a generalization of McCormick’s relaxation technique, is presented. Problems within the important class of reaction-diffusion systems may be optimized with these tools. © 2016 The Authors. Optimal Control Applications and Methods published by John Wiley & Sons, Ltd.

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1. INTRODUCTION

Reaction-diffusion systems can be modeled using semilinear parabolic partial differential equations (PDEs). An important and well-known example is the heat equation with source term nonlinear in the temperature. One may be faced with the task of fitting such a model to experimental data by formulating an optimization problem. The resulting optimization problem is typically nonconvex, making it desirable to develop a global optimization method for problems involving this class of differential equations, to ensure that the best possible fit can be obtained and that the descriptive power of this class of important models can be robustly evaluated. Alternatively, one may be interested in coming up with the best possible (i.e., global) solution to a design problem involving this important class of differential equations. Unlike stochastic global optimization methods, such as genetic algorithms and simulated annealing, deterministic global optimization using a branch-and-bound algorithm can provide a guarantee that the global optimum has been identified to within a finite tolerance. This is achieved when the algorithm converges, because it represents a constructive procedure for locating the global optimum. The critical component of such an algorithm is the construction of parametric bounds on the PDE solution.

The problem of developing parametric bounds for the solutions of parametric ordinary differential equations (ODEs) has received much attention in the literature. It grew out of the study of
general differential inequalities [1]. Harrison [2] first described a technique to construct interval pointwise in time bounds on the solutions of parametric ODEs, building on a result due to Walter [1]. Unfortunately, it was found in practice that most real systems do not satisfy a stringent condition of quasimonotonicity (which requires the off-diagonal entries of each source function’s Jacobian to preserve its sign in its domain), in which case these bounds are often too weak to be useful. This is due to the wrapping effect of interval analysis [2, 3], the difficulty stemming from employing bounds parallel to the coordinate axes. This motivated the demonstration of the construction of affine in the parameter bounds on the solutions of parametric ODEs in [4]. These bounds employ McCormick’s relaxation technique, are significantly stronger under nonquasimonotonicity, and are trivially both convex and concave in the parameter. Unfortunately, they include arbitrary user-specified components that directly influence the quality of the bounds and may be unsuitable under high nonlinearity in the parameter [5]. This motivated the construction of nonlinear convex lower and concave upper in the parameter bounds for ODEs using a generalization of McCormick’s relaxation technique in [5]. It is also possible to suppress the wrapping effect using validated integrators based on Taylor models [6]. Other parallel studies aimed at employing differential inequalities to develop parametric bounds for ODEs include [7, 8] and [9].

While differential inequalities have also been studied extensively in the PDE context [10–12], the problem of extending them to developing parametric bounds on PDEs has been, to the best of our knowledge, completely ignored. Differential inequalities have been used in the context of the method of lower and upper solutions [13, 14] to prove the existence and uniqueness of solutions for various classes of PDEs [10–12]. To the best of our knowledge, they have not yet been used to develop parametric bounds, an important gap that this work aims to begin addressing.

In this paper, two novel techniques for bounding the solutions of parametric weakly coupled second-order semilinear parabolic PDEs are developed. The first provides a theorem to construct interval bounds, while the second provides a theorem to construct lower bounds convex and upper bounds concave in the parameter. The convex/concave bounds can be significantly tighter than the interval bounds because of the wrapping effect suffered by interval analysis in dynamical systems. However, the construction of the interval bounds is an important first step towards the construction of convex/concave bounds. Both types of bounds are computationally cheap to construct, requiring solving auxiliary systems twice and four times larger than the original system, respectively. An illustrative numerical example of bound construction and use for deterministic global optimization within a simple serial branch-and-bound algorithm, implemented numerically using interval arithmetic and a generalization of McCormick’s relaxation technique, is presented. To the best of our knowledge, this is the first example of such bounds for this class of problems.

The particular motivation that drove this work is optimization of semiconductor problems (which are based on the drift-diffusion-Poisson system of equations). Particular examples of such problems include recovery of inorganic semiconductor doping profiles from data [15, 16], design of inorganic semiconductor doping profiles to minimize leakage currents [17], and thickness optimization of bulk heterojunction organic photovoltaic devices [18, 19]. More generally, problems within the important class of reaction-diffusion systems, where the diffusion coefficients are not state dependent, may be optimized with these tools.

The rest of this paper is organized as follows. In Section 2, the problem is defined mathematically, and the construction of the different types of bounds is motivated by outlining how they are used by a deterministic branch-and-bound global optimization procedure. In Section 3, theorems for constructing the different types of bounds are proved. Finally, Section 4 presents an illustrative numerical example.

2. PRELIMINARIES

2.1. Parametric semilinear parabolic partial differential equation system

Theory is developed in one spatial dimension for simplicity, but the same results can be directly extended to multiple spatial dimensions. Denote the spatial coordinate by \( x \in \mathbb{R} \). Let \( \Omega \) be the bounded open spatial domain in \( \mathbb{R} \), with boundary \( \partial \Omega \) and closure \( \bar{\Omega} \). For any \( t_f > 0 \), denote the
temporal domain by $T \equiv (0, t_f]$ and the temporospatial domain by $Q \equiv \Omega \times T$, denoting its
closure by $\bar{Q}$. Let $\Gamma \equiv \partial \Omega \times T$ and let $p \in P \equiv [p^L, p^U]$ denote the parameter vector. Intervals
between vector functions are componentwise and pointwise in their domain. Denote by $C(Q)$ the
space of functions continuous in $Q$, and by $C^{m,l}(\bar{Q})$ the space of functions with derivatives up to
$m^{th}$ order with respect to $x$ and up to $l^{th}$ order with respect to $t$ continuous in $\bar{Q}$.

