Deterministic Global Optimization for Dynamic Systems Using Interval Analysis

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Outline

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Background

- Many practically important physical systems are modeled by ODE systems.
- Optimization problems involving these models may be stated as

$$
\begin{aligned}
\min_{\boldsymbol{\theta}, \boldsymbol{x}_\mu} \quad & \phi\left[\boldsymbol{x}_\mu(\boldsymbol{\theta}), \boldsymbol{\theta};\ \mu = 0, 1, \ldots, r\right] \\
\text{s.}t. \quad & \dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta}) \\
& \boldsymbol{x}_0 = \boldsymbol{x}_0(\boldsymbol{\theta}) \\
& \boldsymbol{x}_\mu(\boldsymbol{\theta}) = \boldsymbol{x}(t_\mu, \boldsymbol{\theta}) \\
& t \in [t_0, t_r] \\
& \boldsymbol{\theta} \in \boldsymbol{\Theta}
\end{aligned}
$$

- Sequential approach: Eliminate $\boldsymbol{x}_\mu$ using parametric ODE solver, obtaining an unconstrained problem in $\boldsymbol{\theta}$
- May be multiple local solutions – need for global optimization

Deterministic Global Optimization of Dynamic Systems

Much recent interest, mostly combining branch-and-bound and relaxation techniques, e.g.,

- Esposito and Floudas (2000): α-BB approach
  - Rigorous values of α not used: no theoretical guarantees
- Chachuat and Latifi (2003): Theoretical guarantee of ϵ-global optimality
- Papamichail and Adjiman (2002, 2004): Theoretical guarantee of ϵ-global optimality
- Singer and Barton (2006): Theoretical guarantee of ϵ-global optimality
  - Use convex underestimators and concave overestimators to construct two bounding IVPs, which are then solved to obtain lower and upper bounds on the state trajectories.
  - Bounding IVPs are not solved rigorously, so state bounds are not computationally guaranteed.

Deterministic Global Optimization of Dynamic Systems

Our approach: Branch-and-reduce algorithm based on interval analysis and using Taylor models

- Basic ideas
  - Use local optimizations to obtain an upper bound $\widehat{\phi}$ on the global minimum
  - Compute Taylor models of the state variables using a new validated solver for parametric ODEs (VSPODE) (Lin and Stadtherr, 2006)
  - Compute the Taylor model T_ϕ of the objective function
  - Perform constraint propagation procedure using $T_\phi \leq \widehat{\phi}$, to reduce the parameter (decision variable) space $\mathbf{\Theta}$
  - Use branch-and-bound
- Can implement to obtain either an ϵ-global minimum, or (using interval Newton approach) the exact ($\epsilon = 0$) global minimum

Interval Analysis

- A real interval $X = [a, b] = \{x \in \Re \mid a \leq x \leq b\}$ is a segment on the real number line.

- An interval vector $\boldsymbol{X} = (X_1, X_2, ..., X_n)^T$ is an n-dimensional rectangle.

- Basic interval arithmetic for $X = [a, b]$ and $Y = [c, d]$ is

$$X \text{ op } Y = \{x \text{ op } y \mid x \in X,\ y \in Y\}$$

- Interval elementary functions (e.g., $\exp(X)$, $\sin(X)$) are also available.

- The *interval extension* $F(\boldsymbol{X})$ encloses all values of $f(\boldsymbol{x})$ for $\boldsymbol{x} \in \boldsymbol{X}$; that is, $\{f(\boldsymbol{x}) \mid \boldsymbol{x} \in \boldsymbol{X}\} \subseteq F(\boldsymbol{X})$

- Interval extensions computed using interval arithmetic may lead to overestimation of function range (the interval “dependency” problem).

