Reachability Bounds for Global and Robust Optimization of Parametric ODEs Via Implicit Methods

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Dynamic Optimization

- One common form of the dynamic optimization problem

$$
\begin{aligned}
\phi^* = \; & \min_{\mathbf{p}\in P\subset\mathbb{R}^{n_p}} \phi(\mathbf{x}(\mathbf{p},t_f),\mathbf{p}) \\
\text{s.t.} \quad & \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}(\mathbf{p},t),\mathbf{p},t), \quad \forall t \in I = [t_0,t_f] \\
& \mathbf{x}(\mathbf{p},t) = \mathbf{x}_0(\mathbf{p}) \\
& \mathbf{g}(\mathbf{x}(\mathbf{p},t),\mathbf{p}) \le \mathbf{0}, \quad \forall t \in I = [t_0,t_f]
\end{aligned}
$$

- That is we seek an optimal satisfying the ODE-IVP problem along with any constraints.
    - $\mathbf{x}$ – state variables
    - $\mathbf{p}$ – decision variables

Global optimization of stiff dynamical systems

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Abstract
We present a deterministic global optimization method for nonlinear programming formulations constrained by stiff systems of ordinary differential equation (ODE) initial value problems (IVPs). The examples arise from dynamic optimization problems exhibiting both fast and slow transient phenomena commonly encountered in model-based systems engineering applications. The proposed approach utilizes unconditionally stable implicit integration methods to reformulate the ODE-constrained problem

Wilhelm, ME; Le, AV; and Stuber. MD. "Global Optimization of Stiff Dynamical Systems." In Press for *AIChE Journal: Futures Issue (2019)*

1 | INTRODUCTION

Dynamic optimization problems of the form:

$$
\begin{aligned}
& \phi^* = \min_{\mathbf{p}\in P\subset\mathbb{R}^{n_p}} \phi(\mathbf{x}(\mathbf{p},t_f),\mathbf{p}) \\
& \text{s.t. } \dot{\mathbf{x}}(\mathbf{p},t) = \mathbf{f}(\mathbf{x}(\mathbf{p},t),\mathbf{p},t), \quad \forall t \in I = [t_0,t_f] \\
& \mathbf{x}(\mathbf{p},t_0) = \mathbf{x}_0(\mathbf{p}) \\
& \mathbf{g}(\mathbf{x}(\mathbf{p},t_f),\mathbf{p}) \le \mathbf{0}
\end{aligned} \tag{1}
$$

are of extreme importance to process systems engineers and the broader model-based systems engineering community as they can be formulated for a variety of systems whose transient behavior is of particular interest, from optimal control to mechanistic model validation. The first major complicating detail of the optimization formulation (1) is that it is constrained by a system of ordinary differential equation–initial value problems (ODE–IVPs). Therefore, simply verifying a feasible point requires the solution of a system of ODE–IVPs. The second major complicating detail is that (1) is a nonconvex program, in general, and therefore verifying optimality requires deterministic global optimization. The focus of this paper is on solving (1) to guaranteed global optimality (or declaration of infeasibility). The methods developed in this work are of specific importance when the ODE–IVP system is stiff.

Methods for solving (1) rigorously to global optimality rely on the spatial branch-and-bound (B&B) framework[1,2] or some variant. The B&B algorithm requires the ability to calculate rigorous upper and lower bounds on the global optimal solution value. An upper bound can be calculated by simply evaluating $\phi(\mathbf{x}(\cdot,t_f),\cdot)$ at any feasible point. However, calculating rigorous lower bounds poses significant challenges as this step requires that rigorous and accurate global bounds are known or are readily calculable for all variables and functions of (1). For standard nonconvex nonlinear programs (NLPs) (i.e., without dynamical systems constraints), rigorous lower bounds on the optimal solution value are obtained by calculating convex and concave relaxations of the functions and solving a corresponding convex lower-bounding problem. Applying this approach to a dynamic optimization

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Parametric ODE-IVP

Parametric ODE-IVP Formulation

$$\dot{\mathbf{x}} = \frac{d\mathbf{x}}{dt}(\mathbf{p}, t) = \mathbf{f}(\mathbf{x}(\mathbf{p}, t), \mathbf{p}, t), \quad t \in I = [t_0, t_f], \ \mathbf{p} \in P$$

$$\mathbf{x}(\mathbf{p}, t_0) = \mathbf{x}_0(\mathbf{p}), \quad \mathbf{p} \in P$$

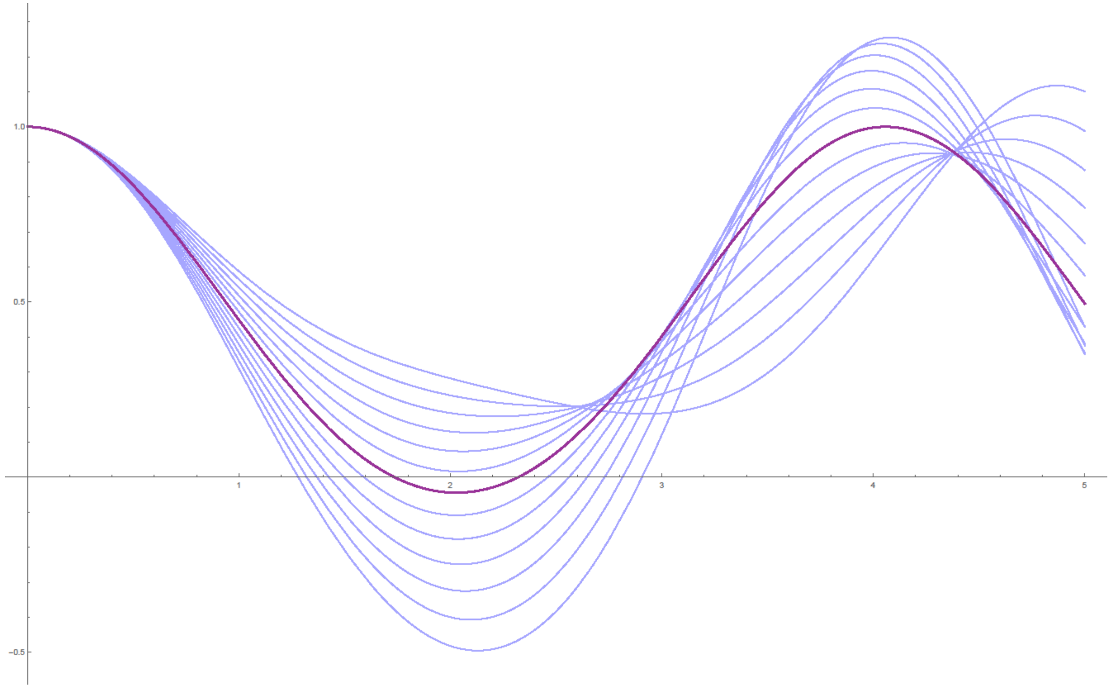
where $\mathbf{f}: D \times \Pi \times \mathrm{T} \to \mathbb{R}^{n_x}$ and $x_0: P \to D$
with $D \subset \mathbb{R}^{n_x}$, $\Pi \subset \mathbb{R}^{n_p}$, and $\mathrm{T} \subset \mathbb{R}$ open
with $P \in \mathbb{I}\Pi$ and $\mathrm{I} \in \mathbb{I}\mathrm{T}$

Assumptions (Well-posed)

1. $\mathbf{x}_0: P \to D$ is locally Lipschitz continuous on P

2. $\mathbf{f}$ is continuously differential on $D \times \Pi \times \mathrm{T}$

Parametric ODE-IVP Solution



A solution is any continuous $\mathbf{x} : P \times I \to D$ such that, for every $\mathbf{p} \in P,\ \mathbf{x}(\mathbf{p},\cdot) : \mathrm{T} \to D$ is continuous differentiable and satisfies the parametric ODE-IVP on I.

Review (Dynamic Optimization)

Discretization [1] *:*

- The domain is separated into K finite elements.
- The derivative terms are approximated by difference forms wherever they appear within the formulation.

$$\left.\frac{dx}{dt}\right|_{t_{k+1}} = \frac{x_{k+1} - x_k}{h}$$

$$g\left(\left.\frac{dx}{dt}\right|_{t_{k+1}}, f(x_{k+1}, p_{k+1})\right) = 0$$

$$k = 0, \dots, K-1$$

Collocation [1] *:*

- The domain is separated into K finite elements.
- The solution in each finite element is then approximated by a polynomial of order $N+1$

$$\left.\frac{dx}{dt}\right|_{t_{kj}} = \frac{1}{h_i}\sum_{j=0}^{K}\frac{dl_j(\tau_i)}{d\tau}, \qquad x_{i+1,0} = \sum_{j=0}^{N} l_j(1)x_{kj}$$

$$g\left(\left.\frac{dx}{dt}\right|_{t_{kj}}, f(x_{ki}, p_{ki})\right) = 0, \qquad t_{kj} = t_{k-1} + \tau_j h$$

$$k = 0, \dots, K-1, \qquad i = 0, \dots, N-1,$$

1. Biegler, L.T.: **Nonlinear Programming: Concepts, Algorithms, and Applications to Chemical Processes.** SIAM, Philadelphia (2010)

Review (Dynamic Optimization)

Discretization [1] *:*

- ○ The domain is separated into K finite elements.
- ○ The derivative ter…
  difference form…
  the formulatio…

$$\left.\frac{dx}{dt}\right|_{t_{k+1}} = \ldots$$

$$g\left(\left.\frac{dx}{dt}\right|_{t_{k}\ldots}\right. \ldots$$

$$k = 0, \ldots, K - 1$$

Collocation [1] *:*

- ○ The domain is separated into K finite elements.
- ○ The solution in each finite element is then
  …ial of order $N + 1$

$$\ldots_{i+1,0} = \sum_{j=0}^{N} l_j(1) x_{kj}$$

$$t_{kj} = t_{k-1} + \tau_j h$$

$$\ldots, N - 1,$$

- Either method introduces a significant number of variables and potentially nonlinear equations
- Results in complicated high dimension problems that may be challenging for modern global optimizers to solve.

1. Biegler, L.T.: **Nonlinear Programming: Concepts, Algorithms, and Applications to Chemical Processes.** SIAM, Philadelphia (2010)

Review (Relaxing ODEs)

Taylor-Series Integrators[3]

$$\mathbf{x}(\tau_{q+1},\mathbf{p}) \in \underbrace{\mathbf{x}(\tau_q,\mathbf{p}) + \sum_{j=1}^{p} \frac{h^j}{j!}\mathbf{f}^{(j)}(\mathbf{x}(\tau_q,\mathbf{p}),\mathbf{p})}_{\text{Taylor Series}} + \underbrace{\frac{h^{p+1}}{(p+1)!}\mathbf{f}^{(p+1)}(\mathrm{X}(\tau_q),\mathrm{P})}_{\text{Remainder Bound}}$$

Differential Inequalities[4]

$$\dot{\mathbf{x}}^{cv}(t,\mathbf{p}) = \mathbf{f}^{cv}(t,\mathbf{p},\mathbf{x}^{cv}(t,\mathbf{p}),\mathbf{x}^{cc}(t,\mathbf{p})), \quad \mathbf{x}^{cv}(t_0,\mathbf{p}) = \mathbf{x}_0^{cv}(\mathbf{p})$$
$$\dot{\mathbf{x}}^{cc}(t,\mathbf{p}) = \mathbf{f}^{cc}(t,\mathbf{p},\mathbf{x}^{cv}(t,\mathbf{p}),\mathbf{x}^{cc}(t,\mathbf{p})), \quad \mathbf{x}^{cc}(t_0,\mathbf{p}) = \mathbf{x}_0^{cc}(\mathbf{p})$$

Discretize-and-Relax[5]

- A two-stage method.
- Calculates valid relaxations across a time step and then refines relaxation at each point.

❑ Each of these approaches allows relaxation of ODE to be calculated with respect to **p**.

❑ Results in a lower dimensional problem.

