Quadratic Underestimators of Differentiable McCormick Relaxations for Deterministic Global Optimization

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Outline

Optimizing Simulations

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We commonly encounter problems that can be described by simulations. These simulations often haven a greatly reduced problem dimension compared to problems represented explicitly as closed-form equations since intermediate variables must be introduced in the latter approach, $n_p << n_x < n_y$. Examples:

- Regressions with embedded ODE (**Chemical Kinetics**) [1]
- Yield optimization of flowsheets (**Process Design**)

Full-Space

$$f^* = \min_{\mathbf{y} \in Y \subset \mathbb{R}^{n_y}} f(\mathbf{y})$$
$$\text{s.t. } \mathbf{h}(\mathbf{y}) = \mathbf{0}$$
$$\mathbf{g}(\mathbf{y}) \leq \mathbf{0}$$

Reduced-Space

$$f^* = \min_{\mathbf{p} \in P} f(\mathbf{x}(\mathbf{p}), \mathbf{p})$$
$$\text{s.t. } \mathbf{g}(\mathbf{x}(\mathbf{p}), \mathbf{p}) \leq \mathbf{0}$$

1 Stuber, M. et al. Optimization Methods and Software, 2015, 30, 424-460

Dealing with Nonconvexity

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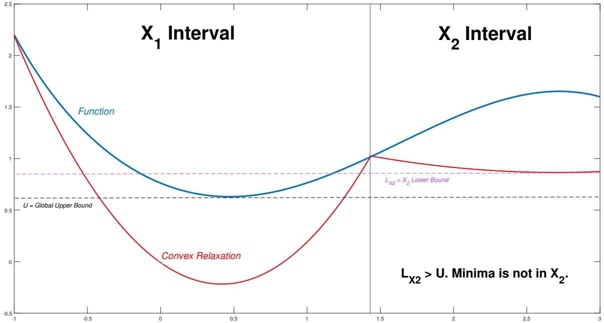
- Many simulations exhibit significant nonconvexity.
- NP-hard and solved via branch-and-bound variations [2].



2 Horst, R. & H. Tuy. Global Optimization: Deterministic Approaches, 2013

Relaxing Algorithms

- One approach to generating these lower bounds is via the use of set-valued arithmetics.
- Using these approaches an enclosure of the image of a function is defined along with operators that take these objects as inputs and output a new enclosure (method overloading).
- Approaches include are interval arithmetic [3], affine arithmetic [4], and McCormick operators [5].

3 Moore, R.E. Introduction to Interval Analysis, 2009

4 De Figueiredo, L.H. et al. Numerical Algorithms, 2004, 37, 147-158

5 Mitsos, A. et al. SIAM Journal of Optimization, 2009, 20, 573-601

McCormick Operators

McCormick Composition Rule [5]:

Let $Z \subset \mathbb{R}^n$, $X \subset \mathbb{R}$ be nonempty convex. The composite function $g = \phi \circ f$ s.t. $f : Z \rightarrow \mathbb{R}$ is continuous, $F : X \rightarrow \mathbb{R}$, $f(Z) \subset X$. Let $f^{cv}, f^{cc} : Z \rightarrow \mathbb{R}$ be relaxations of f on Z. Let $\phi^{cv}, \phi^{cc} : X \rightarrow \mathbb{R}$ be relaxations of ϕ on X. Let $\xi^*_{\text{min}}/\xi^*_{\text{max}}$ be a min/max of ϕ^{cv}/ϕ^{cc} on X.

$$g^{cv} : Z \rightarrow \mathbb{R} : z \mapsto \phi^{cv}(\text{mid}(f^{cv}, f^{cc}, \xi^*_{\text{min}}))$$
$$g^{cc} : Z \rightarrow \mathbb{R} : z \mapsto \phi^{cc}(\text{mid}(f^{cv}, f^{cc}, \xi^*_{\text{max}}))$$

- Usually second-order convergent and tighter than interval bounds [5,6].
- Desirable to minimize clustering about optima in branch and bound algorithm [7].
- Rules for propagating differentiable relaxations have been introduced [8].

5 Mitsos, A. et al. SIAM Journal of Optimization, 2009, 20, 573-601

6 Bompadre, A. et al. Journal of Global Optimization, 2012, 52, 1-28

7 Kannan, R. et al. Journal of Global Optimization, 2017, 69, 629-676

8 Khan, K. et al. Journal of Global Optimization, 2017, 67(4), 687-729

Lower Bounds from Subproblems

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No agreement exists in the literature on the best optimization problem to construct with these relaxations [8,9,10]. Affine relaxations may be weaker but the linear solvers are more robust and faster which may justify evaluating more nodes.

