A Nonsmooth Approach for Generating Convex Relaxations of Dynamic Systems

Yingkai Song and Kamil A. Khan
Department of Chemical Engineering, McMaster University, Hamilton, ON, Canada

Summary. We propose a new approach for generating convex and concave relaxations for the solutions of parametric ordinary differential equations (ODEs), for use in global dynamic optimization and reachability analysis. These relaxations are described as the solutions of an auxiliary nonsmooth ODE system with embedded convex optimization problems. The resulting relaxations are indeed valid relaxations, are convex, and converge rapidly to the original system as the parametric subdomain shrinks. The new approach is compatible with any relaxations for the original right-hand side, and tighter such relaxations will necessarily translate into tighter relaxations for state variables. Especially, if generalized McCormick relaxations are used, the new approach is guaranteed to yield tighter relaxations than a state-of-the-art ODE relaxation approach [1], and thus may reduce the number of iterations for overarching global dynamic optimization. Further implications and examples are discussed.

Background and Motivation

Global dynamic optimization is useful in a wide variety of engineering applications such as parameter estimation, global optimal control, and optimization-based worst-case uncertainty analysis. Compared with stochastic methods for global optimization, deterministic global optimization methods have the advantage that a globally optimal solution is guaranteed to be found within a predefined tolerance in finite computation time. However, current deterministic global dynamic optimization methods based on branch-and-bound [2] can only solve problems of modest size. Thus, improved techniques are sought to extend these methods to problems of practical interest.

One computational bottleneck for global dynamic optimization is generating convex and concave relaxations for state variables with respect to decision variables, termed *state relaxations* [1]. These relaxations are useful for computing lower bounds for the global optimal objective value, which are required in deterministic global optimization algorithms. Moreover, state relaxations could also help construct convex enclosures for the reachable set which is useful in applications involving reachability analysis such as fault detection and robust optimal control. Hence, there is a need in global dynamic optimization to develop efficient and accurate computational tools for generating state relaxations automatically.

State relaxations should have desirable convergence and tightness properties. The relaxations supplied to a branch-and-bound global optimization method must converge rapidly to the underlying model as the decision space is subdivided or else the overall global optimization method will be impeded by cluster effects, in which the method will branch many times on intervals that either contain or are near a global minimum [3]. This notion of rapid convergence has been formalized as *second-order pointwise convergence* [4]. Tighter state relaxations could construct tighter lower bounds for the global optimal objective value, and thus may reduce the overall computational time by reducing the number of required iterations. In reachability analysis, tighter enclosures of the reachable set could reduce the sets' conservatism, which could lead to earlier detection of faults or less conservative control inputs.

New Relaxation Approach

Consider a parametric ODE system of the form

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

where $\mathbf{x}$ denotes dependent state variables and $\mathbf{p}$ denotes system parameters.

We propose a new approach for constructing state relaxations $\mathbf{x}^{cv}(t,\mathbf{p})$ and $\mathbf{x}^{cc}(t,\mathbf{p})$ for states $\mathbf{x}(t,\mathbf{p})$ with respect to $\mathbf{p}$. These relaxations are described as the solutions of an auxiliary ODE system whose right-hand side comprises convex optimization problems with embedded relaxations for $\mathbf{f}$. The auxiliary system is nonsmooth because of the nonsmooth nature of optimal-valued functions. The advantages of this approach are presented as follows. First, if the relaxations for $\mathbf{f}$ have second-order pointwise convergence, then the resulting state relaxations inherit this desirable convergence property which could help avoid cluster effects. Secondly, the new approach is compatible with various relaxations for $\mathbf{f}$, such as αBB relaxations [5] and generalized McCormick relaxations [6], while previously established approaches are typically limited by one particular type of relaxations. Thirdly, tighter relaxations for $\mathbf{f}$ necessarily translate into tighter state relaxations. Thus, it is worthwhile from a dynamic optimization or reachability analysis standpoint to seek tighter relaxation methods for closed-form functions since doing so necessarily translates into superior descriptions of reachable sets for dynamic systems. Especially, if the generalized McCormick relaxations are employed, the new approach necessarily yields tighter state relaxations than a state-of-the-art ODE relaxation approach by Scott and Barton [1], and thus may reduce the number of required iterations for overarching global dynamic optimization.

Proof-of-concept Implementation

Two numerical examples are presented to illustrate the convergence and tightness properties of the new state relaxations. The examples are implemented in MATLAB, using the ODE solver `ode15s` and the local optimization solver `fmincon`.