3. Rihm, Robert. **Interval methods for initial value problems in ODEs.** *Topics in Validated Computations* (1994): 173-207.
4. Joseph K Scott, Paul I Barton. **Improved relaxations for the parametric solutions of ODEs using differential inequalities.** *Journal of Global Optimization*. 2013 (57): 143–176.
5. A.M. Sahlodin, Benoît Chachaut. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics*, 61 (179): 803 – 820, 2011

Implicit Integration of Problem

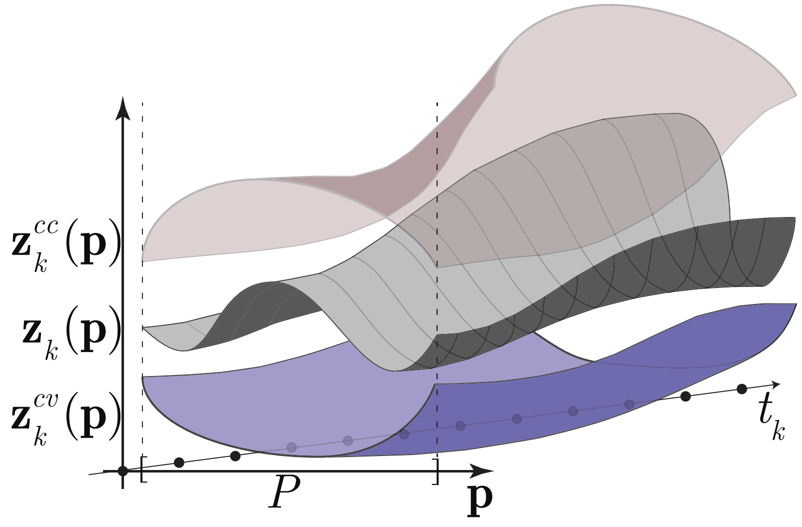
Generalized form of the dynamic optimization problem:

$$\phi^* = \min_{\mathbf{p}\in P\subset\mathbb{R}^{n_p}} \phi(\mathbf{x}(\mathbf{p},\tau_0),\mathbf{x}(\mathbf{p},\tau_1),\ldots,\mathbf{x}(\mathbf{p},\tau_q),\ldots\mathbf{x}(\mathbf{p},\tau_Q),\mathbf{p})$$

$$\text{s.t.} \quad \dot{\mathbf{x}}(\mathbf{p},t) = \mathbf{f}(\mathbf{x}(\mathbf{p},t),\mathbf{p},t), \qquad \forall t \in I \subset [t_0, t_f]$$

$$\dot{\mathbf{x}}(\mathbf{p},t) = \mathbf{x}_0(\mathbf{p})$$

$$g(\mathbf{x}(\mathbf{p},\tau_0),\mathbf{x}(\mathbf{p},\tau_1),\ldots,\mathbf{x}(\mathbf{p},\tau_q),\ldots\mathbf{x}(\mathbf{p},\tau_Q),\mathbf{p}) \le \mathbf{0}$$



Implicit Integration Scheme

Full-space Algebraic Form ($n_x \times K + n_p$ dimensions) :

$$\phi^* = \min_{(\hat{\mathbf{z}},\mathbf{p})\in Z\times P} \phi(\hat{\mathbf{z}},\mathbf{p})$$

$$\text{s.t.} \quad \mathbf{h}(\hat{\mathbf{z}},\mathbf{p}) = \mathbf{0}$$

$$\mathbf{z}_0 = \mathbf{x}_0(\mathbf{p})$$

$$\mathbf{g}(\hat{\mathbf{z}},\mathbf{p}) \le \mathbf{0}$$

Block-sequential solution and relaxation

Implicit Function Form (n_p Dimensions)

$$\phi^* = \min_{\mathbf{p}\in P} \phi(\mathbf{z}(\mathbf{p}),\mathbf{p})$$

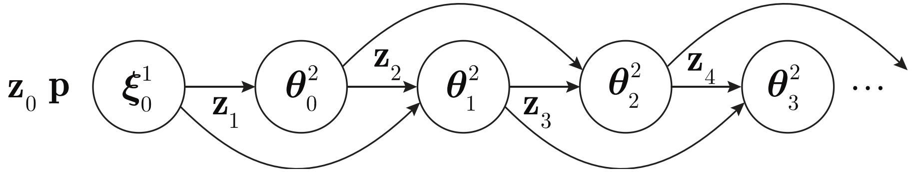
$$\text{s.t.} \quad \mathbf{g}(\mathbf{z}(\mathbf{p}),\mathbf{p}) \le \mathbf{0}$$

Implicit Linear Multistep Method

- An s-step PILMS method can be defined by the equation[6,7]:

$$\boxed{\hat{\mathbf{z}}_{k+s} + \sum_{i=0}^{s-1} a_i \hat{\mathbf{z}}_{k+i} - \Delta t \sum_{j=0}^{s} b_j\, \mathbf{f}(\hat{\mathbf{z}}_{k+j}, \mathbf{p}, t_{k+j}) = \mathbf{0}}$$

$$\begin{aligned}
\mathbf{h}_1 &= \boldsymbol{\xi}_0^1 = (h_1, h_2, h_3, h_4, h_5)\\
\mathbf{h}_2 &= \boldsymbol{\theta}_0^2 = (h_6, h_7, h_8, h_9, h_{10})\\
\mathbf{h}_3 &= \boldsymbol{\theta}_1^2 = (h_{11}, h_{12}, h_{13}, h_{14}, h_{15})\\
&\vdots\\
\mathbf{h}_K &= \boldsymbol{\theta}_{K-2}^2 = (h_{5K-4}, h_{5K-3}, h_{5K-2}, h_{5K-2}, h_{5K})
\end{aligned}$$



- Specific methods for each choice of $\{a_i\}_{i=0}^{s-1}$ and $\{b_j\}_{j=0}^{s}$.
- Adams Moulton arises from $a_{s-1} = -1$, $\{a_i\}_{i=0}^{s-2} = 0$.

$$\boxed{\boldsymbol{\xi}_k^s(\hat{\mathbf{z}}_{k+s}, \ldots, \hat{\mathbf{z}}_k, \mathbf{p}) = \hat{\mathbf{z}}_{k+s} + \sum_{i=0}^{s-1} a_i \hat{\mathbf{z}}_{k+i} - \Delta t b_j \mathbf{f}(\hat{\mathbf{z}}_{k+s}, \mathbf{p}, t_{k+s}) = \mathbf{0}}$$

- Backwards Difference Formula comes from

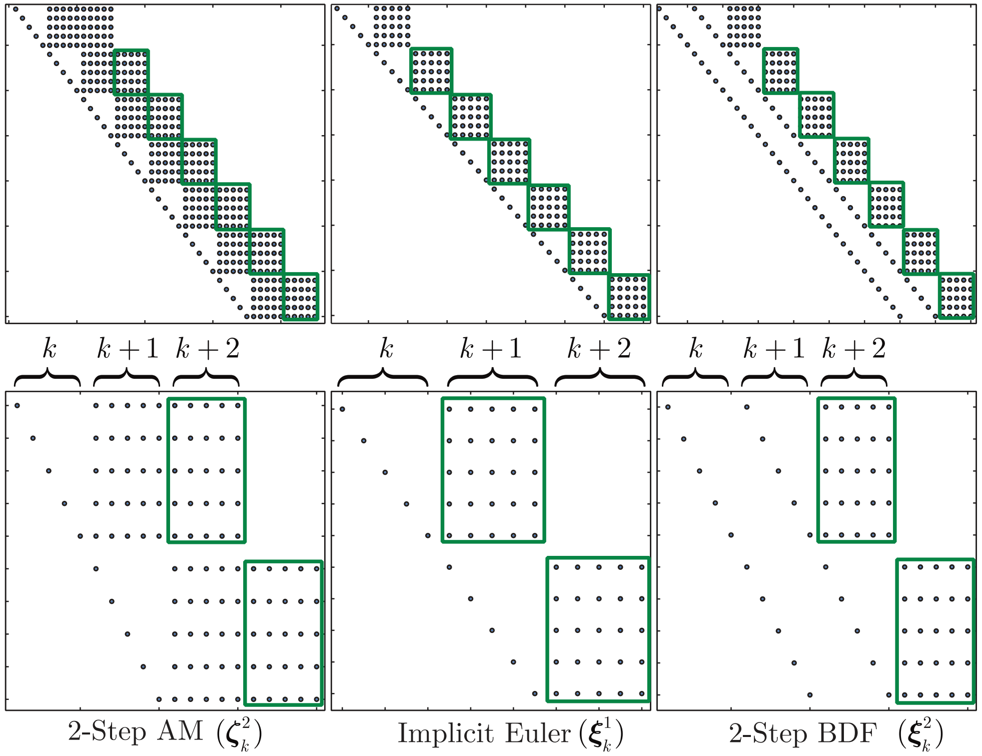
$$\boxed{\boldsymbol{\zeta}_k^s(\hat{\mathbf{z}}_{k+s}, \ldots, \hat{\mathbf{z}}_k, \mathbf{p}) = \hat{\mathbf{z}}_{k+s} - \hat{\mathbf{z}}_{k+s-1} - \Delta t \sum_{i=0}^{s} b_j \mathbf{f}(\hat{\mathbf{z}}_{k+j}, \mathbf{p}, t_{k+j}) = \mathbf{0}}$$

6. Gautschi W. **Numerical Analysis**. Springer Science & Business Media, New York; 2012.
7. Hairer E, Wanner G. **Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems.** Springer, Heidelberg; 1991.

Two Step PILMS Methods

- Two-step PILMS methods exhibit unconditional A-stability[6,7]

- The three implicit approaches considered can be expressed in terms of a series of block solves given by:



Implicit Euler[6,7]:

$$\boldsymbol{\xi}_k^1(\hat{\mathbf{z}}_{k+1}, \hat{\mathbf{z}}_k, \mathbf{p}) = \hat{\mathbf{z}}_{k+1} - \hat{\mathbf{z}}_k - \Delta t \mathbf{f}(\hat{\mathbf{z}}_{k+1}, \mathbf{p}, t_{\boldsymbol{k+1}})$$

Two-step Adam's Moulton method[6,7]:

$$\boldsymbol{\xi}_k^2(\hat{\mathbf{z}}_{k+2}, \hat{\mathbf{z}}_{k+1}, \hat{\mathbf{z}}_k, \mathbf{p}) = \hat{\mathbf{z}}_{k+2} - \tfrac{4}{3}\hat{\mathbf{z}}_{k+1} + \tfrac{1}{3}\,\hat{\mathbf{z}}_k - \tfrac{2}{3}\Delta t \mathbf{f}(\hat{\mathbf{z}}_{k+2}, \mathbf{p}, t_{\boldsymbol{k+2}})$$

Two-step BDF method[6,7]:

$$\boldsymbol{\zeta}_k^2(\hat{\mathbf{z}}_{k+2}, \hat{\mathbf{z}}_{k+1}, \hat{\mathbf{z}}_k, \mathbf{p}) = \hat{\mathbf{z}}_{k+2} - \hat{\mathbf{z}}_{k+1} - \tfrac{1}{2}\Delta t\big(\mathbf{f}(\hat{\mathbf{z}}_{k+2}, \mathbf{p}, t_{\boldsymbol{k+2}}) + \mathbf{f}(\hat{\mathbf{z}}_{k+1}, \mathbf{p}, t_{\boldsymbol{k+1}})\big)$$

6. Gautschi W. **Numerical Analysis**. Springer Science & Business Media, New York; 2012.
7. Hairer E, Wanner G. **Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems.** Springer, Heidelberg; 1991.

Assumptions

1. There exists a unique function $\mathbf{z}: P \rightarrow D^{K+1}$ with $\mathbf{h}(\mathbf{z}(\mathbf{p}), \mathbf{p}) = \mathbf{0}$, and an interval $X \in ID$ such that $\mathbf{z}(\mathbf{p})$ is unique in X^{K+1} for all $\mathbf{p} \in P$.

2. Derivative information $\nabla h_i, i = 1, \dots, n_x K$ is available, say by automatic differentiation, and is factorable.

3. A matrix $\mathbf{Y}_k \in \mathbb{R}^{n_x \times n_x}$ is known such that $M_k = \mathbf{Y}_k J_k^S(X, P)$ satisfies $0 \notin M_{k,ii}$ for all $i \in \{1, \dots, n_x\}$ and for all k, where $J_k^S(X, P)$ is an inclusion monotonic interval extension of $\mathrm{J}_\mathrm{k}^\mathrm{S}$ on $X \times P$.

<u>Hardest assumption to verify:</u>

- *We've developed block sequential analogs to the sufficient conditions presented in Neumaier.*[8]
- *Parametric interval methods can be used to provide sharper tests.*[8,9]
- *These can further be combined with bisection methods.*[10,11]

Can the interval extension of J_k^S be preconditioned such that it contains no singular matrices on its domain?

8. Neumaier A. **Interval methods for systems of equations**, vol.37. Cambridge university press, 1990.
9. Krawczyk R. **Interval iterations for including a set of solutions.** Computing 1984 Mar 32 (1): 13–31.
10. R. B. Kearfott. **Abstract generalized bisection and a cost bound.** *Mathematics of Computation*, 49 (179): 187 – 202, 1987
11. Stuber MD. **Evaluation of Process Systems Operating Envelopes.** PhD Dissertation, MIT, 2013.

Development of Relaxations

- The parametric mean-valued form[12] of a block is given by:

$$\boxed{\nabla_{\mathbf{x}} h_j(\mathbf{y}^j(\mathbf{p}),\mathbf{p})^T(\mathbf{z}_k(\mathbf{p})-\boldsymbol{\gamma}(\mathbf{p})) = -h_j(\boldsymbol{\gamma}(\mathbf{p}),\mathbf{p}), \quad j=(k-1)n_x+1,\dots,kn_x}$$

where $\gamma: P \to D$ and $\mathbf{y}^j: P \to D$ such that for some $\lambda: P \to (0,1)$,

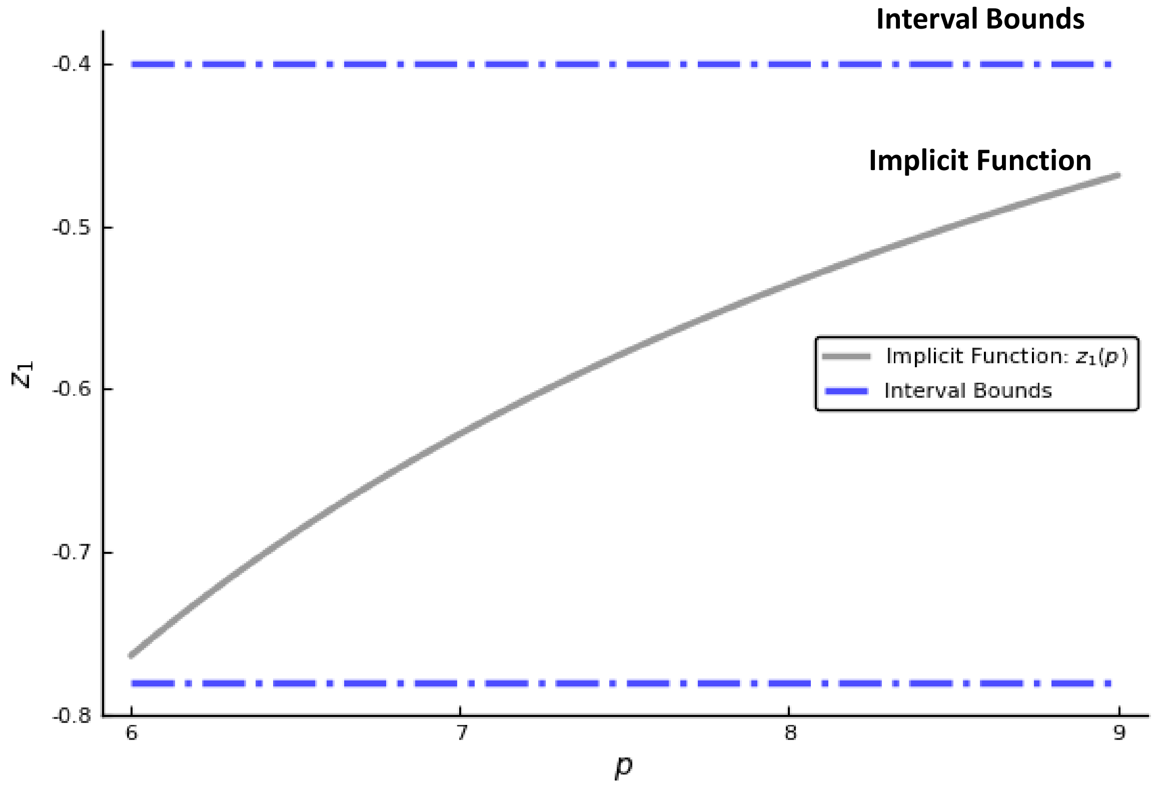
$$\boxed{\mathbf{y}^j(\mathbf{p}) = \lambda(\mathbf{p})\mathbf{z}_k(\mathbf{p}) + (1-\lambda(\mathbf{p}))\boldsymbol{\gamma}(\mathbf{p}), \quad \forall\, \mathbf{p} \in P}$$

- This suggests that a parametric analog of the Newton-Raphson fixed point method may be used to compute relaxation.