For each $p \in P$, and every $i \in I_u \equiv \{1, \ldots, n_u\}$, define an operator as follows:

$$L_i u_{i,p}(x,t) \equiv a_i(x,t) \frac{\partial^2 u_{i,p}}{\partial x^2}(x,t) + b_i(x,t) \frac{\partial u_{i,p}}{\partial x}(x,t), \ \forall (x,t) \in Q. \quad (1)$$

Then, define an operator as follows:

$$L_i u_{i,p}(x,t) = \frac{\partial u_{i,p}}{\partial t}(x,t) - L_i u_{i,p}(x,t), \ \forall (x,t) \in Q. \quad (2)$$

If, for every $i \in I_u$, $a_i$ is positive in $Q$, the operators $L_i$ and $L_i$ are said to be elliptic and
parabolic, respectively. Then, the coupled system of a finite number $n_u$ of equations

$$\begin{align*}
L_i u_{i,p}(x,t) &= f_i(u_p(x,t), x, t, p), \ \forall (x,t) \in Q, \\
B_i u_{i,p}(x,t) &= h_i(x, t, p), \ \forall (x,t) \in \Gamma, \\
u_{i,p}(x,0) &= u_{i,0}(x, p), \ \forall x \in \bar{\Omega}
\end{align*} \quad (3)$$

is parabolic. This system is weakly coupled in the sense that the coupling source function $f$ does not depend on state spatial derivatives. Dependence of the state variable $u_p \in \mathbb{R}^{n_u}$ on $p$ is denoted by
the subscript to indicate that it is implicit. $B_i$ denotes a linear boundary operator of the form:

$$B_i u_{i,p}(x,t) \equiv \alpha_i(x,t) \frac{\partial u_{i,p}}{\partial v}(x,t) + \beta_i(x,t) u_{i,p}(x,t), \ \forall (x,t) \in \Gamma, \quad (4)$$

with $\frac{\partial u_{i,p}}{\partial v} (\cdot, t)$ for each $t \in T$ denoting the outward normal spatial derivative of $u_{i,p} (\cdot, t)$ on $\partial \Omega$, and

$$\alpha_i(x,t) \geq 0, \ \beta_i(x,t) \geq 0, \ \alpha_i(x,t) + \beta_i(x,t) > 0, \ \forall (x,t) \in \Gamma. \quad (5)$$

We next briefly summarize some standard continuity and consistency assumptions required for
the existence of a solution to (3) as follows. The coefficients of operator $L_i$ and the functions $h_i, u_{i,0}$
are assumed to be Hölder continuous in their respective domains $\forall i$. The coefficients of the operator
$B_i$ are assumed to be continuous in their domain $\forall i$. The initial conditions $u_{i,0}$ satisfy the boundary
conditions at $t = 0 \ \forall i$. The functions $f_i$ are assumed to be Hölder continuous in $Q \ \forall i$. Additionally,
some regularity is expected for the boundary surface $\partial \Omega$ in the sense that each of its points can be
represented locally by a function satisfying a Hölder continuity condition. An exhaustive discussion of these well-studied existence conditions is outside the scope of this work, and we refer the interested reader to Section 2.1 of [10], for instance, for more details.

For notational brevity, it is convenient to rewrite (3) as follows:

$$\begin{align*}
L_i u_{i,p} &= f_i(u_p, x, t, p) \text{ in } Q, \\
B_i u_{i,p} &= h_i(x, t, p) \text{ on } \Gamma, \\
u_{i,p}(x,0) &= u_{i,0}(x, p) \text{ in } \bar{\Omega}.
\end{align*} \quad (6)$$

2.2. A simple serial branch-and-bound method

Here, a procedure for deterministic branch-and-bound global optimization is outlined, to motivate
the constructions of parametric bounds on $u_p$. The classic reference for branch-and-bound theory is [20].

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Consider an optimization problem of the form:

\[
p_{\text{opt}} = \arg \min_{p \in P} \left\{ O(p) = \sum_{(x,t) \in \tilde{Q}^M} \phi(u_p(x,t)) \right\}. \tag{7}
\]

\[
\text{s.t.} \quad \forall t \in T, \forall i \in I_u, \\
L_i u_{i,p} = f_i(u_p, x, t, p) \quad \text{in} \ Q, \\
B_i u_{i,p} = h_i(x, t, p) \quad \text{on} \ \Gamma, \\
u_{i,p}(x, 0) = u_{i,0}(x, p) \quad \text{in} \ \tilde{Q}.
\]

Here, \( O \) denotes a potentially nonconvex objective function, for example, least squares or maximum likelihood in parameter estimation problems. Moreover, \( \tilde{Q}^M \) denotes a set of points in \( \tilde{Q} \) at which experimental measurements are taken. Standard optimization software (e.g., \( \text{fmincon} \) in MATLAB) can only yield a locally optimal solution \( O_{\text{loc}} \) in the vicinity of the initial guess. A branch-and-bound algorithm can determine the globally optimal solution \( O_{\text{opt}} \) to within some finite absolute convergence tolerance \( \epsilon_O \), by recursively bounding the solution on progressively smaller subintervals of the parameter space.

A local optimizer can be used to obtain an upper bound by initializing it anywhere on the subinterval (another approach is to just evaluate the objective function anywhere on the subinterval). The corresponding lower bound can be obtained in one of two ways. Assume that a pointwise in \( \tilde{Q} \) interval bound \( [u_p^L, u_p^U] \) on \( u_p \) is available (the construction of such bounds is addressed later on in this paper). Standard interval arithmetic [3] can then be used to propagate it (along with \( P \) through \( \phi \) to obtain a corresponding interval bound \( [O^L, O^U] \) on \( O \). \( O^L \) can then be taken to lower bound \( O \), and hence its global minimum, on the subinterval. Alternatively, assume that a pointwise in \( \tilde{Q} \) bound \( [u_p^{CV}, u_p^{CC}] \) on \( u_p \) is available, with \( u_p^{CV} \) being convex and \( u_p^{CC} \) being concave on \( P \) (the construction of such bounds is addressed later on in this paper). Then, a generalization of McCormick’s relaxation technique can be applied to obtain an interval bound \( [O^{CV}(p), O^{CC}(p)] \) on \( O(p) \) for each \( p \in P \), with \( O^{CV} \) being convex and \( O^{CC} \) being concave on \( P \). \( O^{CV} \) can then be locally optimized on the subinterval to yield a lower bound on the global minimum (this step uses the well-known fact that the local minimum of a convex function is its global minimum).

To aid visualization, the different types of bounds are illustrated in Figure 1 for a univariate objective function. A generalization of McCormick’s relaxation technique will be used to construct \( [u_p^{CV}, u_p^{CC}] \) later on in this paper and will be discussed in more detail at that time. If the objective lower bound on any subinterval is higher than the least upper bound known so far (LUB, or the incumbent solution), the global solution cannot exist on it, and the subinterval is excluded from further consideration. If the least lower bound on the remaining subintervals is not within \( \epsilon_O \) of the LUB, one subinterval is bisected on a uniformly randomly selected parameter into two intervals to be bounded and added to the active interval list. The process is initiated with \( P \) and continued until the least lower bound is within \( \epsilon_O \) of LUB. At this point, an optimal solution is available as the parameter corresponding to the LUB (this solution, by construction, is known to be within \( \epsilon_O \) of the global solution).