- **Standard McCormick Operators**
  - Nonsmooth NLP [1] ⇒ Nonsmooth NLP solver (e.g. Proximal Methods[9])
  - Relax Further [5] ⇒ Linear Program (e.g. CPLEX [10])
- **Differentiable NLP [5]**
  - Solve with Interior point method (e.g. Ipopt [11])
  - Further relax to QCQP ⇒ Interior point method

1 Stuber, M. et al. Optimization Methods and Software, 2015, 30, 424-460

5 Mitsos, A. et al. SIAM Journal of Optimization, 2009, 20, 573-601

8 Khan, K. et al. Journal of Global Optimization, 2017, 67(4), 687-729

9 L. Luksan et al. ACM Transactions on Mathematical Software 27 (2001), 193-213

10 IBM ILOG CPLEX Optimizer, 2017

11 Wächter, A. et al. Mathematical Programming, 2006, 106(1), 25-57

Outline

m-Convex Function [12]

Let $f : Z \subset \mathbb{R}^n \rightarrow \mathbb{R}$ be a proper, closed, m-convex, Whitney-1 differentiable, locally Lipschitz continuous function. At every point $x \in \text{int}(Z)$ there is a second-order quadratic expansion in the form

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{y} - \mathbf{x}) + \frac{m}{2}||\mathbf{y} - \mathbf{x}||_2^2 \quad (1)$$

- In many cases, m-convexity is required for superlinear convergence of optimization methods [12].

12 Vial, J.P. et al. Mathematics of Operations Research,8(2), 231-259

QCQP Relaxations

The quadratically-constrained quadratic programming (QCQP) relaxation of a nonlinear program is given below:

$$
\begin{aligned}
&\min_{\mathbf{y},\eta} \eta \\
\text{s.t.}\quad & f^{cv}(\mathbf{y}_0) + (\mathbf{y}-\mathbf{y}_0)^T \nabla f^{cv}(\mathbf{y}_0) + \frac{m_{f^{cv}}}{2}||\mathbf{y}-\mathbf{y_0}||_2^2 \leq \eta \\
& \mathbf{h}^{cc}(\mathbf{y}_0) + (\mathbf{y}-\mathbf{y}_0)^T \nabla \mathbf{h}^{cc}(\mathbf{y}_0) + \frac{m_{\mathbf{h}^{cc}}}{2}||\mathbf{y}-\mathbf{y_0}||_2^2 \geq \mathbf{0} \\
& \mathbf{h}^{cv}(\mathbf{y}_0) + (\mathbf{y}-\mathbf{y}_0)^T \nabla \mathbf{h}^{cv}(\mathbf{y}_0) + \frac{m_{\mathbf{h}^{cv}}}{2}||\mathbf{y}-\mathbf{y_0}||_2^2 \leq \mathbf{0} \\
& \mathbf{g}^{cv}(\mathbf{y}_0) + (\mathbf{y}-\mathbf{y}_0)^T \nabla \mathbf{g}^{cv}(\mathbf{y}_0) + \frac{m_{\mathbf{g}^{cv}}}{2}||\mathbf{y}-\mathbf{y_0}||_2^2 \leq \mathbf{0}
\end{aligned}
$$

Quadratic Bounds Algebra

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Addition of m-Convex Function [12]

Let $f : Z \subset \mathbb{R}^n \to \mathbb{R}$ be a m-convex and $g : Z \subset \mathbb{R}^n \to \mathbb{R}$ be convex on Z then $f + g$ is p-convex on Z with $p \geq m$.

Linearity of m-Convex Function [12]

Let $f_1, f_2 : Z \subset \mathbb{R}^n \to \mathbb{R}$ be m_1-convex and m_2-convex, respectively. Let α_1, α_2 be positive real numbers then $\alpha_1 f_1 + \alpha_2 f_2$ is $(\alpha_1 m_1 + \alpha_2 m_2)$-convex.

Additive Inverse of m-Convex Function [12]

The function $f : Z \subset \mathbb{R}^n \to \mathbb{R}$ is m-concave on Z if and only if $-f$ is m-convex on Z.

12 Vial, J.P. et al. Mathematics of Operations Research,8(2), 231-259

Propagating m-Convexity Bounds [12]

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Composition of m-Convex Function

Let $f : Z \subset \mathbb{R}^n \to \mathbb{R}$ be a m-convex and $g : Z \subset R \to \mathbb{R}$ be a monotone convex increasing function on Z. Suppose g' is bounded below by β then $g \circ f$ is $m\beta$-convex.

Basic McCormick Scheme Fails

We know that $x \to x$ isn't m-convex. The composition rule fails to imply m-convexity.