12. Stuber MD, Scott JK, Barton PI. **Convex and concave relaxations of implicit functions.** Optimization Methods and Software2015;30(3):424–460.

Block relaxation algorithm

1. Initialize the relaxations, $\mathbf{z}_k^0$, and subgradients, $\mathbf{s}_{z_k}^0$, from interval bounds.



procedure BLOCKRELAX($\mathbf{h}_k, X, P, \mathbf{z}_{k-1}^{cv}, \mathbf{z}_{k-1}^{cc}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cc}, \mathbf{z}_{k-2}^{cv}, \mathbf{z}_{k-2}^{cc}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cc}, r$)

1. $\mathbf{z}_k^{0,cv}, \mathbf{z}_k^{0,cc}, \mathbf{s}_{\mathbf{z}_k}^{0,cv}, \mathbf{s}_{\mathbf{z}_k}^{0,cc} \leftarrow \mathbf{x}^L, \mathbf{x}^U, 0, 0$

for $j \leftarrow 0$ **to** $r-1$ **do**

$\lambda \leftarrow \lambda \in [0,1], \bar{\mathbf{p}} \leftarrow \mathbf{p} \in P$

$\mathbf{c}, \mathbf{C}, \mathbf{s_c}, \mathbf{s_C} \leftarrow \mathtt{Aff}(\ldots)$ ▹ Subroutine defined in [23]

$\mathbf{z}_k^{j,a}(\mathbf{p}) \leftarrow \mathbf{c} + \mathbf{s_c}^{\mathsf{T}}(\mathbf{p} - \bar{\mathbf{p}}), \ \forall \mathbf{p} \in P$ ▹ Affine relaxation lower bound

$\mathbf{z}_k^{j,A}(\mathbf{p}) \leftarrow \mathbf{C} + \mathbf{s_C}^{\mathsf{T}}(\mathbf{p} - \bar{\mathbf{p}}), \ \forall \mathbf{p} \in P$ ▹ Affine relaxation upper bound

$\gamma^j(\cdot) \leftarrow \lambda \mathbf{z}_k^{j,a}(\cdot) + (1-\lambda)\mathbf{z}_k^{j,A}(\cdot)$

$\mathbf{s}_\gamma^j \leftarrow \lambda \mathbf{s_c} + (1-\lambda)\mathbf{s_C}$

$\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathbf{u_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots\ldots\ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$ ▹ **B** matrix defined in [23] w.r.t. $\mathbf{h}_k$ and $\mathbf{J}_k$

$\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathbf{o_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots\ldots\ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$

$\mathbf{s}_\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathcal{S}_{\mathbf{u}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

$\mathbf{s}_\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathcal{S}_{\mathbf{o}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

$\mathbf{z}_k^{j+1,cv}(\cdot) \leftarrow \bar{\mathbf{u}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$

$\mathbf{z}_k^{j+1,cc}(\cdot) \leftarrow \bar{\mathbf{o}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$

$\mathbf{s}_\mathbf{z}^{j+1,cv}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{u}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$

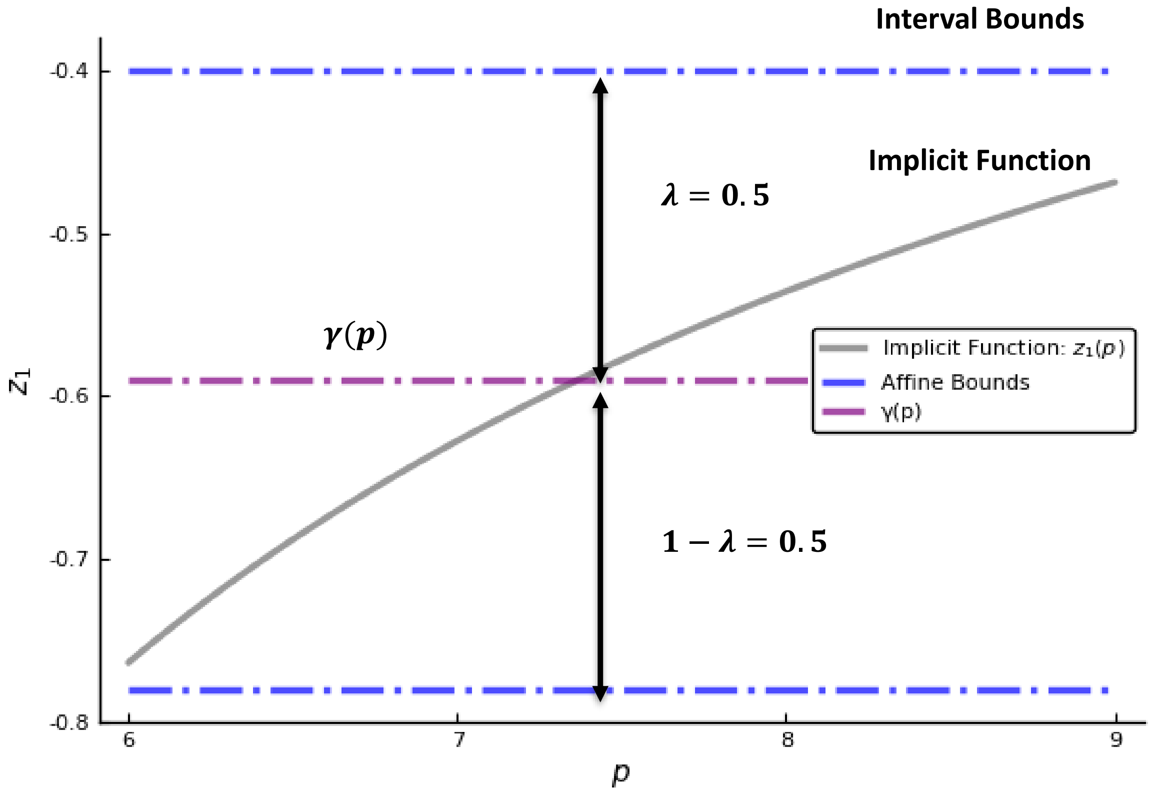
$\mathbf{s}_\mathbf{z}^{j+1,cc}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{o}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$

end for

return $\mathbf{z}_k^{r,cc}(\cdot), \mathbf{z}_k^{r,cc}(\cdot), \mathbf{s}_\mathbf{z}^{r,cv}(\cdot), \mathbf{s}_\mathbf{z}^{r,cc}(\cdot)$

Block relaxation algorithm

2. Compute affine function between current relaxations and respective subgradients



procedure BLOCKRELAX$(\mathbf{h}_k, X, P, \mathbf{z}^{cv}_{k-1}, \mathbf{z}^{cc}_{k-1}, \mathbf{s}^{cv}_{\mathbf{z}_{k-1}}, \mathbf{s}^{cc}_{\mathbf{z}_{k-1}}, \mathbf{z}^{cv}_{k-2}, \mathbf{z}^{cc}_{k-2}, \mathbf{s}^{cv}_{\mathbf{z}_{k-2}}, \mathbf{s}^{cc}_{\mathbf{z}_{k-2}}, r)$

1\.

$\quad \mathbf{z}_k^{0,cv}, \mathbf{z}_k^{0,cc}, \mathbf{s}_{\mathbf{z}_k}^{0,cv}, \mathbf{s}_{\mathbf{z}_k}^{0,cc} \leftarrow \mathbf{x}^L, \mathbf{x}^U, 0, 0$

$\quad$ **for** $j \leftarrow 0$ **to** $r-1$ **do**

2\.

$\qquad \lambda \leftarrow \lambda \in [0,1], \bar{\mathbf{p}} \leftarrow \mathbf{p} \in P$

$\qquad \mathbf{c}, \mathbf{C}, \mathbf{s_c}, \mathbf{s_C} \leftarrow \mathtt{Aff}(\ldots)$ ▹ Subroutine defined in [23]

$\qquad \mathbf{z}_k^{j,a}(\mathbf{p}) \leftarrow \mathbf{c} + \mathbf{s_c}^{\mathsf{T}}(\mathbf{p} - \bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▹ Affine relaxation lower bound

$\qquad \mathbf{z}_k^{j,A}(\mathbf{p}) \leftarrow \mathbf{C} + \mathbf{s_C}^{\mathsf{T}}(\mathbf{p} - \bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▹ Affine relaxation upper bound

$\qquad \gamma^j(\cdot) \leftarrow \lambda \mathbf{z}_k^{j,a}(\cdot) + (1-\lambda)\mathbf{z}_k^{j,A}(\cdot)$

$\qquad \mathbf{s}_\gamma^j \leftarrow \lambda \mathbf{s_c} + (1-\lambda)\mathbf{s_C}$

$\qquad \mathbf{M}^{j,cv}(\cdot) \leftarrow \mathbf{u_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$ ▹ B matrix defined in [23] w.r.t. $\mathbf{h}_k$ and $\mathbf{J}_k$

$\qquad \mathbf{M}^{j,cc}(\cdot) \leftarrow \mathbf{o_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$

$\qquad \mathbf{s}_{\mathbf{M}}^{j,cv}(\cdot) \leftarrow \mathcal{S}_{\mathbf{u}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

$\qquad \mathbf{s}_{\mathbf{M}}^{j,cc}(\cdot) \leftarrow \mathcal{S}_{\mathbf{o}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

$\qquad \mathbf{z}_k^{j+1,cv}(\cdot) \leftarrow \bar{\mathbf{u}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$

$\qquad \mathbf{z}_k^{j+1,cc}(\cdot) \leftarrow \bar{\mathbf{o}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$

$\qquad \mathbf{s}_{\mathbf{z}}^{j+1,cv}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{u}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_{\mathbf{z}}^{j,cv}(\cdot), \mathbf{s}_{\mathbf{z}}^{j,cc}(\cdot), \cdot)$

$\qquad \mathbf{s}_{\mathbf{z}}^{j+1,cc}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{o}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_{\mathbf{z}}^{j,cv}(\cdot), \mathbf{s}_{\mathbf{z}}^{j,cc}(\cdot), \cdot)$

$\quad$ **end for**

$\quad$ **return** $\mathbf{z}_k^{r,cc}(\cdot), \mathbf{z}_k^{r,cc}(\cdot), \mathbf{s}_{\mathbf{z}}^{r,cv}(\cdot), \mathbf{s}_{\mathbf{z}}^{r,cc}(\cdot)$

Block relaxation algorithm

3. Compute $\mathbf{M}$, the relaxation of a preconditioned Jacobian and respective subgradients

The functions $\mathbf{M}_k : P \to M_k$, and $\mathbf{B}_k : X \times \cdots \times X \times P \to M_k$ be defined for $k \in \{1, \ldots, K\}$ corresponding to each timestep are defined by:

$$\mathbf{M}_k(\cdot) = \mathbf{B}_k\left(\mathbf{y}^{(k-1)n_x+1}(\cdot), \ldots, \mathbf{y}^{kn_x}(\cdot), \cdot\right) \equiv \mathbf{Y}_k \begin{pmatrix} \nabla_{\mathbf{x}} h_{(k-1)n_x+1}(\mathbf{y}^{(k-1)n_x+1}(\cdot), \cdot)^{\mathrm{T}} \\ \nabla_{\mathbf{x}} h_{(k-1)n_x+2}(\mathbf{y}^{(k-1)n_x+2}(\cdot), \cdot)^{\mathrm{T}} \\ \vdots \\ \nabla_{\mathbf{x}} h_{kn_x}(\mathbf{y}^{kn_x}(\cdot), \cdot)^{\mathrm{T}} \end{pmatrix}$$

- The points $(\mathbf{y}^j(\mathbf{p}), \mathbf{p}) \in X \times P$ are the points at which the gradients of $\nabla_x h_j(\cdot,\cdot)$ are evaluated.
- $\mathbf{Y}_k$ is a matrix which preconditions the system satisfying assumption 3 ($\mathbf{M}_k$ enclosures no singular matrix)

procedure BLOCKRELAX($\mathbf{h}_k, X, P, \mathbf{z}^{cv}_{k-1}, \mathbf{z}^{cc}_{k-1}, \mathbf{s}^{cv}_{\mathbf{z}_{k-1}}, \mathbf{s}^{cc}_{\mathbf{z}_{k-1}}, \mathbf{z}^{cv}_{k-2}, \mathbf{z}^{cc}_{k-2}, \mathbf{s}^{cv}_{\mathbf{z}_{k-2}}, \mathbf{s}^{cc}_{\mathbf{z}_{k-2}}, r$)