Figure 1. Different types of bounds for the objective function \( O \).
A sample illustrative iteration of the procedure, with the convex bound being employed to lower bound the objective on each subinterval, is shown in Figure 2. We see that we need to construct bounds for the PDE solution that are either constant in the parameter (i.e., an interval bound) or convex lower and concave upper in the parameter (bounds also typically referred to as convex and concave relaxations, or simply relaxations, in the global optimization literature).

3. BOUNDS

3.1. Background theorems

Here, key theorems necessary to construct the bounds are collected. The following existence-comparison theorem is key for the construction of the interval bounds. Unless made explicit otherwise, the order relation \( \preceq \) should henceforth be taken to be componentwise and pointwise in the domain for vector functions.

We first restate a positivity lemma for parabolic operators from [10]. This lemma is a consequence of the maximum principle for parabolic operators (2).

**Theorem 1**

Let a function \( u_p \in C^{2,1}(Q) \cap C(\bar{Q}) \) be such that

\[
\begin{align*}
\mathcal{L}u_p + cu_p &\geq 0 \text{ in } Q, \\
B u_p &\geq 0 \text{ on } \Gamma, \\
u_p(x, 0) &\geq 0 \text{ in } \bar{Q},
\end{align*}
\]

where \( c \equiv c(x, t) \) is a bounded function in \( Q \). Then, \( u_p \geq 0 \) in \( \bar{Q} \).

**Proof**

See Lemma 2.2.1 in [10].

Next, we restate a theorem due to Pao [10].

**Theorem 2**

Consider (6) for some \( p \in P \) and assume that a pair of functions \( v \) and \( w \) in \( C^{2,1}(Q) \cap C(\bar{Q}) \), ordered as \( v \preceq w \), satisfy the following inequality for each \( i \):

\[
\begin{align*}
\mathcal{L}_i v_i &\leq f_i(z, x, t, p)|_{z_i = v_i}, \forall z \in [v, w] \text{ in } Q, \\
\mathcal{B}_i v_i &\leq h_i(x, t, p) \text{ on } \Gamma, \\
v_i(x, 0) &\leq u_{i,0}(x, p) \text{ in } \Omega, \\
\mathcal{L}_i w_i &\geq f_i(z, x, t, p)|_{z_i = w_i}, \forall z \in [v, w] \text{ in } Q, \\
\mathcal{B}_i w_i &\geq h_i(x, t, p) \text{ on } \Gamma, \\
\mathcal{B}_i w_i &\leq u_{i,0}(x, p) \text{ in } \Omega.
\end{align*}
\]

with it being assumed that each \( f_i \) is Lipschitz in the state on \([v, w]\), that is, \( \exists K_i \in \mathbb{R}_+ \) such that
\begin{equation}
|f_i(x^1, x, t, p) - f_i(x^2, x, t, p)| \leq K_1 \sum_{j=1}^{n_u} |y^1_j - y^2_j|, \quad \forall (x^1, x^2) \in [v, w] \times [v, w].
\end{equation}

Then, there exists a unique solution \( u_p \) to (6), and it is ordered as \( v \leq u_p \leq w \).

**Proof**

See Theorem 8.9.3 in [10]. The author of that work, Pao, proved the theorem by constructing a monotone sequence of functions, with \( w \) and \( v \) as the initial condition for the iteration, to converge to \( u_p \) from above and below, respectively.

Next, we prove an original theorem, utilizing the previous two theorems, that will be required to construct the interval bounds.

**Theorem 3**

Consider (6) for some \( p \in P \) and assume that a pair of functions \( v \) and \( w \) in \( C^{2,1} (Q) \cap C (\bar{Q}) \) satisfy the following inequality \( \forall i \in I_0 \):

\begin{align}
\mathcal{L}_i v_i &\leq f_i(z, x, t, p)|_{z_i = v_i}, \quad \forall z \in \min(v, w), \max(v, w) \text{ in } Q, \\
\mathcal{B}_i v_i &\leq h_i(x, t, p) \text{ on } \Gamma, \\
v_i(x, 0) &\leq u_i(0, x, p) \text{ in } \Omega, \\
\mathcal{L}_i v_i &\geq f_i(z, x, t, p)|_{z_i = w_i}, \quad \forall z \in \min(v, w), \max(v, w) \text{ in } Q, \\
\mathcal{B}_i v_i &\geq h_i(x, t, p) \text{ on } \Gamma, \\
w_i(x, 0) &\leq u_i(0, x, p) \text{ in } \Omega,
\end{align}

with it being assumed that each \( f_i \) is differentiable in the state on \( \min(v, w), \max(v, w) \) and is Lipschitz in the state on \( \min(v, w), \max(v, w) \) (condition 10). Then, such a pair of functions is necessarily ordered as \( v \leq w \). Moreover, there exists a unique solution \( u_p \) to (6), and it is ordered as \( v \leq u_p \leq w \).

**Proof**

First, we show that such a pair of functions is necessarily ordered as \( v \leq w \). For this purpose, subtract the top half of (11) from the lower half, and observe that the following inequality \( \forall i \in I_0 \) is directly implied:

\begin{align}
\mathcal{L}_i (w_i - v_i) &\geq \left( f_i(z, x, t, p)|_{z_i = w_i} - f_i(z, x, t, p)|_{z_i = v_i} \right), \quad \forall z \in \min(v, w), \max(v, w) \text{ in } Q, \\
\mathcal{B}_i (w_i - v_i) &\geq 0 \text{ on } \Gamma, \\
(w_i - v_i)(x, 0) &\geq 0 \text{ in } \Omega.
\end{align}