Need to Track Linearity Properties to Start

For $z_j = f(z_i)$ such that z_i is affine, calculate m by rule for f then propagate m values using previously defined rules.

13 Vial, J.P. et al. Mathematics of Operations Research,8(2), 231-259

Generating m-values

Composition with Affine Functions

Let $f : Z \subset \mathbb{R}^n \to \mathbb{R}$ be a m-convex and $g : Z \subset \mathbb{R}^n \to \mathbb{R}$ is affine then $f \circ g$ is m-convex on Z.

- Define point, gradient, monotonicity flag, convexity flag, and interval bounds for variable.
- Define ruleset for computing m for each operator based on convexity flag and monotonicity.
- Propagate further bounds by composition rules.

13 Vial, J.P. et al. Mathematics of Operations Research,8(2), 231-259

Convergence Order: Spoilers!

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Theorem: Second-Order Pointwise Convergence

Consider a nonempty open set $Z \subset \mathbb{R}^n$, a nonempty compact set $Q \subset Z$, and a $C^{1,1}$ function $f : Z \to \mathbb{R}$. For each interval $\mathbf{w} \in \mathbb{IR}^n \cup \mathbb{Q} = \mathbb{IQ}$, a convex underestimator $f_w^C : \mathbf{w} \to R$ of f on w, suppose that there exists a scalar $\tau^C > 0$ for which

$$\sup_{z \in \mathbf{w}} \left(f(z) - f_{\mathbf{w}}^C(z) \right) \leq \tau^C wid(\mathbf{w})^2, \qquad \forall \mathbf{w} \in \mathbb{IQ}$$

Then, for each $\alpha \in [0, 1)$, there exists $\tau_\alpha > 0$ for which

$$\sup_{z \in \mathbf{w}} f(z) - (f_{\mathbf{w}}^C(\epsilon) + \langle \nabla f(z), z - \epsilon \rangle) + \langle A(z - \epsilon), z - \epsilon \rangle \leq \tau^C wid(\mathbf{w})^2, \quad \forall \mathbf{w} \in \mathbb{IQ}, \quad \forall \epsilon \in s_\alpha(\mathbf{w})) \tag{3}$$

That is to say, the quadratic underestimator inherits second-order point-wise convergence from the second-order point-wise convergence of the subdifferential.

Convergence Order of Subdifferential [13]

Consider a nonempty open set $Z \subset \mathbb{R}^n$, a nonempty compact set $Q \subset Z$, and a $C^{1,1}$ function $f : Z \to \mathbb{R}$. For each interval $\mathbf{w} \in \mathbb{IR}^n \cup \mathbb{Q} = \mathbb{IQ}$, a convex underestimator $f^C_w : \mathbf{w} \to R$ of f on w, suppose that there exists a scalar $\tau^C > 0$ for which

$$\sup_{z \in \mathbf{w}} \left(f(z) - f^C_{\mathbf{w}}(z) \right) \leq \tau^C wid(\mathbf{w})^2, \qquad \forall \mathbf{w} \in \mathbb{IQ}$$

Then, for each $\alpha \in [0, 1)$, there exists $\tau_\alpha > 0$ for which

$$\sup_{z \in \mathbf{w}} \left(f(z) - (f^C_{\mathbf{w}}(\epsilon) + \langle s, z - \epsilon \rangle) \right) \leq \tau^C wid(\mathbf{w})^2,$$

$$\forall \mathbf{w} \in \mathbb{IQ}, \qquad \forall \epsilon \in s_\alpha(\mathbf{w}), \qquad \forall s \in \partial f^C_{\mathbf{w}}(\epsilon)$$

Proof.

Note that $\nabla f(\mathbf{x}) \in \partial f^C_{\mathbf{w}}(\epsilon)$ and $\langle A(z - \epsilon), z - \epsilon \rangle \geq 0$ since A is positive semidefinite. Then $f(z) - (f^C_{\mathbf{w}}(\epsilon) + \langle s, z - \epsilon \rangle + \langle A(z - \epsilon), z - \epsilon \rangle) \leq f(z) - (f^C_{\mathbf{w}}(\epsilon) + \langle s, z - \epsilon \rangle)$ and the quadratic underestimator inherits second-order pointwise convergence. □

13 K. Khan, Subtangent-Based Approaches for Optimization of Parametric Process Systems, AIChE Annual Meeting, October 30, 2018