1. $\mathbf{z}^{0,cv}_k, \mathbf{z}^{0,cc}_k, \mathbf{s}^{0,cv}_{\mathbf{z}_k}, \mathbf{s}^{0,cc}_{\mathbf{z}_k} \leftarrow \mathbf{x}^L, \mathbf{x}^U, 0, 0$

for $j \leftarrow 0$ **to** $r-1$ **do**

2.
$\lambda \leftarrow \lambda \in [0,1], \bar{\mathbf{p}} \leftarrow \mathbf{p} \in P$
$\mathbf{c}, \mathbf{C}, \mathbf{s_c}, \mathbf{s_C} \leftarrow \mathtt{Aff}(\ldots)$ ▹ Subroutine defined in [23]
$\mathbf{z}^{j,a}_k(\mathbf{p}) \leftarrow \mathbf{c} + \mathbf{s_c}^{\mathrm{T}}(\mathbf{p} - \bar{\mathbf{p}}), \ \forall \mathbf{p} \in P$ ▹ Affine relaxation lower bound
$\mathbf{z}^{j,A}_k(\mathbf{p}) \leftarrow \mathbf{C} + \mathbf{s_C}^{\mathrm{T}}(\mathbf{p} - \bar{\mathbf{p}}), \ \forall \mathbf{p} \in P$ ▹ Affine relaxation upper bound
$\gamma^j(\cdot) \leftarrow \lambda \mathbf{z}^{j,a}_k(\cdot) + (1-\lambda)\mathbf{z}^{j,A}_k(\cdot)$
$\mathbf{s}^j_\gamma \leftarrow \lambda \mathbf{s_c} + (1-\lambda)\mathbf{s_C}$

3.
$\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathbf{u_B}(\mathbf{z}^{j,a}_k(\cdot), \mathbf{z}^{j,A}_k(\cdot), \ldots, \ldots, \mathbf{z}^{j,a}_k(\cdot), \mathbf{z}^{j,A}_k(\cdot), \cdot)$ ▹ B matrix defined in [23] w.r.t. $\mathbf{h}_k$ and $\mathbf{J}_k$
$\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathbf{o_B}(\mathbf{z}^{j,a}_k(\cdot), \mathbf{z}^{j,A}_k(\cdot), \ldots, \ldots, \mathbf{z}^{j,a}_k(\cdot), \mathbf{z}^{j,A}_k(\cdot), \cdot)$
$\mathbf{s}^{j,cv}_{\mathbf{M}}(\cdot) \leftarrow \mathcal{S}_{\mathbf{u}_B}(\mathbf{z}^{j,a}_k(\cdot), \mathbf{z}^{j,A}_k(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}^{j,a}_k(\cdot), \mathbf{z}^{j,A}_k(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$
$\mathbf{s}^{j,cc}_{\mathbf{M}}(\cdot) \leftarrow \mathcal{S}_{\mathbf{o}_B}(\mathbf{z}^{j,a}_k(\cdot), \mathbf{z}^{j,A}_k(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}^{j,a}_k(\cdot), \mathbf{z}^{j,A}_k(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

$\mathbf{z}^{j+1,cv}_k(\cdot) \leftarrow \bar{\mathbf{u}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}^{j,cv}_k(\cdot), \mathbf{z}^{j,cc}_k(\cdot), \mathbf{z}^{cv}_{k-1}(\cdot)\mathbf{z}^{cc}_{k-1}(\cdot), \mathbf{z}^{cv}_{k-2}(\cdot)\mathbf{z}^{cc}_{k-2}(\cdot), \cdot)$
$\mathbf{z}^{j+1,cc}_k(\cdot) \leftarrow \bar{\mathbf{o}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}^{j,cv}_k(\cdot), \mathbf{z}^{j,cc}_k(\cdot), \mathbf{z}^{cv}_{k-1}(\cdot)\mathbf{z}^{cc}_{k-1}(\cdot), \mathbf{z}^{cv}_{k-2}(\cdot)\mathbf{z}^{cc}_{k-2}(\cdot), \cdot)$
$\mathbf{s}^{j+1,cv}_{\mathbf{z}}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{u}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}^j_\gamma, \mathbf{s}^j_\gamma, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}^{j,cv}_k(\cdot), \mathbf{z}^{j,cc}_k(\cdot), \mathbf{s}^{j,cv}_{\mathbf{z}}(\cdot), \mathbf{s}^{j,cc}_{\mathbf{z}}(\cdot), \cdot)$
$\mathbf{s}^{j+1,cc}_{\mathbf{z}}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{o}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}^j_\gamma, \mathbf{s}^j_\gamma, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}^{j,cv}_k(\cdot), \mathbf{z}^{j,cc}_k(\cdot), \mathbf{s}^{j,cv}_{\mathbf{z}}(\cdot), \mathbf{s}^{j,cc}_{\mathbf{z}}(\cdot), \cdot)$

end for

return $\mathbf{z}^{r,cc}_k(\cdot), \mathbf{z}^{r,cc}_k(\cdot), \mathbf{s}^{r,cv}_{\mathbf{z}}(\cdot), \mathbf{s}^{r,cc}_{\mathbf{z}}(\cdot)$

Block relaxation algorithm

4(a). Compute relaxation of $\boldsymbol{\psi}_k$ (a valid relaxation of $\boldsymbol{z}_k^{j+1}$) and the respective subgradients thereof.

Let $\mathbf{b}_k: X \times X \times X \times P \to \mathbb{R}^{n_x}$ such that $\mathbf{b}_k = \mathbf{Y}_k \theta_{k-2}^{s}$ with $\theta \in \{\xi, \zeta\}$, $s \in \{1,2\}$, and $2 \le k \le K$. Define the function $\psi_k: X \times M \times X \times X \times P \to \mathbb{R}^{n_x}$ such that $\forall(\tilde{\boldsymbol{\gamma}}, \tilde{\mathbf{M}}, \tilde{\mathbf{z}}_k, \tilde{\mathbf{z}}_{k-1}, \tilde{\mathbf{z}}_{k-2}, \mathbf{p}) \in X \times M \times X \times X \times P$, we have $\psi_k(\tilde{\boldsymbol{\gamma}}, \tilde{\mathbf{M}}, \tilde{\mathbf{z}}_k, \tilde{\mathbf{z}}_{k-1}, \tilde{\mathbf{z}}_{k-2}, \mathbf{p}) = \tilde{\mathbf{z}}_k^*$,where the i[th] component of $\tilde{\mathbf{z}}_k^*$ is given by the loop:

for $\quad i = 1, \ldots, n_x \quad$ do

$$\tilde{z}_{k,i}^* := \tilde{\gamma}_i - \frac{b_{k,i}(\tilde{\gamma}, \mathbf{z}_{k-1}(\mathbf{p}), \mathbf{z}_{k-2}(\mathbf{p}), \mathbf{p}) + \sum_{j<i} \tilde{m}_{ij}\left(\overline{z}_{k,j}^* - \tilde{\gamma}_j\right) + \sum_{j>i} \tilde{m}_{ij}\left(\tilde{z}_{k,j} - \tilde{\gamma}_j\right)}{\tilde{m}_{ii}}$$

end

procedure BlockRelax($\mathbf{h}_k, X, P, \mathbf{z}_{k-1}^{cv}, \mathbf{z}_{k-1}^{cc}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cc}, \mathbf{z}_{k-2}^{cv}, \mathbf{z}_{k-2}^{cc}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cc}, r$)

1. $\quad \mathbf{z}_k^{0,cv}, \mathbf{z}_k^{0,cc}, \mathbf{s}_{\mathbf{z}_k}^{0,cv}, \mathbf{s}_{\mathbf{z}_k}^{0,cc} \leftarrow \mathbf{x}^L, \mathbf{x}^U, 0, 0$

for $j \leftarrow 0$ **to** $r-1$ **do**

2. $\quad \lambda \leftarrow \lambda \in [0,1], \bar{\mathbf{p}} \leftarrow \mathbf{p} \in P$

$\quad \mathbf{c}, \mathbf{C}, \mathbf{s_c}, \mathbf{s_C} \leftarrow \mathtt{Aff}(\ldots)$ ▹ Subroutine defined in [23]

$\quad \mathbf{z}_k^{j,a}(\mathbf{p}) \leftarrow \mathbf{c} + \mathbf{s_c}^{\mathsf{T}}(\mathbf{p} - \bar{\mathbf{p}}), \ \forall \mathbf{p} \in P$ ▹ Affine relaxation lower bound

$\quad \mathbf{z}_k^{j,A}(\mathbf{p}) \leftarrow \mathbf{C} + \mathbf{s_C}^{\mathsf{T}}(\mathbf{p} - \bar{\mathbf{p}}), \ \forall \mathbf{p} \in P$ ▹ Affine relaxation upper bound

$\quad \gamma^j(\cdot) \leftarrow \lambda \mathbf{z}_k^{j,a}(\cdot) + (1-\lambda)\mathbf{z}_k^{j,A}(\cdot)$

$\quad \mathbf{s}_\gamma^j \leftarrow \lambda \mathbf{s_c} + (1-\lambda)\mathbf{s_C}$

3. $\quad \mathbf{M}^{j,cv}(\cdot) \leftarrow \mathbf{u_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots\ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$ ▹ B matrix defined in [23] w.r.t. $\mathbf{h}_k$ and $\mathbf{J}_k$

$\quad \mathbf{M}^{j,cc}(\cdot) \leftarrow \mathbf{o_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots\ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$

$\quad \mathbf{s}_{\mathbf{M}}^{j,cv}(\cdot) \leftarrow \mathcal{S}_{\mathbf{u}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

$\quad \mathbf{s}_{\mathbf{M}}^{j,cc}(\cdot) \leftarrow \mathcal{S}_{\mathbf{o}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

4. $\quad \mathbf{z}_k^{j+1,cv}(\cdot) \leftarrow \bar{\mathbf{u}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$

$\quad \mathbf{z}_k^{j+1,cc}(\cdot) \leftarrow \bar{\mathbf{o}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$

$\quad \mathbf{s}_{\mathbf{z}}^{j+1,cv}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{u}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_{\mathbf{z}}^{j,cv}(\cdot), \mathbf{s}_{\mathbf{z}}^{j,cc}(\cdot), \cdot)$

$\quad \mathbf{s}_{\mathbf{z}}^{j+1,cc}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{o}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_{\mathbf{z}}^{j,cv}(\cdot), \mathbf{s}_{\mathbf{z}}^{j,cc}(\cdot), \cdot)$

end for

return $\mathbf{z}_k^{r,cc}(\cdot), \mathbf{z}_k^{r,cc}(\cdot), \mathbf{s}_{\mathbf{z}}^{r,cv}(\cdot), \mathbf{s}_{\mathbf{z}}^{r,cc}(\cdot)$

Block relaxation algorithm

4(a). Compute relaxation of $\boldsymbol{\psi}_k$ (a valid relaxation of $\boldsymbol{z}_k^{j+1}$) and the respective subgradients thereof.

Let $\mathbf{b}$ … $\in$

$\{1,2\}$ …

$\mathbb{R}^{n_x}$ s … e

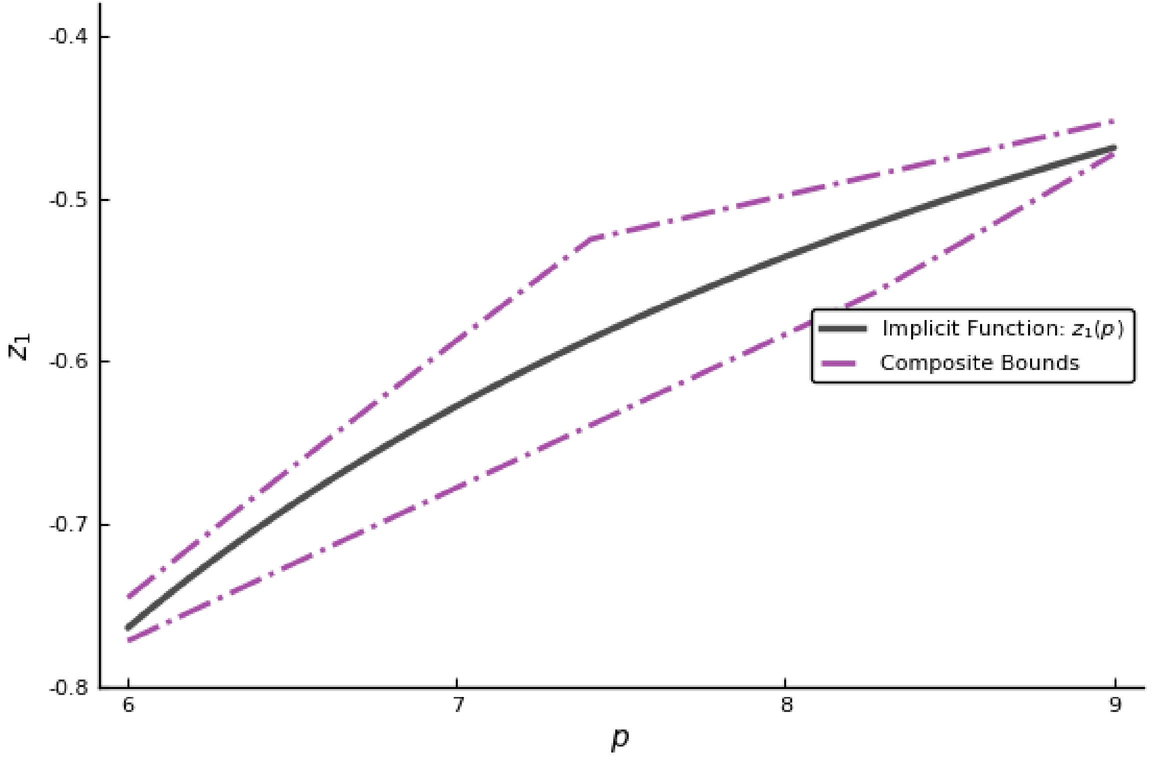
$\psi_k(\tilde{\boldsymbol{\gamma}}$ …

by th …

for

$\tilde{z}$ … $_i\,\tilde{m}_{ij}\left(\tilde{z}_{k,j}-\tilde{\gamma}_j\right)$

end



procedure BLOCKRELAX($\mathbf{h}_k, X, P, \mathbf{z}_{k-1}^{cv}, \mathbf{z}_{k-1}^{cc}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cc}, \mathbf{z}_{k-2}^{cv}, \mathbf{z}_{k-2}^{cc}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cc}, r$)