Whenever \( w_i = v_i \), the right-hand side of (12) is 0. Next, observe that whenever \( w_i \neq v_i \), the mean value theorem can be applied to deduce the following inequality \( \forall i \):

\begin{align}
\mathcal{L}_i (w_i - v_i) &\geq \frac{\partial f_i}{\partial z_i} (z, x, t, p)|_{z_i = \eta} (w_i - v_i), \quad \forall z \in \min(v, w), \max(v, w) \text{ in } Q, \\
\mathcal{B}_i (w_i - v_i) &\geq 0 \text{ on } \Gamma, \\
(w_i - v_i)(x, 0) &\geq 0 \text{ in } \Omega,
\end{align}

where \( \eta \) is an intermediate value (pointwise in \( Q \)) between \( v_i \) and \( w_i \) for each \( z \) in \( \min(v, w), \max(v, w) \). It is well-known that Lipschitz functions that are differentiable have bounded first derivatives (see any standard textbook on analysis, such as [21]). Thus, \( \frac{\partial f_i}{\partial z_i} \) is bounded in \( Q \) for each \( z \) in \( \min(v, w), \max(v, w) \). Then, by the positivity lemma for (6) (Theorem 1), it follows that \( w_i - v_i \geq 0, \forall i \in I_0 \), that is, that \( v \leq w \). Having shown this, the existence of a unique solution \( u_p \) ordered as \( v \leq u_p \leq w \) is a direct consequence of Theorem 2.
The following theorem is key for the construction of the convex/concave relaxations.

**Theorem 4**
Consider the pair of scalar PDEs:

\[
\begin{align*}
\mathcal{L}_i u_{i,p} &= f_i(x, t, \mathbf{p}) \text{ in } Q, \\
\mathcal{B}_i u_{i,p} &= h_i(x, t, \mathbf{p}) \text{ on } \Gamma, \\
\ u_{i,p}(x, 0) &= u_{i,0}(x, \mathbf{p}) \text{ in } \tilde{\Omega},
\end{align*}
\]

for \( i \in \{1, 2\} \). Assume that, for some \( \mathbf{p} \in P \), the following inequality holds:

\[
\begin{align*}
f_1(x, t, \mathbf{p}) &\leq f_2(x, t, \mathbf{p}) \text{ in } Q, \\
h_1(x, t, \mathbf{p}) &\leq h_2(x, t, \mathbf{p}) \text{ on } \Gamma, \\
u_{1,0}(x, \mathbf{p}) &\leq u_{2,0}(x, \mathbf{p}) \text{ in } \tilde{\Omega}.
\end{align*}
\]

Then, the solutions are ordered as \( u_{1,p} \leq u_{2,p} \).

**Proof**
See Theorem 2.2.1 in [10].

### 3.2. Interval bound

We next construct an interval bound on the solution to (6).

**Theorem 5**
Consider a pair of functions \( u^L \) and \( u^U \) satisfying the following inequality \( \forall i \in I_u \):

\[
\begin{align*}
\mathcal{L}_i u_i^L &\leq \inf_{u^L(x,t) \leq u^U(x,t), \ z_i = u_i^L(x,t), \ p \in P} \{f_i(z, x, t, \mathbf{p})\} \text{ in } Q, \\
\mathcal{B}_i u_i^L &\leq \inf_{p \in P} \{h_i(x, t, \mathbf{p})\} \text{ on } \Gamma, \\
u_i^L(x, 0) &\leq \inf_{p \in P} \{u_{i,0}(x, \mathbf{p})\} \text{ in } \tilde{\Omega}, \\
\mathcal{L}_i u_i^U &\geq \sup_{u^L(x,t) \leq u^U(x,t), \ z_i = u_i^U(x,t), \ p \in P} \{f_i(z, x, t, \mathbf{p})\} \text{ in } Q, \\
\mathcal{B}_i u_i^U &\geq \sup_{p \in P} \{h_i(x, t, \mathbf{p})\} \text{ on } \Gamma, \\
u_i^U(x, 0) &\geq \sup_{p \in P} \{u_{i,0}(x, \mathbf{p})\} \text{ in } \tilde{\Omega},
\end{align*}
\]

with it being assumed that each \( f_i \) is differentiable in the state on \( (u^L, u^U) \) and is Lipschitz in the state on \( [u^L, u^U] \), that is, \( \exists K_i \in \mathbb{R}_+ \) such that

\[
|f_i(y^1, x, t, \mathbf{p}) - f_i(y^2, x, t, \mathbf{p})| \leq K_i \sum_{j=1}^{n_u} |y^1_j - y^2_j|, \ \forall (y^1, y^2) \in [u^L, u^U] \times [u^L, u^U].
\]

Then, there exists a unique solution \( u_{\mathbf{p}} \) to (6) for each \( \mathbf{p} \in P \), ordered as \( u^L \leq u_{\mathbf{p}} \leq u^U \).

**Proof**
For each \( \mathbf{p} \in P \), \( u^L \) and \( u^U \) satisfy the hypotheses of Theorem 3. □

Consider the following simple example application of this theorem.
Example 1

Consider the following scalar PDE for some \( p \in P \):

\[
\frac{\partial u}{\partial t}(x, t) - \frac{\partial^2 u}{\partial x^2}(x, t) = e^{p^3}, \forall (x, t) \in Q.
\]  

(18)

with the boundary and initial conditions not being parameter dependent. An auxiliary system satisfying (16) is obtained as follows:

\[
\frac{\partial u^L}{\partial t}(x, t) - \frac{\partial^2 u^L}{\partial x^2}(x, t) = e^{(p^L)^3}, \forall (x, t) \in Q,
\]

\[
\frac{\partial u^U}{\partial t}(x, t) - \frac{\partial^2 u^U}{\partial x^2}(x, t) = e^{(p^U)^3}, \forall (x, t) \in Q.
\]  

(19)

with the same initial and boundary conditions as the original PDE. Here, we have used the fact that the source function is monotonically increasing in \( p \) to deduce that

\[
e^{p^3} \in \left[ e^{(p^L)^3}, e^{(p^U)^3} \right], \forall p \in P.
\]  

(20)

In general, standard interval arithmetic can be used to obtain an interval bound for the range of the right-hand side, thereby obtaining a valid auxiliary system satisfying (16), with a variety of software tools (e.g., INTLAB for MATLAB [22]) being available to automate the process. Note, however, that Taylor bounding methods [6, 23] may also be used, provided the right-hand side source functions are sufficiently differentiable, as required by Taylor arithmetic.