Taylor Models

- Taylor Model $T_f = (p_f, R_f)$: Bounds a function $f(\boldsymbol{x})$ over $\boldsymbol{X}$ using a q-th order Taylor polynomial p_f and an interval remainder bound R_f.
- Could obtain T_f using a truncated Taylor series:

$$p_f = \sum_{i=0}^{q} \frac{1}{i!} \left[(\boldsymbol{x} - \boldsymbol{x}_0) \cdot \triangledown \right]^i f(\boldsymbol{x}_0)$$

$$R_f = \frac{1}{(q+1)!} \left[(\boldsymbol{x} - \boldsymbol{x}_0) \cdot \triangledown \right]^{q+1} F\left[\boldsymbol{x}_0 + (\boldsymbol{x} - \boldsymbol{x}_0)\zeta \right]$$

where,

$$\boldsymbol{x}_0 \in \boldsymbol{X}; \quad \zeta \in [0, 1]$$

$$[\boldsymbol{g} \cdot \triangledown]^k = \sum_{\substack{j_1 + \cdots + j_m = k \\ 0 \le j_1, \cdots, j_m \le k}} \frac{k!}{j_1! \cdots j_m!} g_1^{j_1} \cdots g_m^{j_m} \frac{\partial^k}{\partial x_1^{j_1} \cdots \partial x_m^{j_m}}$$

- Can also compute Taylor models by using Taylor model operations (Makino and Berz, 1996)

Taylor Model Operations

- Let T_f and T_g be the Taylor models of the functions $f(x)$ and $g(x)$, respectively, over the interval $x \in X$.
- Addition: $T_{f \pm g} = (p_{f \pm g}, R_{f \pm g}) = (p_f \pm p_g, R_f \pm R_g)$
- Multiplication: $T_{f \times g} = (p_{f \times g}, R_{f \times g})$ with $p_{f \times g} = p_f \times p_g - p_e$ and $R_{f \times g} = B(p_e) + B(p_f) \times R_g + B(p_g) \times R_f + R_f \times R_g$
- $B(p)$ indicates an interval bound on the function p.
- Reciprocal operation and intrinsic functions can also be defined.
- Store and operate on coefficients of p_f only. Floating point errors are accumulated in R_f.
- Beginning with Taylor models of simple functions, Taylor models of very complicated functions can be computed.
- Compared to other rigorous bounding methods (e.g., interval arithmetic), Taylor models often yield sharper bounds for modest to complicated functional dependencies (Makino and Berz, 1999).

Taylor Models – Range Bounding

- Exact range bounding of the interval polynomials – NP hard
- Direct evaluation of the interval polynomials – overestimation
- Focus on bounding the dominant part (1st and 2nd order terms)
- Exact range bounding of a general interval quadratic – also worst-case exponential complexity
- A compromise approach – Exact bounding of 1st order and diagonal 2nd order terms

$$B(p) = \sum_{i=1}^{m} \left[a_i \left(X_i - x_{i0} \right)^2 + b_i (X_i - x_{i0}) \right] + S$$

$$= \sum_{i=1}^{m} \left[a_i \left(X_i - x_{i0} + \frac{b_i}{2a_i} \right)^2 - \frac{b_i^2}{4a_i} \right] + S,$$

where S is the interval bound of other terms by direct evaluation

Taylor Models – Constraint Propagation

- Consider constraint $c(\boldsymbol{x}) \leq 0$, $\boldsymbol{x} \in \boldsymbol{X}$. Goal – Eliminate parts of $\boldsymbol{X}$ in which constraint cannot be satisfied
- For each $i = 1, 2 \cdots, m$, shrink X_i using:

$$B(T_c) = B(p_c) + R_c = a_i \left(X_i - x_{i0} + \frac{b_i}{2a_i} \right)^2 - \frac{b_i^2}{4a_i} + S_i \leq 0$$

$$\Longrightarrow \quad a_i U_i^2 \leq V_i, \quad \text{with } U_i = X_i - x_{i0} + \frac{b_i}{2a_i} \text{ and } V_i = \frac{b_i^2}{4a_i} - S_i$$