1. $\mathbf{z}_k^{0,cv}, \mathbf{z}_k^{0,cc}, \mathbf{s}_{\mathbf{z}_k}^{0,cv}, \mathbf{s}_{\mathbf{z}_k}^{0,cc} \leftarrow \mathbf{x}^L, \mathbf{x}^U, \mathbf{0}, \mathbf{0}$

for $j \leftarrow 0$ **to** $r-1$ **do**

2. $\lambda \leftarrow \lambda \in [0,1], \bar{\mathbf{p}} \leftarrow \mathbf{p} \in P$

$\mathbf{c}, \mathbf{C}, \mathbf{s_c}, \mathbf{s_C} \leftarrow \mathtt{Aff}(\ldots)$ ▹ Subroutine defined in [23]

$\mathbf{z}_k^{j,a}(\mathbf{p}) \leftarrow \mathbf{c} + \mathbf{s_c}^{\mathsf{T}}(\mathbf{p}-\bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▹ Affine relaxation lower bound

$\mathbf{z}_k^{j,A}(\mathbf{p}) \leftarrow \mathbf{C} + \mathbf{s_C}^{\mathsf{T}}(\mathbf{p}-\bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▹ Affine relaxation upper bound

$\gamma^j(\cdot) \leftarrow \lambda \mathbf{z}_k^{j,a}(\cdot) + (1-\lambda)\mathbf{z}_k^{j,A}(\cdot)$

$\mathbf{s}_\gamma^j \leftarrow \lambda \mathbf{s_c} + (1-\lambda)\mathbf{s_C}$

3. $\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathbf{u_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$ ▹ B matrix defined in [23] w.r.t. $\mathbf{h}_k$ and $\mathbf{J}_k$

$\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathbf{o_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$

$\mathbf{s}_\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathcal{S}_{\mathbf{u}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

$\mathbf{s}_\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathcal{S}_{\mathbf{o}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

4. $\mathbf{z}_k^{j+1,cv}(\cdot) \leftarrow \mathbf{\bar{u}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$

$\mathbf{z}_k^{j+1,cc}(\cdot) \leftarrow \mathbf{\bar{o}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$

$\mathbf{s}_\mathbf{z}^{j+1,cv}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{u}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$

$\mathbf{s}_\mathbf{z}^{j+1,cc}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{o}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$

end for

return $\mathbf{z}_k^{r,cc}(\cdot), \mathbf{z}_k^{r,cc}(\cdot), \mathbf{s}_\mathbf{z}^{r,cv}(\cdot), \mathbf{s}_\mathbf{z}^{r,cc}(\cdot)$

Block relaxation algorithm

4(b). Compute composite relaxation of $\boldsymbol{\psi}_k$ (a valid relaxation of $\mathbf{z}_k^{j+1}$) and the respective subgradients thereof.

Let $\mathbf{u}_\phi$,$\mathbf{o}_\phi$ be composite relaxations of ϕ on $X \times P$. The functions $\mathbf{u}_\phi, \mathbf{o}_\phi$: $\mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times P \rightarrow \mathbb{R}^{n_x}$ will be defined as:

$$\bar{\mathbf{u}}_\phi(\mathbf{z}^{cv}, \mathbf{z}^{cc}, \mathbf{p}) \equiv \max\left\{\mathbf{z}^{cv}, \mathbf{u}_\phi(\mathbf{z}^{cv}, \mathbf{z}^{cc}, \mathbf{p})\right\}$$

$$\bar{\mathbf{o}}_\phi(\mathbf{z}^{cv}, \mathbf{z}^{cc}, \mathbf{p}) \equiv \min\left\{\mathbf{z}^{cc}, \mathbf{o}_\phi(\mathbf{z}^{cv}, \mathbf{z}^{cc}, \mathbf{p})\right\}$$

$\forall(\mathbf{z}^{cv}, \mathbf{z}^{cc}, \mathbf{p}) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times P$

Relaxation at next step is composite relaxation of GS result and prior relaxation.

procedure BLOCKRELAX($\mathbf{h}_k, X, P, \mathbf{z}_{k-1}^{cv}, \mathbf{z}_{k-1}^{cc}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cc}, \mathbf{z}_{k-2}^{cv}, \mathbf{z}_{k-2}^{cc}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cc}, r$)

1.
$\mathbf{z}_k^{0,cv}, \mathbf{z}_k^{0,cc}, \mathbf{s}_{\mathbf{z}_k}^{0,cv}, \mathbf{s}_{\mathbf{z}_k}^{0,cc} \leftarrow \mathbf{x}^L, \mathbf{x}^U, 0, 0$

for $j \leftarrow 0$ **to** $r-1$ **do**

2.
$\lambda \leftarrow \lambda \in [0,1], \bar{\mathbf{p}} \leftarrow \mathbf{p} \in P$
$\mathbf{c}, \mathbf{C}, \mathbf{s_c}, \mathbf{s_C} \leftarrow \mathtt{Aff}(\ldots)$ ▸ Subroutine defined in [23]
$\mathbf{z}_k^{j,a}(\mathbf{p}) \leftarrow \mathbf{c} + \mathbf{s_c}^{\mathsf{T}}(\mathbf{p} - \bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▸ Affine relaxation lower bound
$\mathbf{z}_k^{j,A}(\mathbf{p}) \leftarrow \mathbf{C} + \mathbf{s_C}^{\mathsf{T}}(\mathbf{p} - \bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▸ Affine relaxation upper bound
$\gamma^j(\cdot) \leftarrow \lambda \mathbf{z}_k^{j,a}(\cdot) + (1-\lambda)\mathbf{z}_k^{j,A}(\cdot)$
$\mathbf{s}_\gamma^j \leftarrow \lambda \mathbf{s_c} + (1-\lambda)\mathbf{s_C}$

3.
$\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathbf{u_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$ ▸ B matrix defined in [23] w.r.t. $\mathbf{h}_k$ and $\mathbf{J}_k$
$\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathbf{o_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$
$\mathbf{s}_\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathcal{S}_{\mathbf{u}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$
$\mathbf{s}_\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathcal{S}_{\mathbf{o}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

4.
$\mathbf{z}_k^{j+1,cv}(\cdot) \leftarrow \bar{\mathbf{u}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$
$\mathbf{z}_k^{j+1,cc}(\cdot) \leftarrow \bar{\mathbf{o}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$
$\mathbf{s}_\mathbf{z}^{j+1,cv}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{u}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$
$\mathbf{s}_\mathbf{z}^{j+1,cc}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{o}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$

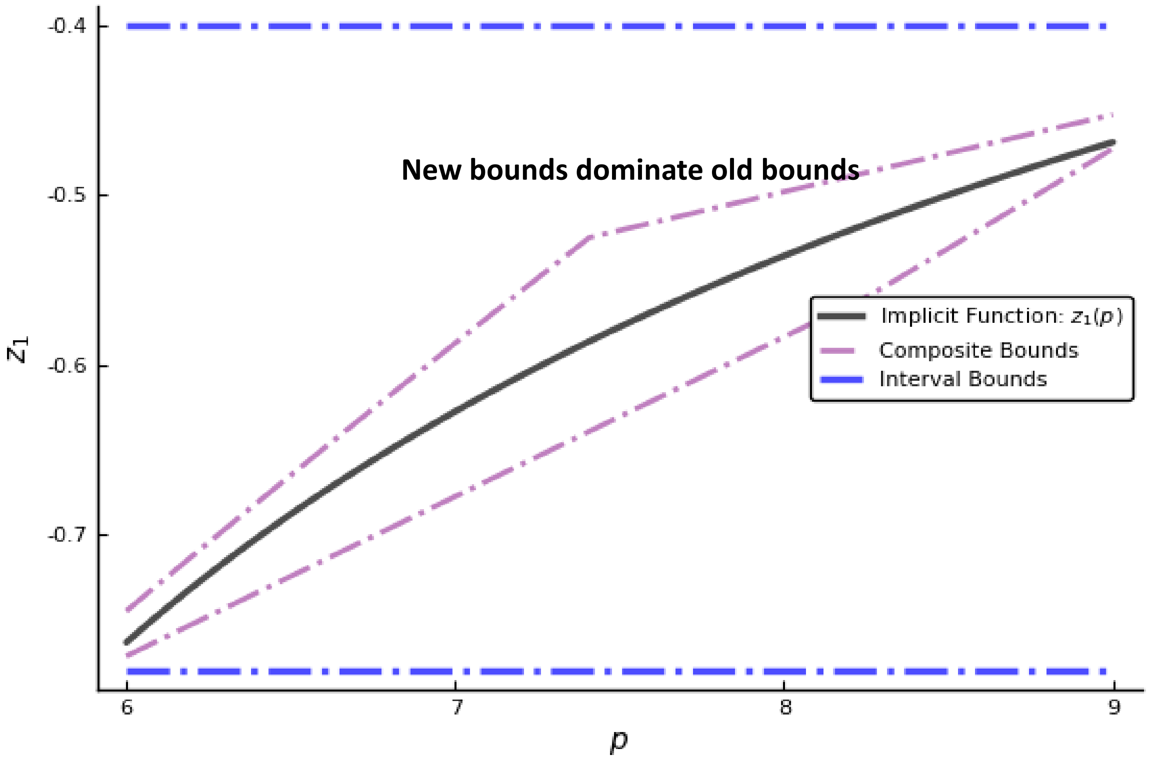
end for

return $\mathbf{z}_k^{r,cc}(\cdot), \mathbf{z}_k^{r,cc}(\cdot), \mathbf{s}_\mathbf{z}^{r,cv}(\cdot), \mathbf{s}_\mathbf{z}^{r,cc}(\cdot)$

12. Stuber MD, Scott JK, Barton PI. **Convex and concave relaxations of implicit functions.** Optimization Methods and Software2015;30(3):424–460.

Block relaxation algorithm

4(b). Compute composite relaxation of $\boldsymbol{\psi}_k$ (a valid relaxation of $\boldsymbol{z}_k^{j+1}$) and the respective subgradients thereof.



procedure BlockRelax($\mathbf{h}_k, X, P, \mathbf{z}_{k-1}^{cv}, \mathbf{z}_{k-1}^{cc}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cc}, \mathbf{z}_{k-2}^{cv}, \mathbf{z}_{k-2}^{cc}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cc}, r$)

1. $\mathbf{z}_k^{0,cv}, \mathbf{z}_k^{0,cc}, \mathbf{s}_{\mathbf{z}_k}^{0,cv}, \mathbf{s}_{\mathbf{z}_k}^{0,cc} \leftarrow \mathbf{x}^L, \mathbf{x}^U, 0, 0$