3.3. Relaxations

In this subsection, it is assumed that an interval bound \([u^L, u^U]\) has been constructed as specified in the previous subsection (this also establishes the existence of a unique solution \( u_p \) for each \( p \in P \)). We are interested in constructing convex and concave relaxations of each \( u_{i,p} \) on \( P \), that is, a pair of functions \( u^c_{i,p} \) and \( u^{cc}_{i,p} \) that are respectively convex and concave on \( P \) pointwise in \( \bar{Q} \) and respectively lower bounds and upper bounds pointwise in \( \bar{Q} \) for each \( p \in P \). The following theorem is used to achieve this.

Theorem 6

For some \( p \in P \), consider a pair of functions \( u^c_{p} \) and \( u^{cc}_{p} \) satisfying the following equality \( \forall i \in I_u \):

\[
\mathcal{L}_i u^c_{i,p} = f_i^{CV} (u^c_{p}, u^{cc}_{p}, x, t, p) \text{ in } Q,
\]

\[
\mathcal{B}_i u^c_{i,p} = h_i^{CV} (x, t, p) \text{ on } \Gamma,
\]

\[
u^c_{i,p}(x, 0) = u^c_{i,0} (x, p) \text{ in } \bar{Q},
\]

\[
\mathcal{L}_i u^{cc}_{i,p} = f_i^{CC} (u^c_{p}, u^{cc}_{p}, x, t, p) \text{ in } Q,
\]

\[
\mathcal{B}_i u^{cc}_{i,p} = h_i^{CC} (x, t, p) \text{ on } \Gamma,
\]

\[
u^{cc}_{i,p}(x, 0) = u^{cc}_{i,0} (x, p) \text{ in } \bar{Q}.
\]  

(21)

Here, the superscripts \( CV \) and \( CC \) should be taken to mean that these functions are respectively valid convex relaxations and concave relaxations of the original right-hand side functions, provided \( u^c_{p} \) and \( u^{cc}_{p} \) are respectively valid convex and concave relaxations of \( u_p \). Moreover, assume that
each \( f_i^{CV} \) and \( f_i^{CC} \) is globally Lipschitz in \( u_p^{cv} \) and \( u_p^{cc} \), that is, \( \exists K_i^{CV} \in \mathbb{R}_+ \) and \( \exists K_i^{CC} \in \mathbb{R}_+ \) such that

\[
|f_i^{CV}(y^1, y^3, x, t, p) - f_i^{CV}(y^2, y^4, x, t, p)| \\
\leq K_i^{CV} \left( \sum_{j=1}^{n_u} |y_j^1 - y_j^2| + \sum_{j=1}^{n_u} |y^3_j - y^4_j| \right), \quad \forall (y^1, y^2, y^3, y^4) \in \mathbb{R}^{n_u} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_u}.
\]

(22)

Then, \( u_p^{cv} \) and \( u_p^{cc} \) are valid convex relaxations and concave relaxations of \( u_p \), respectively.

**Proof**

For each \( p \in P \), under the assumed global Lipschitz continuity of each \( f_i^{CV} \) and \( f_i^{CC} \) in \( u_p^{cv} \) and \( u_p^{cc} \), the sequence in \( C^{2,1}(Q) \cap C(\bar{Q}) \), with successive iterates defined by the following:

\[
\begin{align*}
\mathcal{L}_i u_{i,p}^{cv,k+1} &= f_i^{CV}(u_p^{cv,k}, u_p^{cc,k}, x, t, p) \quad \text{in} \quad Q, \\
B_i u_{i,p}^{cv,k+1} &= h_i^{CV}(x, t, p), \quad \forall (x, t) \in \Gamma, \\
u_{i,p}^{cv,k+1}(x,0) &= u_i(0, x), \quad \forall x \in \bar{\Omega}, \\
\mathcal{L}_i u_{i,p}^{cc,k+1} &= f_i^{CC}(u_p^{cv,k}, u_p^{cc,k}, x, t, p) \quad \text{in} \quad Q, \\
B_i u_{i,p}^{cc,k+1} &= h_i^{CC}(x, t, p), \quad \forall (x, t) \in \Gamma, \\
u_{i,p}^{cc,k+1}(x,0) &= u_i(0, x), \quad \forall x \in \bar{\Omega},
\end{align*}
\]

(23)

\( \forall i \in I_u \) converges to the unique solution \( u_p^{cv} \) and \( u_p^{cc} \) to (21) from any initial estimate in \( C^{2,1}(Q) \cap C(\bar{Q}) \). See Theorem 8.9.1 in [10] for proof. The formal reason behind this is that the mapping between successive iterates is a contraction mapping on the Banach space \( C^{2,1}(Q) \cap C(\bar{Q}) \). For every \( p \in P \), choose \( u_p^{cv,0} \) and \( u_p^{cc,0} \) to be \( u^L \) and \( u^U \), respectively. Assume that the following inequalities hold at step \( k \) for any distinct parameter pair \( p_1, p_2 \in P \) and any \( \lambda \in (0, 1) \):

\[
\begin{align*}
u_p^{cv,k} &\leq u_p^{cc,k}, \quad \forall p \in P, \\
u_{\lambda p_1 + (1-\lambda)p_2}^{cv,k} &\leq \lambda u_p^{cv,k} + (1-\lambda) u_p^{cc,k} \\
\lambda u_p^{cc,k} + (1-\lambda) u_p^{cv,k} &\leq u_{\lambda p_1 + (1-\lambda)p_2}^{cc,k}.
\end{align*}
\]

(24)

Note that these are valid at \( k = 0 \). These inequalities capture the fact that \( u_p^{cv,k} \) and \( u_p^{cc,k} \) are valid relaxations of \( u_p \), and hence \( f_i^{CV}, h_i^{CV}, u_i^{cv,0}, f_i^{CC}, h_i^{CC} \) and \( u_i^{cc,0} \) are valid relaxations of their respective functions at step \( k \). Simultaneously, consider the following sequence:

\[
\begin{align*}
\mathcal{L}_i u_{i,p}^{k+1} &= f_i(u_p^{k}, x, t, p) \quad \text{in} \quad Q, \\
B_i u_{i,p}^{k+1} &= h_i(x, t, p) \quad \text{on} \quad \Gamma, \\
u_{i,p}^{k+1}(x,0) &= u_{i,0}(x, p) \quad \text{in} \quad \bar{\Omega},
\end{align*}
\]