Example 1
Consider the following parametric ODE system:

$$\dot{x}(t,p) = p(x^2-1), \quad x(0,p) \quad = -2,$$

with $t_f = 0.15$ and $-1 \le p \le 1$. State relaxations are constructed by the new approach using αBB relaxations of the right-hand side function. Figure 1 shows that the resulting relaxations have second-order pointwise convergence, where X^C denotes the enclosure formed by state relaxations, and P denotes the parametric subdomain.

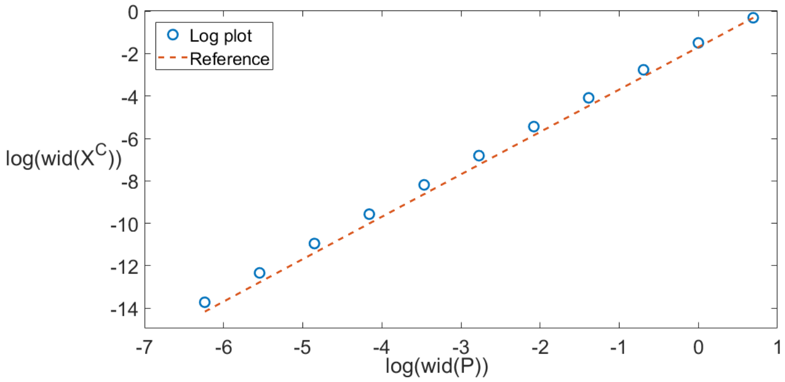

Figure 1: A log-log plot of width of the enclosure formed by state relaxations at $t := t_f$ versus width of the parameter's domain (*circles*) and a reference line with a slope of 2 (*dashed*).

Example 2
The following example is modified from a bioreaction model in [7] by adding more nonlinearities:

$$\begin{aligned} \dot{x}_1(t,p) &= \left(\frac{1.2x_2}{px_2^2+x_2+7.1} - 0.18\right)x_1, & x_1(0,p) &= 0.82, \\ \dot{x}_2(t,p) &= 0.36(5.7-x_2) - \frac{12.636x_2x_1}{px_2^2+x_2+7.1} + \frac{1}{x_1} - x_2^2 + x_1^2x_2, & x_2(0,p) &= 0.8, \end{aligned}$$

with $t_f = 15$ and $0.4 \le p \le 0.6$. State relaxations are constructed by the new approach using generalized McCormick relaxations and by the approach of Scott and Barton [1]. Figure 2 shows that the new state relaxations are tighter than Scott–Barton relaxations for this example.

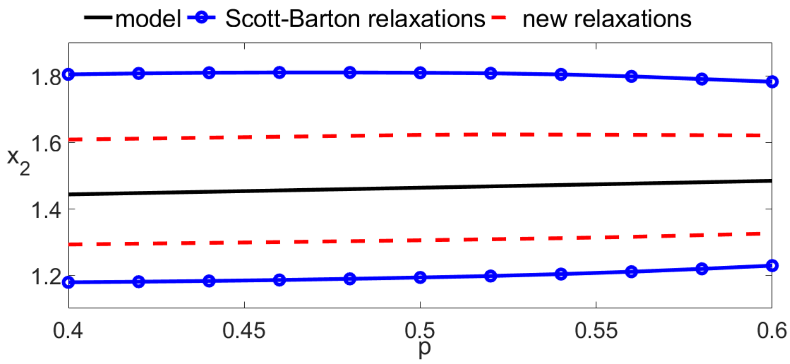

Figure 2: The final state $x_2(t_f, p)$ vs. p (*black-solid*), along with corresponding Scott–Barton relaxations (*blue-circled*) and new relaxations (*red-dashed*), plotted as functions of p at $t := t_f$.

References

[1] Scott J. K., Barton P. I. (2013) Improved relaxations for the parametric solutions of ODEs using differential inequalities. *J. Glob. Optim.* **57**(1): 143-176.

[2] Falk J. E., Soland R. M. (1969) An algorithm for separable nonconvex programming problems. *Manage. Sci.* **15**(9): 550-569.

[3] Wechsung A., Schaber S. D., Barton, P. I. (2014) The cluster problem revisited. *J. Glob. Optim.* **58**(3): 429-438.

[4] Bompadre A., Mitsos, A. (2012) Convergence rate of McCormick relaxations. *J. Glob. Optim.* **52**(1): 1-28.

[5] Adjiman C., Dallwig S., Floudas C., Neumaier A. (1998) A global optimization method αBB, for general twice-differentiable constrained NLPs: I. Theoretical Advances. *Comput. Chem. Eng.* **22**(9): 1137-1158.

[6] Scott J. K., Stuber M. D., Barton P. I. (2011) Generalized McCormick relaxations. *J. Glob. Optim.* **51**(4): 569-606.

[7] Bastin G., Dochain D. (1991) On-line Estimation and Adaptive Control of Bioreactors. Elsevier, Amsterdam.