for $j \leftarrow 0$ **to** $r-1$ **do**

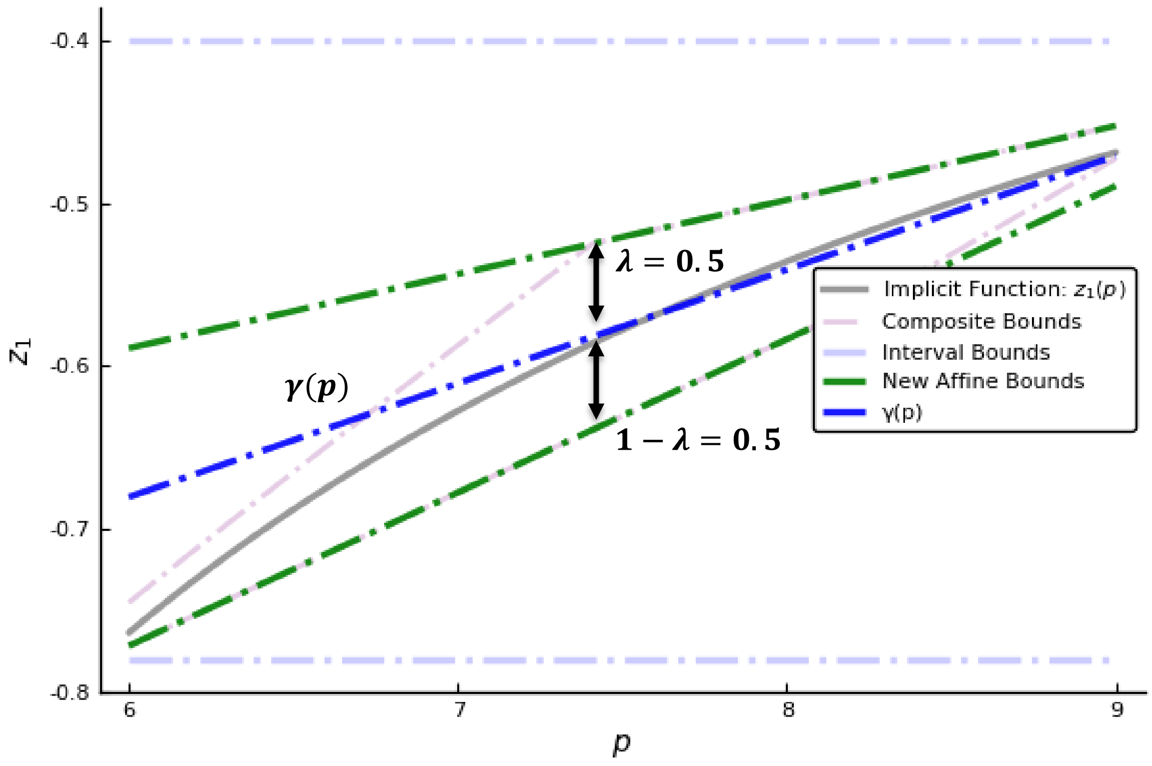
2. $\lambda \leftarrow \lambda \in [0,1], \bar{\mathbf{p}} \leftarrow \mathbf{p} \in P$
   $\mathbf{c}, \mathbf{C}, \mathbf{s_c}, \mathbf{s_C} \leftarrow \mathtt{Aff}(\ldots)$ ▹ Subroutine defined in [23]
   $\mathbf{z}_k^{j,a}(\mathbf{p}) \leftarrow \mathbf{c} + \mathbf{s_c}^{\mathrm{T}}(\mathbf{p} - \bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▹ Affine relaxation lower bound
   $\mathbf{z}_k^{j,A}(\mathbf{p}) \leftarrow \mathbf{C} + \mathbf{s_C}^{\mathrm{T}}(\mathbf{p} - \bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▹ Affine relaxation upper bound
   $\gamma^j(\cdot) \leftarrow \lambda \mathbf{z}_k^{j,a}(\cdot) + (1-\lambda)\mathbf{z}_k^{j,A}(\cdot)$
   $\mathbf{s}_\gamma^j \leftarrow \lambda \mathbf{s_c} + (1-\lambda)\mathbf{s_C}$
3. $\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathbf{u_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots\ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$ ▹ B matrix defined in [23] w.r.t. $\mathbf{h}_k$ and $\mathbf{J}_k$
   $\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathbf{o_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots\ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$
   $\mathbf{s}_\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathcal{S}_{\mathbf{u}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$
   $\mathbf{s}_\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathcal{S}_{\mathbf{o}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$
4. $\mathbf{z}_k^{j+1,cv}(\cdot) \leftarrow \bar{\mathbf{u}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$
   $\mathbf{z}_k^{j+1,cc}(\cdot) \leftarrow \bar{\mathbf{o}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$
   $\mathbf{s}_\mathbf{z}^{j+1,cv}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{u}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$
   $\mathbf{s}_\mathbf{z}^{j+1,cc}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{o}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$

end for

return $\mathbf{z}_k^{r,cc}(\cdot), \mathbf{z}_k^{r,cc}(\cdot), \mathbf{s}_\mathbf{z}^{r,cv}(\cdot), \mathbf{s}_\mathbf{z}^{r,cc}(\cdot)$

Block relaxation algorithm

2. Compute affine function between current relaxations and respective subgradients



procedure BLOCKRELAX($\mathbf{h}_k, X, P, \mathbf{z}^{cv}_{k-1}, \mathbf{z}^{cc}_{k-1}, \mathbf{s}^{cv}_{\mathbf{z}_{k-1}}, \mathbf{s}^{cc}_{\mathbf{z}_{k-1}}, \mathbf{z}^{cv}_{k-2}, \mathbf{z}^{cc}_{k-2}, \mathbf{s}^{cv}_{\mathbf{z}_{k-2}}, \mathbf{s}^{cc}_{\mathbf{z}_{k-2}}, r$)

1. $\mathbf{z}_k^{0,cv}, \mathbf{z}_k^{0,cc}, \mathbf{s}_{\mathbf{z}_k}^{0,cv}, \mathbf{s}_{\mathbf{z}_k}^{0,cc} \leftarrow \mathbf{x}^L, \mathbf{x}^U, 0, 0$

for $j \leftarrow 0$ **to** $r-1$ **do**

2. $\lambda \leftarrow \lambda \in [0,1], \bar{\mathbf{p}} \leftarrow \mathbf{p} \in P$
   $\mathbf{c}, \mathbf{C}, \mathbf{s_c}, \mathbf{s_C} \leftarrow \mathtt{Aff}(\ldots)$ ▹ Subroutine defined in [23]
   $\mathbf{z}_k^{j,a}(\mathbf{p}) \leftarrow \mathbf{c} + \mathbf{s_c}^{\mathrm{T}}(\mathbf{p} - \bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▹ Affine relaxation lower bound
   $\mathbf{z}_k^{j,A}(\mathbf{p}) \leftarrow \mathbf{C} + \mathbf{s_C}^{\mathrm{T}}(\mathbf{p} - \bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▹ Affine relaxation upper bound
   $\gamma^j(\cdot) \leftarrow \lambda \mathbf{z}_k^{j,a}(\cdot) + (1-\lambda)\mathbf{z}_k^{j,A}(\cdot)$
   $\mathbf{s}_\gamma^j \leftarrow \lambda \mathbf{s_c} + (1-\lambda)\mathbf{s_C}$

3. $\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathbf{u_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$ ▹ **B** matrix defined in [23] w.r.t. $\mathbf{h}_k$ and $\mathbf{J}_k$
   $\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathbf{o_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$
   $\mathbf{s}_\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathcal{S}_{\mathbf{u}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$
   $\mathbf{s}_\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathcal{S}_{\mathbf{o}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

4. $\mathbf{z}_k^{j+1,cv}(\cdot) \leftarrow \bar{\mathbf{u}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$
   $\mathbf{z}_k^{j+1,cc}(\cdot) \leftarrow \bar{\mathbf{o}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$
   $\mathbf{s}_\mathbf{z}^{j+1,cv}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{u}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$
   $\mathbf{s}_\mathbf{z}^{j+1,cc}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{o}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$

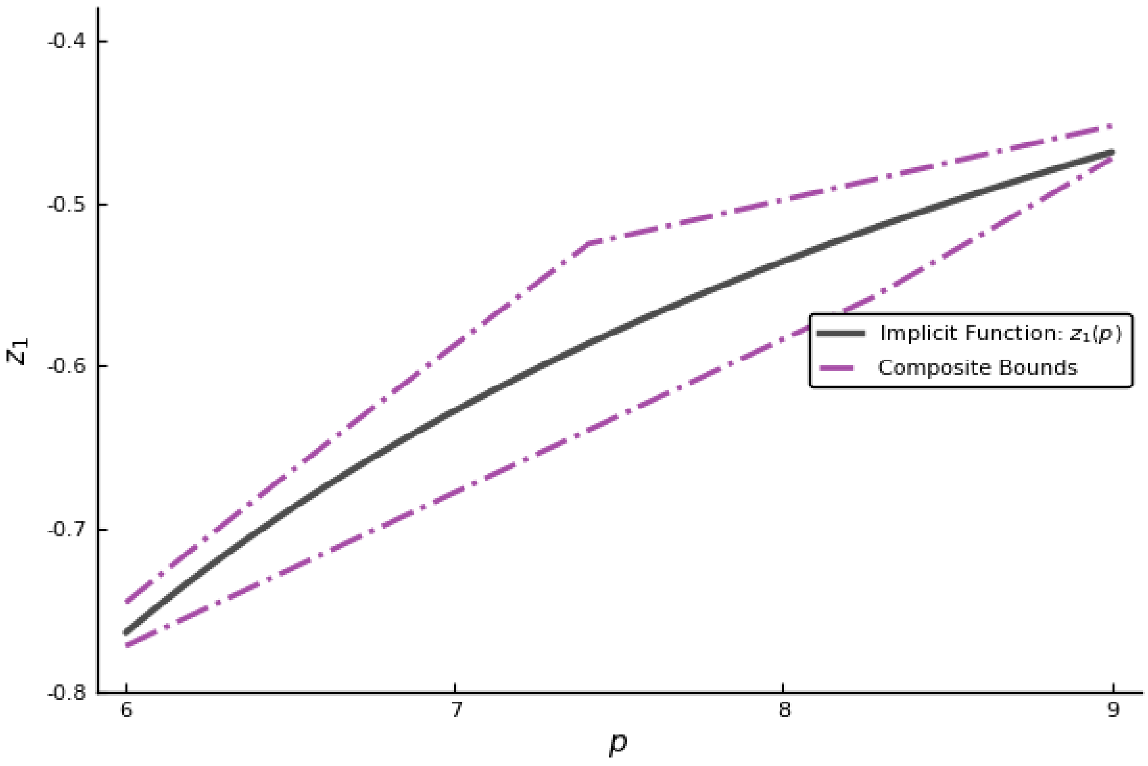
end for

return $\mathbf{z}_k^{r,cc}(\cdot), \mathbf{z}_k^{r,cc}(\cdot), \mathbf{s}_\mathbf{z}^{r,cv}(\cdot), \mathbf{s}_\mathbf{z}^{r,cc}(\cdot)$

Next iteration...

Block relaxation algorithm

4(b). Compute composite relaxation of $\boldsymbol{z}_k^{j+1}$ and the respective subgradients thereof.



procedure BLOCKRELAX$(\mathbf{h}_k, X, P, \mathbf{z}_{k-1}^{cv}, \mathbf{z}_{k-1}^{cc}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-1}}^{cc}, \mathbf{z}_{k-2}^{cv}, \mathbf{z}_{k-2}^{cc}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cv}, \mathbf{s}_{\mathbf{z}_{k-2}}^{cc}, r)$

1.

$\mathbf{z}_k^{0,cv}, \mathbf{z}_k^{0,cc}, \mathbf{s}_{\mathbf{z}_k}^{0,cv}, \mathbf{s}_{\mathbf{z}_k}^{0,cc} \leftarrow \mathbf{x}^L, \mathbf{x}^U, 0, 0$

for $j \leftarrow 0$ **to** $r-1$ **do**

Next iteration...

2.

$\lambda \leftarrow \lambda \in [0,1], \bar{\mathbf{p}} \leftarrow \mathbf{p} \in P$

$\mathbf{c}, \mathbf{C}, \mathbf{s_c}, \mathbf{s_C} \leftarrow \mathtt{Aff}(\ldots)$ ▹ Subroutine defined in [23]

$\mathbf{z}_k^{j,a}(\mathbf{p}) \leftarrow \mathbf{c} + \mathbf{s_c}^{\mathrm{T}}(\mathbf{p} - \bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▹ Affine relaxation lower bound

$\mathbf{z}_k^{j,A}(\mathbf{p}) \leftarrow \mathbf{C} + \mathbf{s_C}^{\mathrm{T}}(\mathbf{p} - \bar{\mathbf{p}}),\ \forall \mathbf{p} \in P$ ▹ Affine relaxation upper bound

$\gamma^j(\cdot) \leftarrow \lambda \mathbf{z}_k^{j,a}(\cdot) + (1-\lambda)\mathbf{z}_k^{j,A}(\cdot)$

$\mathbf{s}_\gamma^j \leftarrow \lambda \mathbf{s_c} + (1-\lambda)\mathbf{s_C}$

3.

$\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathbf{u_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$ ▹ B matrix defined in [23] w.r.t. $\mathbf{h}_k$ and $\mathbf{J}_k$

$\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathbf{o_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \ldots, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \cdot)$

$\mathbf{s}_\mathbf{M}^{j,cv}(\cdot) \leftarrow \mathcal{S}_{\mathbf{u}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

$\mathbf{s}_\mathbf{M}^{j,cc}(\cdot) \leftarrow \mathcal{S}_{\mathbf{o}_B}(\mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \ldots, \mathbf{z}_k^{j,a}(\cdot), \mathbf{z}_k^{j,A}(\cdot), \mathbf{s_c}, \mathbf{s_C}, \cdot)$

4.

$\mathbf{z}_k^{j+1,cv}(\cdot) \leftarrow \bar{\mathbf{u}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$

$\mathbf{z}_k^{j+1,cc}(\cdot) \leftarrow \bar{\mathbf{o}}_\psi(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{z}_{k-1}^{cv}(\cdot)\mathbf{z}_{k-1}^{cc}(\cdot), \mathbf{z}_{k-2}^{cv}(\cdot)\mathbf{z}_{k-2}^{cc}(\cdot), \cdot)$

$\mathbf{s}_\mathbf{z}^{j+1,cv}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{u}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$

$\mathbf{s}_\mathbf{z}^{j+1,cc}(\cdot) \leftarrow \mathcal{S}_{\bar{\mathbf{o}}_\psi}(\gamma^j(\cdot), \gamma^j(\cdot), \mathbf{s}_\gamma^j, \mathbf{s}_\gamma^j, \mathbf{M}^{j,cv}(\cdot), \mathbf{M}^{j,cc}(\cdot), \mathbf{z}_k^{j,cv}(\cdot), \mathbf{z}_k^{j,cc}(\cdot), \mathbf{s}_\mathbf{z}^{j,cv}(\cdot), \mathbf{s}_\mathbf{z}^{j,cc}(\cdot), \cdot)$

end for

return $\mathbf{z}_k^{r,cc}(\cdot), \mathbf{z}_k^{r,cc}(\cdot), \mathbf{s}_\mathbf{z}^{r,cv}(\cdot), \mathbf{s}_\mathbf{z}^{r,cc}(\cdot)$

Relaxation Algorithm

1. Compute relaxation of initial conditions using standard McCormick arithmetic.

2. Performance a relaxation in a block sequential fashion to compute relaxations and subgradients at next time step and repeat.