(25)
\( \forall i \in I_u, \) initiated at \( u_p \) such that it remains there \( \forall k \). Some algebra implies from (23) that the following:

\[
L_i \left( \lambda u_{i,p1}^{cv,k+1} + (1 - \lambda) u_{i,p2}^{cv,k+1} \right) = \lambda f_i^{CV} \left( u_{p1}^{cv,k}, u_{p1}^{cc,k}, x, t, p1 \right) + (1 - \lambda) f_i^{CV} \left( u_{p2}^{cv,k}, u_{p2}^{cc,k}, x, t, p2 \right) \text{ in } Q, \]

\[
B_i \left( \lambda u_{i,p1}^{cv,k+1} + (1 - \lambda) u_{i,p2}^{cv,k+1} \right) = \lambda h_i^{CV} \left( x, t, p1 \right) + (1 - \lambda) h_i^{CV} \left( x, t, p2 \right) \text{ on } \Gamma, \]

\[
\left( \lambda u_{i,p1}^{cv,k+1} + (1 - \lambda) u_{i,p2}^{cv,k+1} \right) \left( x, 0 \right) = \lambda u_{i,0}^{CV} \left( x, p1 \right) + (1 - \lambda) u_{i,0}^{CV} \left( x, p2 \right) \text{ in } \Omega, \tag{26}
\]

and the following:

\[
L_i u_{i,\lambda p1 + (1 - \lambda)p2}^{cv,k+1} = f_i^{CV} \left( u_{i,\lambda p1 + (1 - \lambda)p2}^{cv,k}, u_{i,\lambda p1 + (1 - \lambda)p2}^{cc,k}, x, t, \lambda p1 + (1 - \lambda) p2 \right) \text{ in } Q, \]

\[
B_i u_{i,\lambda p1 + (1 - \lambda)p2}^{cv,k+1} = h_i^{CV} \left( x, t, \lambda p1 + (1 - \lambda) p2 \right) \text{ on } \Gamma, \]

\[
u_{i,\lambda p1 + (1 - \lambda)p2}^{cv,k+1} \left( x, 0 \right) = u_{i,0}^{CV} \left( x, \lambda p1 + (1 - \lambda) p2 \right) \text{ in } \Omega, \tag{27}
\]

equalities are valid for any distinct parameter pair \((p1, p2) \in P \times P\) and any \( \lambda \in (0, 1)\). Analogous equalities are valid for the concave overestimating portion. Then, simply comparing right-hand side values between (26) and (27) using Theorem 4 implies that \( u_{i,p1}^{cv,k+1} \leq \lambda u_{i,p2}^{cv,k+1} + (1 - \lambda) u_{i,p2}^{cv,k+1} \). Similarly, comparing right-hand side values between (25) and the top half portion of (23), also using Theorem 4, implies that \( u_{i,p1}^{cv,k+1} \leq u_{i,p2}^{cv,k+1} \). Analogous comparisons guarantee \( u_p \leq u_{p,c,k+1} \), \( \forall p \in P\) and that \( \lambda u_{p,c,k+1} + (1 - \lambda) u_{p,c,k+1} \leq u_{p,c,k+1} + (1 - \lambda) u_{p,c,k+1} \) for any distinct parameter pair \((p1, p2) \in P \times P\) and any \( \lambda \in (0, 1)\). Thus, we know by induction that \( u_p^{cv} \) and \( u_p^{cc} \) are valid relaxations, that is, that

\[
u_p^{cv} \leq u_p \leq u_p^{cc}, \quad \forall p \in P, \]

\[
u_{p,c,k+1}^{cv} \leq \lambda u_{p,c,k+1}^{cv} + (1 - \lambda) u_{p,c,k+1}^{cc}, \]

\[
u_{p,c,k+1}^{cc} \leq \lambda u_{p,c,k+1}^{cc} + (1 - \lambda) u_{p,c,k+1}^{c,c}, \tag{28}
\]

for any distinct parameter pair \((p1, p2) \in P \times P\) and any \( \lambda \in (0, 1)\).

The aforementioned theorem is readily implemented using a generalization of McCormick’s relaxation technique [24], which was used to construct relaxations of ODE solutions in [5] and required the same conditions as we require here. We next briefly describe the technique in the remainder of this section.

McCormick’s composition theorem, originally proved by McCormick in 1976 [25, 26], is the cornerstone of this technique. We do not restate it here, so as not to distract the reader from the core of our contribution, but refer the interested reader to the references stated for more details. The well-known fact that the sum of two convex functions is convex provides a rule for relaxing binary products. A specific rule also exists for relaxing binary products, but it is again not presented explicitly here in the interest of brevity (refer to [25, 26] and [24] for details). These three rules define McCormick’s relaxation technique. The generalization of McCormick’s relaxation technique developed in [24] is analogous to the original McCormick relaxation technique, the exception being that one is also allowed to treat implicit dependence of intermediate functions on the underlying parameters.

Any function that can be expressed as a finite recursive composition of binary sums, binary products, and a given library of intrinsic functions, referred to as a factorable function, may be relaxed using this technique. This is a rather general class of functions, including nearly all functions that can be represented finitely on a computer [26]. This generality is the reason this technique is our preferred technique for implementing numerically Theorem 6. We do note here, however, that the \( \alpha \)BB technique can also be used to implement our theorem. This technique requires twice-differentiability, which implies the Lipschitz continuity condition required by Theorem 6. Indeed, any other relaxation technique that satisfies the required global Lipschitz continuity condition may be directly applicable.
Consider the following simple analytic example to fix these ideas. The purpose of this example is to allow the reader to get a better sense of how Theorem 6 may be used in practice.