Tightening Interval Bounds

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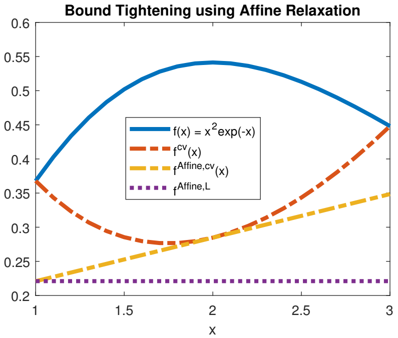
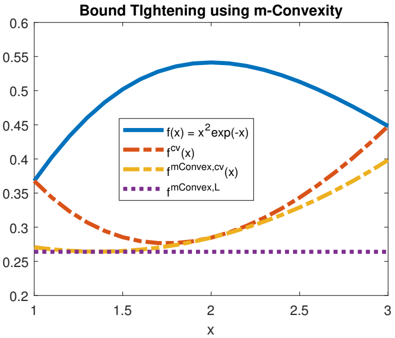
- Subgradients may be used to contract interval bounds [14].
- We know closed form envelopes for univariate and bivariate quadratics [15,16].
- For univariate and bivariate functions these hulls can tighten interval bounds.





14 Najman, J et al. arXiv preprint arXiv:1710.09188, 2017

15 S. Vigerske, Ph.D. diss., Humboldt-UniversitÃďt zu Berlin, 2013

16 F. Domes and A. Neumaier, Constraints 15 (2010), pp. 404-429

Outline

Numerical Results

- We selected twelve problems from the GLOBAL library and literature examples and each subproblem relaxation was compared. The standard EAGO settings were used for all other parameters.
- An absolute tolerance of 10^{-4} was selected as the termination criteria. Ran single threaded on a 3.60GHz Intel Xeon E3-1270 v5 processor with 32GB in Ubuntu 16.04LTS and Julia v1.0. Ipopt v3.12 [11] was used to solve the NLP upper bound problem.
  - Linear lower-problem solved using CPLEX 12.8.0 [10].
  - Quadratic lower-problem solved using Ipopt v3.12.
  - Smooth NLP lower-problem solved using Ipopt v3.12.

10 IBM ILOG CPLEX Optimizer, 2017

11 Wächter, A. et al. Mathematical Programming, 2006, 106(1), 25-57

Numerical Results

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Problem	Variables	Inequalities	Equalities	CPU[s] (Affine)	CPU[s] (Affine + QBT)	CPU[s] (Quadratic)	CPU[s] (Convex NLP)
ex4_1_7	1	0	0	1.0	0.7	0.6	3.5
ex6_2_10	6	0	3	95.2	54.3	81.3	253.2
growthls	3	0	0	5.1	1.2	1.01	15.2
filter	2	0	1	0.6	0.5	2.9	3.1
hydro	30	0	25	0.9	0.4	3.2	6.4
hs62	3	0	1	4.5	4.1	4.7	16.1
st_ph1	6	5	0	0.1	0.1	1.2	2.3
tre	2	0	0	0.15	0.09	0.45	4.4
kinetic[5]	3	0	0	95.1%	96.1%	95.5%	89.2%
heat[5]	1	0	0	1.2	1.01	1.01	15.2
CS I [12]	2	0	9	0.7	0.6	1.6	8.6
CS II [12]	5	12	1	60.7	42.1	28.6	90.4
CS III [12]	8	1	22	71.8%	78.6%	81.3%	51.2%

5 Mitsos, A. et al. SIAM Journal of Optimization, 2009, 20, 573-601

12 Bongartz, D. et al. Journal of Global Optimization, 2017, 20, 761-796

Numerical Results - Trends

- For simulations with an extremely large number of intermediate terms, the m-convexity of the objective and constraints tends to vanish (kinetic/heat) models. M-convexity based bound tighten yields a small improvement in solution times in these cases.

- For smaller problems, with a significant number of quadratic constraints the NLP-subproblem form provides faster solution times.

- For mid-range problems, and simulations with constraints arising from simple intermediate terms the M-convexity problem formulation provides fast solution times.

Conclusions

- We can construct tighter than linear relaxations by propagating strong convexity information.
- Tighter than linear relaxations inherit second-order convergence properties from the McCormick relaxation.
- In general, relaxations that minimize the number of simulation evaluations tend to reduce computational burden for McCormick operator-based optimization.

Future Work

- **Evaluate full incorporation into global algorithms**
  - Develop the notion of numerically safe inequalities
  - Evaluate rules for selecting between nonlinear, quadratic and linear outer-estimators
- **Further theoretical developments**
  - Multiplication operator that propagates m-convexity.
  - Composition operator that propagates m-convexity generally.
  - Explore second-order nonsmooth methods for generating quadratic underestimators.

Acknowledgements

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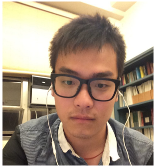
Prof. Matthew Stuber



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Questions?