3. Use relaxations and subgradients available at discrete time points to construct relaxations of the objective and constraints. *Interpolating if necessary.*

---

procedure IVPBOUND($X, P, \mathbf{h}, \mathbf{x}_0, r$)

$\quad \mathbf{z}_0^{cv}, \mathbf{z}_0^{cc}, \mathbf{s}_{\mathbf{z}_0}^{cv}, \mathbf{s}_{\mathbf{z}_0}^{cv} \leftarrow \text{McCormickRelax}(X, P, \mathbf{x}_0(\cdot))$ ▹ Standard McCormick relaxation of $\mathbf{x}_0$ on P

$\quad \mathbf{z}_1^{cv}(\cdot), \mathbf{z}_1^{cc}(\cdot), \mathbf{s}_{\mathbf{z}_1}^{cv}(\cdot), \mathbf{s}_{\mathbf{z}_1}^{cc}(\cdot) \leftarrow \text{BlockRelax}(\mathbf{h}_1, X, P, \mathbf{z}_0^{cv}, \mathbf{z}_0^{cc}, \mathbf{s}_{\mathbf{z}_0}^{cv}, \mathbf{s}_{\mathbf{z}_0}^{cc}, \mathbf{x}^L, \mathbf{x}^U, \mathbf{0}, \mathbf{0}, r)$

$\quad$ **for** $i \leftarrow 2$ **to** K **do**

$\quad\quad \mathbf{z}_i^{cv}(\cdot), \mathbf{z}_i^{cc}(\cdot), \mathbf{s}_{\mathbf{z}_i}^{cv}(\cdot), \mathbf{s}_{\mathbf{z}_i}^{cc}(\cdot) \leftarrow \text{BlockRelax}(\mathbf{h}_i, X, P, \mathbf{z}_{i-1}^{cv}, \mathbf{z}_{i-1}^{cc}, \mathbf{s}_{\mathbf{z}_{i-1}}^{cv}, \mathbf{s}_{\mathbf{z}_{i-1}}^{cc}, \mathbf{z}_{i-2}^{cv}, \mathbf{z}_{i-2}^{cc}, \mathbf{s}_{\mathbf{z}_{i-2}}^{cv}, \mathbf{s}_{\mathbf{z}_{i-2}}^{cc}, r)$

$\quad$ **end for**

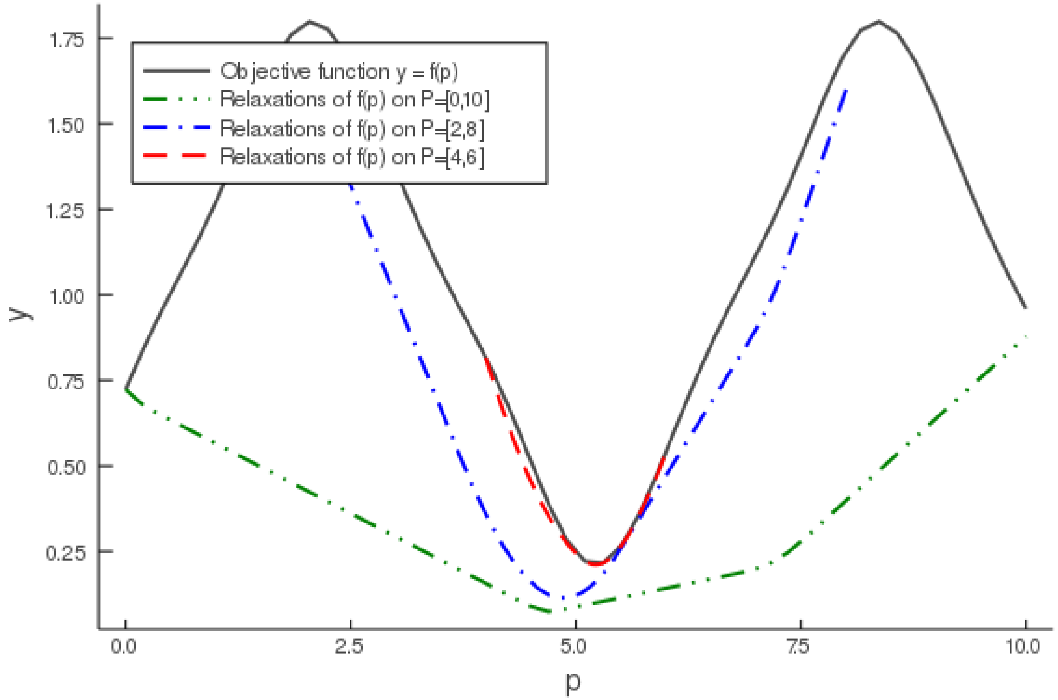
$\quad$ **return** $\mathbf{z}^{cv}(\cdot), \mathbf{z}^{cc}(\cdot), \mathbf{s}_{\mathbf{z}}^{cv}(\cdot), \mathbf{s}_{\mathbf{z}}^{cc}(\cdot)$

end procedure

Exhibits Partition Convergence

Partition Convergence[13]*:*

Consider a nested sequence of intervals $\{P_q\}$, $P_q \subset P$, $q \in \mathbb{N}$, such that $\{P_q\} \to [\bar{\mathbf{p}}, \bar{\mathbf{p}}]$ for some $\bar{\mathbf{p}} \in \boldsymbol{P}$. Let z_q^{cv}, z_q^{cc} be relaxations of z on P_q obtained using the prior algorithm. Let $\phi_q^{cv}(\cdot) = u_\phi(\mathbf{z}_k^{cv}(\cdot), \mathbf{z}_k^{cc}(\cdot), \cdot)$ be a convex relaxation of the objective function ϕ on P_q. Let $\hat{\phi}_q^{cv} = \min_{\mathbf{p} \in P_q} \phi_q^{cv}$, then $\lim_{q\to\infty} \hat{\phi}_q^{cv} = \phi_q^{cv}(\mathbf{z}(\bar{\mathbf{p}}), \bar{\mathbf{p}})$



13. Stuber MD, Scott JK, Barton PI. **Convex and concave relaxations of implicit functions.** Optimization Methods and Software 2015; 30(3):424–460.

Proof of Partition Convergence

- $K = 1$ case is trivially true… Proceed by contradiction.
- Suppose that for $K > 1$, $\lim_{q\to\infty} \hat{\phi}_q^{cv} \neq \phi_q^{cv}(\mathbf{z}(\bar{\mathbf{p}}), \bar{\mathbf{p}})$.
- u_ϕ continuous and exhibits partition convergence as it is constructed using a generalized McCormick relaxation framework[14]. Then

  - Either $\lim_{q\to\infty} \mathbf{z}_{k,q}^{cv} \neq \mathbf{z}_{k,q}(\bar{\mathbf{p}})$ or $\lim_{q\to\infty} \mathbf{z}_{k,q}^{cv} \neq \mathbf{z}_{k,q}(\bar{\mathbf{p}})$ which implies
  - Either $\lim_{q\to\infty} \mathbf{z}_{k-1,q}^{cv} \neq \mathbf{z}_{k-1,q}(\bar{\mathbf{p}})$ or $\lim_{q\to\infty} \mathbf{z}_{k-1,q}^{cv} \neq \mathbf{z}_{k-1,q}(\bar{\mathbf{p}})$ which implies
  - Either $\lim_{q\to\infty} \mathbf{z}_{k-2,q}^{cv} \neq \mathbf{z}_{k-2,q}(\bar{\mathbf{p}})$ or $\lim_{q\to\infty} \mathbf{z}_{k-2,q}^{cv} \neq \mathbf{z}_{k-2,q}(\bar{\mathbf{p}})$ which implies

    …
  - Either $\lim_{q\to\infty} \mathbf{z}_{1,q}^{cv} \neq \mathbf{z}_{1,q}(\bar{\mathbf{p}})$ or $\lim_{q\to\infty} \mathbf{z}_{1,q}^{cv} \neq \mathbf{z}_{1,q}(\bar{\mathbf{p}})$ which is contradiction.

Inductive Proof

14. Scott JK, Stuber MD, Barton PI. **Generalized McCormick relaxations.** Journal of Global Optimization 2011; 51(4): 569–606.

Implementation

- Branch and bound algorithm as an extension to the EAGO global optimizer available at https://github.com/PSORLab/EAGODifferential.jl
- **IntervalArithmetic.jl** for validated interval calculations.
- Relaxations from McCormick submodule of **EAGO.jl**.
- All simulations run on single thread of Intel Xeon E3-1270 v5 3.60/4.00GHz processor with 16GM ECC RAM, Ubuntu 18.04LTS using Julia v1.1.0[15]. Intel MKL 2019 (Update 2) for BLAS/LAPACK.

https://github.com/PSORLab/EAGO.jl

15. Jeff Bezanson, Alan Edelman, Stefan Karpinski and Viral B. Shah **Julia: A Fresh Approach to Numerical Computing**. (2017) *SIAM Review*, 59: 65–98.

A 1D Example

- Consider the 1D pODE-IVP:

$$\frac{dx}{dt}(p,t) = -x^2 + p$$

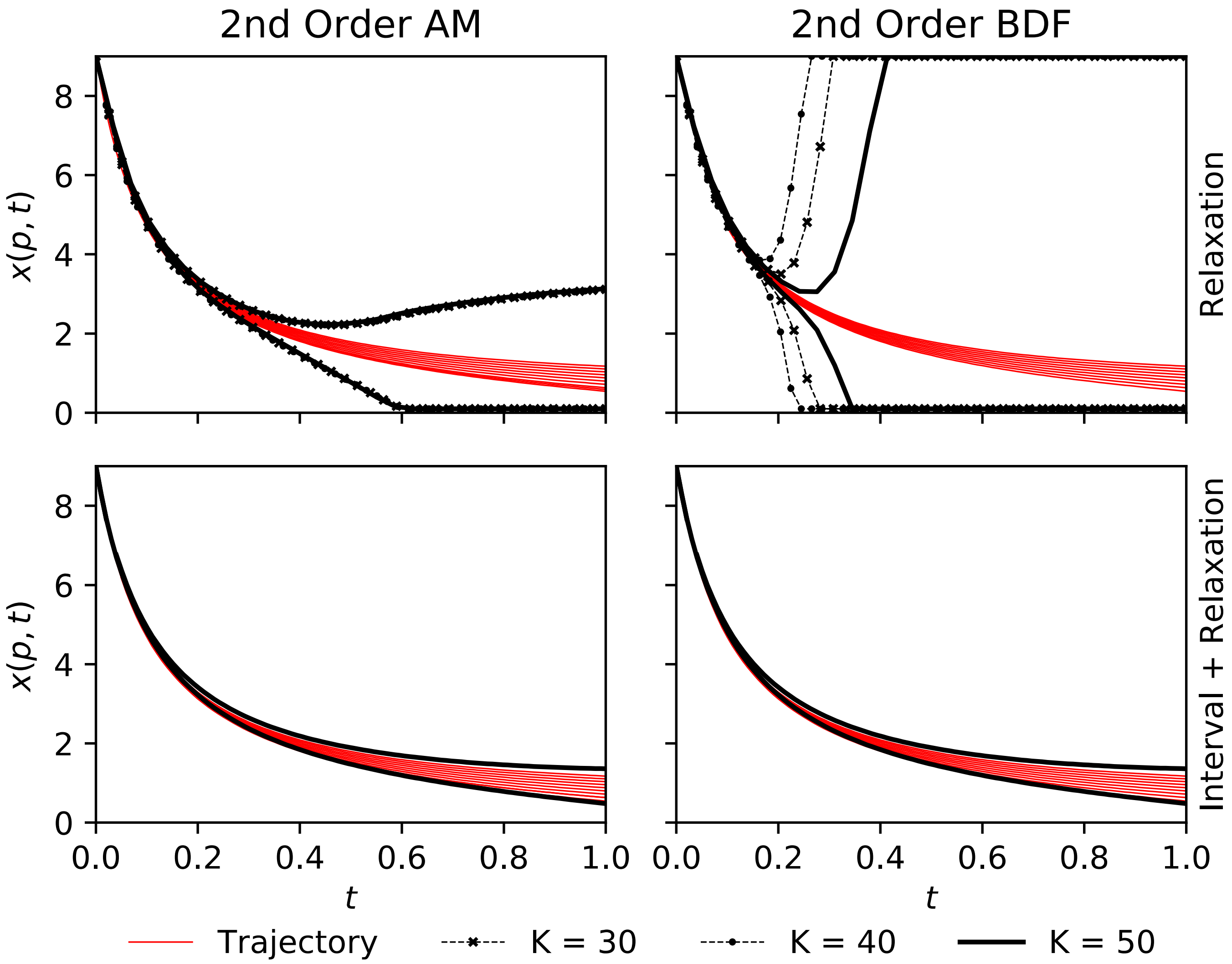
$$x_o(p) = 9$$

$$t \in [0,1], \qquad x \in X = [0.1,9]$$

$$p \in P = [-1,1]$$

- The BDF method enclosure depends heavily on the chosen step size whereas the AM method bounds do not.

- In either case, applying 5 iterations of a corresponding parametric interval method further tightens the relaxations.