**Example 2**
Consider the following function:

\[ g(p) = e^{p^3} + u_p, \forall p \in [-1, 1]. \]  

Here, \( u_p \) is a function whose dependence on \( p \) is not known explicitly, but whose range is known to be bounded on \( P \) by \([u_p^L, u_p^U]\) and whose relaxations are known to be \( u_p^{CV} \) and \( u_p^{CC} \). Truncate these relaxations to lie on \([u_p^L, u_p^U]\) as \( u_p^{CV} = \max(u_p^L, u_p^U) \) and \( u_p^{CC} = \min(u_p^L, u_p^U) \) (recalling that max and min functions preserve convexity and concavity, respectively). We are interested in obtaining a convex relaxation of \( g \) on \( P, g^{CV} \). Then, consider the finite recursive composition:

\[ v_1 = p, \; v_2 = v_3^1, \; v_3 = e^{v_2}, \; v_4 = u_p, \; v_5 = v_3 + v_4, \]

with \( v_5 \) representing the original function \( g \). Use the specified interval for the interval-valued independent variable \( p \) to specify the following:

\[ v_1^L = -1, \; v_1^U = 1, \; v_1^{CV}(p) = p, \; v_1^{CC}(p) = p. \]

Because \( v_2 \) is monotonically increasing in \( v_1 \), deduce

\[ v_2^L = (v_1^L)^3 = -1, \; v_2^U = (v_1^U)^3 = 1. \]

The \( \alpha \)-BB relaxation rule [27] can be used to obtain the following relaxations for \( v_2 \):

\[ v_2^{CV}(v_1) = v_1^3 + 3(v_1^2 - 1), \; v_2^{CC}(v_1) = v_1^3 - 3(v_1^2 - 1). \]

Truncate these to lie on \([v_2^L, v_2^U]\) (recalling that max and min functions preserve convexity and concavity, respectively) as follows:

\[ v_2^{CV}(v_1) = \max(v_1^L, v_2^{CV}(v_1)) = \max(-1, v_1^3 + 3(v_1^2 - 1)), \]

\[ v_2^{CC}(v_1) = \min(v_1^U, v_2^{CC}(v_1)) = \min(1, v_1^3 - 3(v_1^2 - 1)). \]

Because the exponential function is convex, its convex relaxation on its domain is also the exponential function. Moreover, because it is a monotonically increasing function, it attains its infimum at the lower bound of its domain. Then, McCormick’s composition theorem can be applied to relax \( v_3 \) as follows:

\[ v_3^{CV}(v_1) = e^{mid(v_2^{CV}(v_1), v_2^{CC}(v_1), v_2^L)} = e^{mid(\max(-1, v_1^3 + 3(v_1^2 - 1)), \min(1, v_1^3 - 3(v_1^2 - 1)), -1)). \]

Here, \( mid \) is just the median of the three input values. Thus, the convex relaxation of \( v_5 \) is as follows:

\[ v_5^{CV}(v_1) = v_3^{CV}(v_1) + v_4^{CV}(v_1) = e^{mid(\max(-1, v_1^3 + 3(v_1^2 - 1)), \min(1, v_1^3 - 3(v_1^2 - 1)), -1)) + v_4^{CV}(v_1). \]

In other words, the convex relaxation of \( g \) as a function of \( p, g^{CV} \), is given by the following:

\[ g^{CV}(p) = e^{mid(\max(-1, p^3 + 3(p^2 - 1)), \min(1, p^3 - 3(p^2 - 1)), -1)) + \max(u_p^{CV}, u_p^L). \]

Finally, consider the following PDE (with the function we relaxed previously as the source term) for each \( p \in P = [-1, 1] \):

\[ \frac{\partial u_p}{\partial t}(x, t) - \frac{\partial^2 u_p}{\partial x^2}(x, t) = e^{p^3} + u_p, \forall (x, t) \in Q. \]
with initial and boundary conditions that do not carry parameter dependence, and assume that an interval bound \([u^L, u^U]\) has already been constructed for \(u_p\) using Theorem 5. The convex relaxation of \(u_p\) for each \(p \in P\) can then be obtained by solving the following PDE:

\[
\frac{\partial u_{P}^{e}}{\partial t}(x, t) - \frac{\partial^{2} u_{P}^{e}}{\partial x^{2}}(x, t) = \epsilon \text{mid}(\max(-1, p^{3} + 3(p^{2} - 1)), \min(1, p^{3} - 3(p^{2} - 1)), -1) + \max(u_{P}^{e}, u_{L}), \forall (x, t) \in Q,
\]

with the same initial and boundary conditions.

3.4. The case of state spatial derivatives coupled to parameter dependence

When parameter dependence is coupled to the state spatial derivatives, that is, when the elliptic operator in (1) takes the following form for each \(p \in P\):

\[
L_{i}u_{i,p}(x, t, \mathbf{p}) \equiv a_{i}(x, t, \mathbf{p}) \frac{\partial^{2} u_{i,p}}{\partial x^{2}}(x, t) + b_{i}(x, t, \mathbf{p}) \frac{\partial u_{i,p}}{\partial x}(x, t), \forall (x, t) \in Q,
\]

the construction of constant bounds does not change much; that is, one solves the PDE system defined by the following inequalities:

\[
\frac{\partial u_{i}^{L}}{\partial t}(x, t) - \inf_{\mathbf{p} \in P} \left\{ a_{i}(x, t, \mathbf{p}) \frac{\partial^{2} u_{i}^{L}}{\partial x^{2}}(x, t) + b_{i}(x, t, \mathbf{p}) \frac{\partial u_{i}^{L}}{\partial x}(x, t) \right\} \\
\leq \inf_{u^{L}(x, t) \leq u^{L}(x, t), z_{i} = u^{L}(x, t), \mathbf{p} \in P} \{ f_{i}(\mathbf{z}, x, t, \mathbf{p}) \}, \forall (x, t) \in Q,
\]

\[
B_{i}u_{i}^{L}(x, t) \leq \inf_{\mathbf{p} \in P} \{ h_{i}(x, t, \mathbf{p}) \}, \forall (x, t) \in \Gamma,
\]

\[
\frac{\partial u_{i}^{L}}{\partial t}(x, t) - \sup_{\mathbf{p} \in P} \left\{ a_{i}(x, t, \mathbf{p}) \frac{\partial^{2} u_{i}^{L}}{\partial x^{2}}(x, t) + b_{i}(x, t, \mathbf{p}) \frac{\partial u_{i}^{L}}{\partial x}(x, t) \right\} \\
\geq \sup_{u^{L}(x, t) \leq u^{L}(x, t), z_{i} = u^{L}(x, t), \mathbf{p} \in P} \{ f_{i}(\mathbf{z}, x, t, \mathbf{p}) \}, \forall (x, t) \in Q,
\]

\[
B_{i}u_{i}^{L}(x, t) \geq \sup_{\mathbf{p} \in P} \{ h_{i}(x, t, \mathbf{p}) \}, \forall (x, t) \in \Gamma,
\]

\[
u_{i}^{U}(x, 0) \geq \sup_{\mathbf{p} \in P} \{ u_{i,0}^{L}(x, \mathbf{p}) \}, \forall x \in \Omega,
\]

\(\forall i \in I_{u}\) in place of (16). To verify that this is true, one just need to recognize that for each \(\mathbf{p} \in P\), \(u^{L}\) and \(u^{U}\) satisfy the hypotheses of Theorem 3.