Kinetic Problem

Problem Statement

- Fit the rate constants (k_{2f}, k_{3f}, k_4) of oxygen addition to cyclohexadienyl radicals to data. [16]
- First addressed by global by Singer et al.[17]
- Explicit Euler form solved by by Mitsos[18]
- Implicit Euler form addressed in Stuber[19]

pODE IVP:

$$\dot{x}_A = k_1 x_Z x_Y - c_{O2}(k_{2f} + k_{3f})x_A + (k_{2f}/K_2)x_D + (k_{3f}/K_3)x_B - k_5 x_A^2,$$

$$\dot{x}_B = k_{3f} c_{O2} x_A - (k_{3f}/K_3 + k_4)x_B, \quad \dot{x}_D = k_{2f} c_{O2} x_A - (k_{2f}/K_2)x_D,$$

$$\dot{x}_Y = -k_{1s} x_Y x_Z, \quad \dot{x}_Z = -k_1 x_Y x_Z,$$

$$\dot{\boldsymbol{x}}(t=0) = (0, 0, 0, 0.4, 140)$$

Objective Variables

$$f^* = \min_{\boldsymbol{p} \in P} \sum_{i=1}^{n} \left(\mathrm{I}^i - \mathrm{I}^i_{\mathrm{data}}\right)^2$$

$$s.t. \quad \mathrm{I}^i = x_A^i + \frac{2}{21} x_B^i + \frac{2}{21} x_D^i$$

Decision Variables

$$\boldsymbol{p} = (k_{2f}, k_{3f}, k_4)$$

State Variables

$$\boldsymbol{x} = (x_A, x_B, x_D, x_Y, x_Z)$$

Constants

$$k_1, k_{1s}, k_5, K_2, K_3, c_{O2}, \Delta t, n$$

16. J. W. Taylor, et al. **Direct measurement of the fast, reversible addition of oxygen to cyclohexadienyl radicals in nonpolar solvents**, *Phys. Chem. A*, 108 (2004), pp. 7193–7203.
17. A. B. Singer et al., **Global dynamic optimization for parameter estimation in chemical kinetics** A. B. Singer et al., *J. Phys. Chem. A*, 110 (2006), pp. 971–976
18. Mitsos et al. **McCormick-based relaxations of algorithms.** *SIAM Journal on Optimization*, SIAM (2009) 20, 73-601
19. Stuber, M.D. et al. **Convex and concave relaxations of implicit functions.** *Optimization Methods and Software* (2015), 30, 424-460

Implementation

Problem Statement

- Fit the rate ... es
  addition ...
- First add ... $\text{data})^2$
- Explicit ...
- Implicit ... $x_B^i + \frac{2}{21} x_D^i$

pODE IVP:

$\dot{x}_A = k_1 x_Z$ ...

$\dot{x}_B = k_{3f} c$ ... $, x_Z)$

$\dot{x}_Y = -k_{1}$ ...

$\dot{\boldsymbol{x}}(t = 0) =$ ... $_{O2}, \Delta t, n$

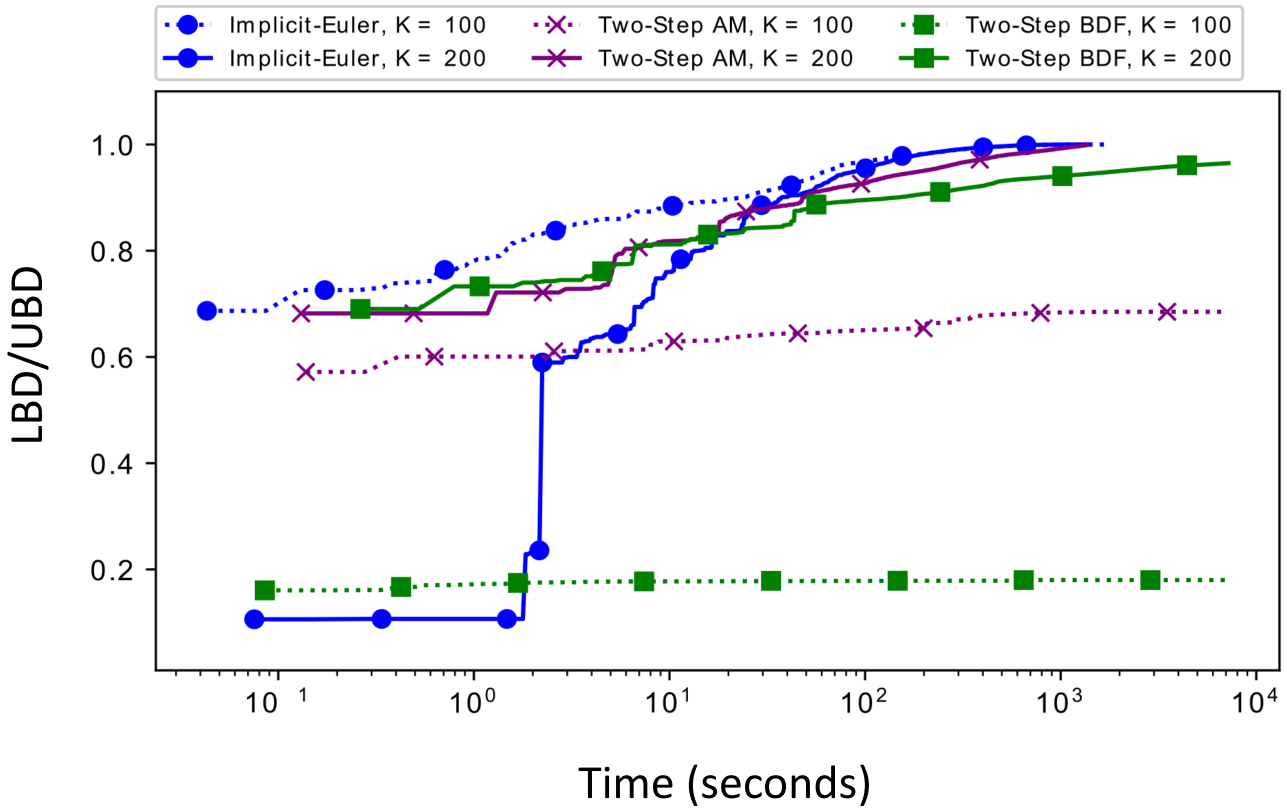
- Affine relaxations used to compute lower bound (CPLEX 12.8).
- Upper-bound computed by integrating ODE at midpoint of active node then evaluating objective & constraints.
- Duality-based bound tightening was performed. Two iterations of each PILMS with was used after five iterations of a block sequential parametric interval method.
- Absolute and relative convergence tolerances for the B&B algorithm of 10^{-2} and 10^{-5}, respectively.

16. J. W. Taylor, et al. **D** ... (2004), pp. 7193–7203.
17. A. B. Singer et al., **Glob** ... 71–976
18. Mitsos et al. **McCormick-based relaxations of algorithms.** *SIAM Journal on Optimization*, SIAM (2009) 20, 73-601
19. Stuber, M.D. et al. **Convex and concave relaxations of implicit functions.** *Optimization Methods and Software* (2015), 30, 424-460

Kinetic Problem

Kinetic problem was solved subject to three discretization schemes for $K = 100$ and $K = 200$.

Solution Method	K	Iterations	Average time per iteration	Solution time	SSE at Solution
Implicit Euler	100	33987	45×10^{-3}s	29.7min	26947.246
	200	23,525	59×10^{-3}s	23.4min	16796.038
2-Step AM	100	62024	12×10^{-2}s	>2 h	N/A*
	200	6068	22×10^{-2}s	22.6min	13077.998
2-Step BDF	100	88408	81×10^{-3}s	>2 h	N/A*
	200	27600	26×10^{-2}s	>2 h	N/A*
Explicit Euler	100	>300,000	23×10^{-4}s	>2 h	N/A
	200	>300,000	24×10^{-4}s	>2 h	N/A



A plug-flow reactor problem

Optimization Problem

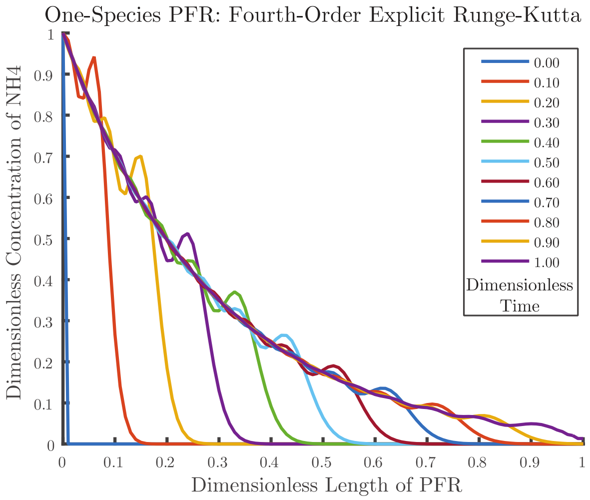
$$\phi^* = \min_{p\in[0,1]} p$$
$$s.t. \quad \hat{x}_K(t = t_f, p) - 0.08 \le 0$$

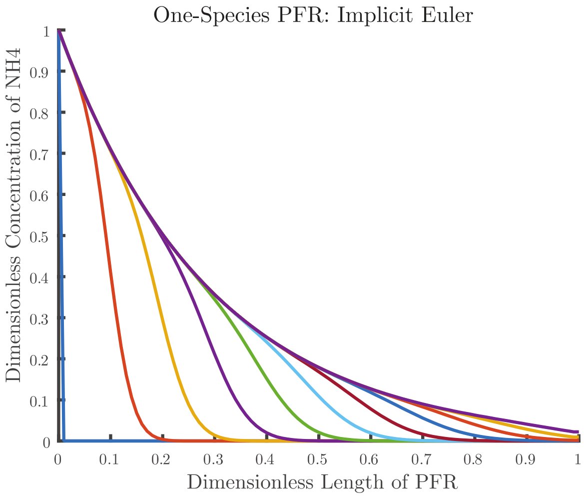
Method of Lines Discretization

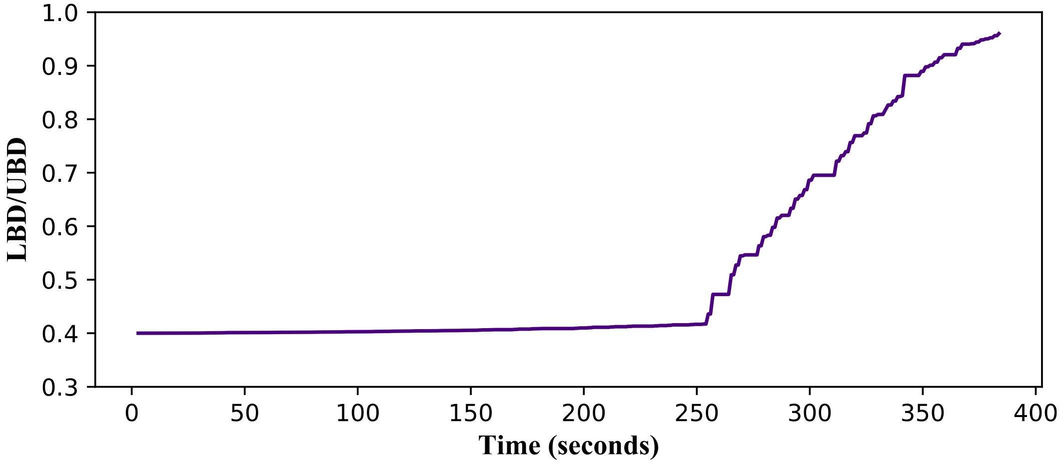
$$\frac{d\hat{\mathbf{x}}}{dt}(p,t) = -\frac{\Delta\hat{\mathbf{x}}}{\Delta y} - Da(p)\hat{\mathbf{x}}$$
$$Da(p) = 0.1 + 0.3p$$

Problem Setup

- Start-up of a single species PFR
- Inlet concentration is 1
- Initial concentration is 0
- Number of timesteps of variable size = 30
- Number of spatial discretization points = 20
- The PFR is sparged and we can module the rate of reaction by changing airflow (p)





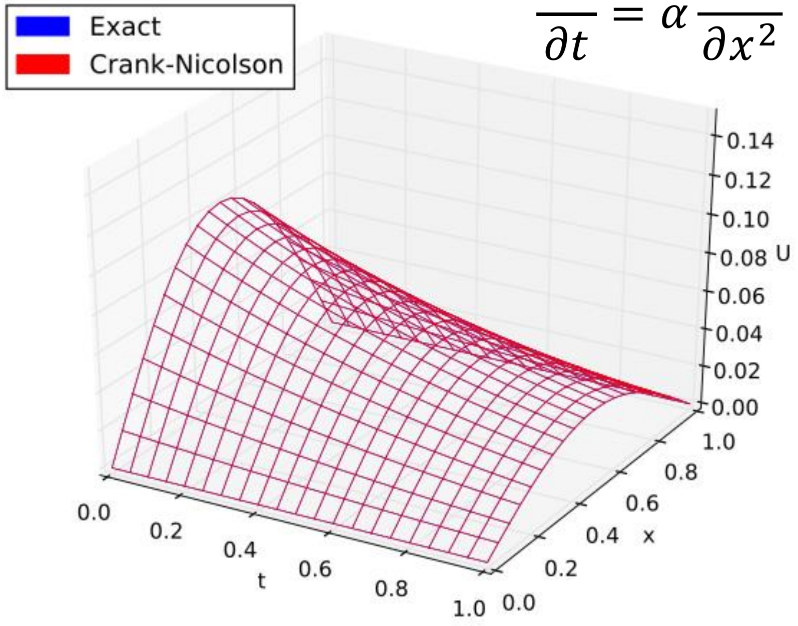


Future Directions

- **Extension to provide enclosure of truncation error.**
  - Interval forms have been addressed.
  - Generalization to relaxations and use in global optimization outstanding.

- **Constructing bounds of PDE constrained systems via relaxation of Crank-Nicolson methods.**

$$\frac{\partial U}{\partial t} = \alpha \frac{\partial^2 U}{\partial x^2}$$



Courtesy of wikimedia commons (https://commons.wikimedia.org/wiki/File:HeatEquationCNApproximate.svg)

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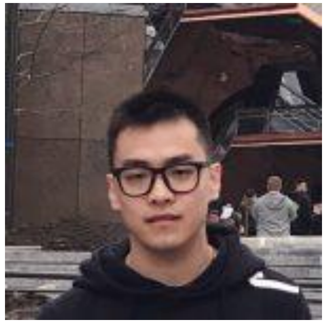

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Fin…

Any Questions?