This case is important for reaction-diffusion systems because optimizing over diffusion coefficients is a very important use-case for this class of problems. However, note that the development of separate convex/concave relaxations for this case is less important, because one can always perform a two-stage optimization: first, over the diffusion coefficients using the system (41), and then over the parameters in the source term using system (21) if nonquasimonotonicity calls for it. In the unlikely scenario that a reaction-diffusion system possesses a source-term dependent on diffusion coefficients (the author of this work is yet to see a physical example), the final chapter of the author’s dissertation [28] conjectures a way to extend system (21) to this case.

4. NUMERICAL DEMONSTRATION

First is a numerical note. Systems are solved using the method of lines, discretizing them on the spatial domain using the three-point-centered finite difference scheme on a uniform grid of spatial nodes and integrating the resulting coupled ODE system forward in time using the \(C + +\) CVODES ODE solver [29]. McCormick relaxations for the right-hand sides are constructed by the open-source \(C + +\) library libMC [26]. Interval arithmetic is performed using a combination of libMC
The local optimizer used is the `fm in c o n` optimizer in MATLAB (which uses the trust-reflective-region method). All C ++ code was linked to MATLAB using its `mex` interface. Note that because in the example, the source function is polynomial in the state, the hypotheses of Theorem 5 are easy to verify.

The following example involves a semilinear parabolic PDE in two variables, coupled through a nonquasimonotone function, so relaxations are constructed along with the interval bounds. It is a modified form of the ODE example in [5].

**Example 3**

Consider the following design problem:

$$
\min_{\mathbf{p} \in \mathcal{P}} \left\{ \frac{1}{n_{\bar{Q}^M}} \sum_{x \in \bar{Q}^M} u_{1,\mathbf{p}}(x, t_f) \right\},
$$

subject to the coupled parabolic system defined for each $\mathbf{p} \in \mathcal{P}$ by the following equations:

$$
\frac{\partial u_{1,\mathbf{p}}}{\partial t}(x, t) - \frac{\partial^2 u_{1,\mathbf{p}}}{\partial x^2}(x, t) = p_1 u_{1,\mathbf{p}}(x, t), \quad \forall (x, t) \in (0, 1) \times (0, 1] ,
$$

$$
\frac{\partial u_{2,\mathbf{p}}}{\partial t}(x, t) - \frac{\partial^2 u_{2,\mathbf{p}}}{\partial x^2}(x, t) = -p_2 \left( u_{1,\mathbf{p}}(x, t) - u_{2,\mathbf{p}}(x, t) + \frac{(u_{2,\mathbf{p}}(x, t))^3}{3} \right), \quad \forall (x, t) \in (0, 1) \times (0, 1] ,
$$

(i.e., $t_f = 1$). Here, $n_{\bar{Q}^M}$ is just the number of points in $\bar{Q}^M$. Time-independent boundary conditions are specified by the following:

$$
u_{1,\mathbf{p}}(0, t) = 1, \quad u_{2,\mathbf{p}}(0, t) = 1, \quad \forall (t, \mathbf{p}) \in (0, 1] \times \mathcal{P},
$$

$$
u_{1,\mathbf{p}}(1, t) = 1, \quad u_{2,\mathbf{p}}(1, t) = 1, \quad \forall (t, \mathbf{p}) \in (0, 1] \times \mathcal{P},
$$

Figure 3. Objective and its bounds for the numerical example in (A) on the left (the objective is red, interval lower bound is black, interval upper bound is magenta, convex lower bound is green, and concave upper bound is blue). In (B) on the right, a slice (where $p_1 = p_2$) through objective to help visualize its nonconvexity.
and initial conditions are specified as a line between these boundary values. $P$ is specified as $[1, 7] \times [1, 7]$. $\Omega^M$ is specified by the uniform spatial grid of 100 points on which the PDE is solved. The objective is visualized, along with its interval/constant bounds and relaxations, on $P$, in Figure 3. We see that all bounds are valid and that the relaxations are significantly better than the interval bounds.

Next, we numerically study the convergence of both types of bounds to the solution at the midpoint of $P$ in Hausdorff metric, that is, the evolution of the quantities:

\[ q \left( \left[ O^L, O^U \right], [O(p_{\text{mpt}}), O(p_{\text{mpt}})] \right) = \max \left( \left| O^L - O(p_{\text{mpt}}) \right|, \left| O^U - O(p_{\text{mpt}}) \right| \right), \]

\[ q \left( \left[ O^C_{\text{p_{mpt}}}, O^C_{\text{p_{mpt}}} \right], [O(p_{\text{mpt}}), O(p_{\text{mpt}})] \right) = \max \left( \left| O^C_{\text{p_{mpt}}} - O(p_{\text{mpt}}) \right|, \left| O^C_{\text{p_{mpt}}} - O(p_{\text{mpt}}) \right| \right), \]

(45)

with the bounds $O^L, O^U, O^C_{p_{\text{mpt}}}, O^C_{p_{\text{mpt}}}$ evaluated on the parameter interval $[p_{\text{mpt}} - \varepsilon_{HM}, p_{\text{mpt}} + \varepsilon_{HM}]$ as $\varepsilon_{HM}$ varies from 3 to 0. Note that $p_{\text{mpt}}$ is just the midpoint of $P$, that is, $[4, 4]$. A similar study was carried out by Bomparde and Mitsos in [30] for McCormick models. The evolution in these quantities can be seen in Figure 4 (on a regular scale in the top panel and on a double logarithmic scale in the bottom panel). The double logarithmic plot suggests a
linear convergence for the interval bounds and a quadratic convergence for the relaxations constructed using general McCormick relaxations.

Finally, we show a sample run of the branch-and-bound algorithm on the problem. Absolute convergence tolerance was chosen as $10^{-4}$, upper bounds were computed via local optimization of the original objective function, and lower bounds were computed via local optimization of the objective function’s convex relaxation. We see in Figure 5 that bounds converge sufficiently close within 14 iterations. The optimal solution is 1.0499, which is attained at [1, 7].

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