$$\Longrightarrow \quad U_i = \begin{cases} \emptyset & \text{if } a_i > 0 \text{ and } \overline{V_i} < 0 \\ \left[-\sqrt{\frac{\overline{V_i}}{a_i}}, \sqrt{\frac{\overline{V_i}}{a_i}} \right] & \text{if } a_i > 0 \text{ and } \overline{V_i} \geq 0 \\ [-\infty, \infty] & \text{if } a_i < 0 \text{ and } \overline{V_i} \geq 0 \\ \left[-\infty, -\sqrt{\frac{\overline{V_i}}{a_i}} \right] \cup \left[\sqrt{\frac{\overline{V_i}}{a_i}}, \infty \right] & \text{if } a_i < 0 \text{ and } \overline{V_i} < 0 \end{cases}$$

$$\Longrightarrow \quad X_i = X_i \cap \left(U_i + x_{i0} - \frac{b_i}{2a_i} \right)$$

Validated Solution of Parametric ODE Systems

- Consider the parametric ODE system

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta})$$

$$\boldsymbol{x}(t_0) = \boldsymbol{x}_0 \in \boldsymbol{X}_0$$

$$\boldsymbol{\theta} \in \boldsymbol{\Theta}$$

- Validated methods:
  - Guarantee there exists a unique solution $\boldsymbol{x}(t)$ in $[t_0, t_f]$, for each $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ and $\boldsymbol{x}_0 \in \boldsymbol{X}_0$
  - Compute an interval $\boldsymbol{X}_j$ that encloses all solutions of the ODE system at t_j for $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ and $\boldsymbol{x}_0 \in \boldsymbol{X}_0$
- Tools are available – VNODE, COSY VI, AWA, etc.
  - May need to treat parameters as additional state variables with zero derivative
- New tool – VSPODE (Lin and Stadtherr, 2006): Deals directly with interval-valued parameters (and also interval-valued initial states)

New Method for Parametric ODEs

- Use interval Taylor series to represent dependence on time. Use Taylor models to represent dependence on uncertain quantities (parameters and initial states).
- Assuming $\boldsymbol{X}_j$ is known, then
  - Phase 1: Same as “standard” approach (e.g., VNODE). Compute a coarse enclosure $\tilde{\boldsymbol{X}}_j$ and prove existence and uniqueness. Use fixed point iteration with Picard operator using high-order interval Taylor series.
  - Phase 2: Refine the coarse enclosure to obtain $\boldsymbol{X}_{j+1}$. Use Taylor models in terms of the uncertain parameters and initial states.
- Implemented in VSPODE (Validating Solver for Parametric ODEs) (Lin and Stadtherr, 2006).

Method for Phase 2

- Represent uncertain initial states and parameters using Taylor models $\boldsymbol{T}_{\boldsymbol{x}_0}$ and $\boldsymbol{T}_{\boldsymbol{\theta}}$, with components

$$T_{x_{i0}} = (m(X_{i0}) + (x_{i0} - m(X_{i0})), [0,0]), \quad i = 1, \cdots, m$$

$$T_{\theta_i} = (m(\Theta_i) + (\theta_i - m(\Theta_i)), [0,0]), \quad i = 1, \cdots, p.$$

- Bound the interval Taylor series coefficients $\boldsymbol{f}^{[i]}$ by computing Taylor models $\boldsymbol{T}_{\boldsymbol{f}^{[i]}}$.
  - Use mean value theorem.
  - Evaluate using Taylor model operations.
- Reduce "wrapping effect" by using a new type of Taylor model involving a parallelpiped remainder bound.
- This results in a Taylor model $\boldsymbol{T}_{\boldsymbol{x}_{j+1}}$ in terms of the initial states $\boldsymbol{x}_0$ and parameters $\boldsymbol{\theta}$.
- Compute the enclosure $\boldsymbol{X}_{j+1} = B(\boldsymbol{T}_{\boldsymbol{x}_{j+1}})$ by bounding over $\boldsymbol{X}_0$ and $\boldsymbol{\Theta}$.

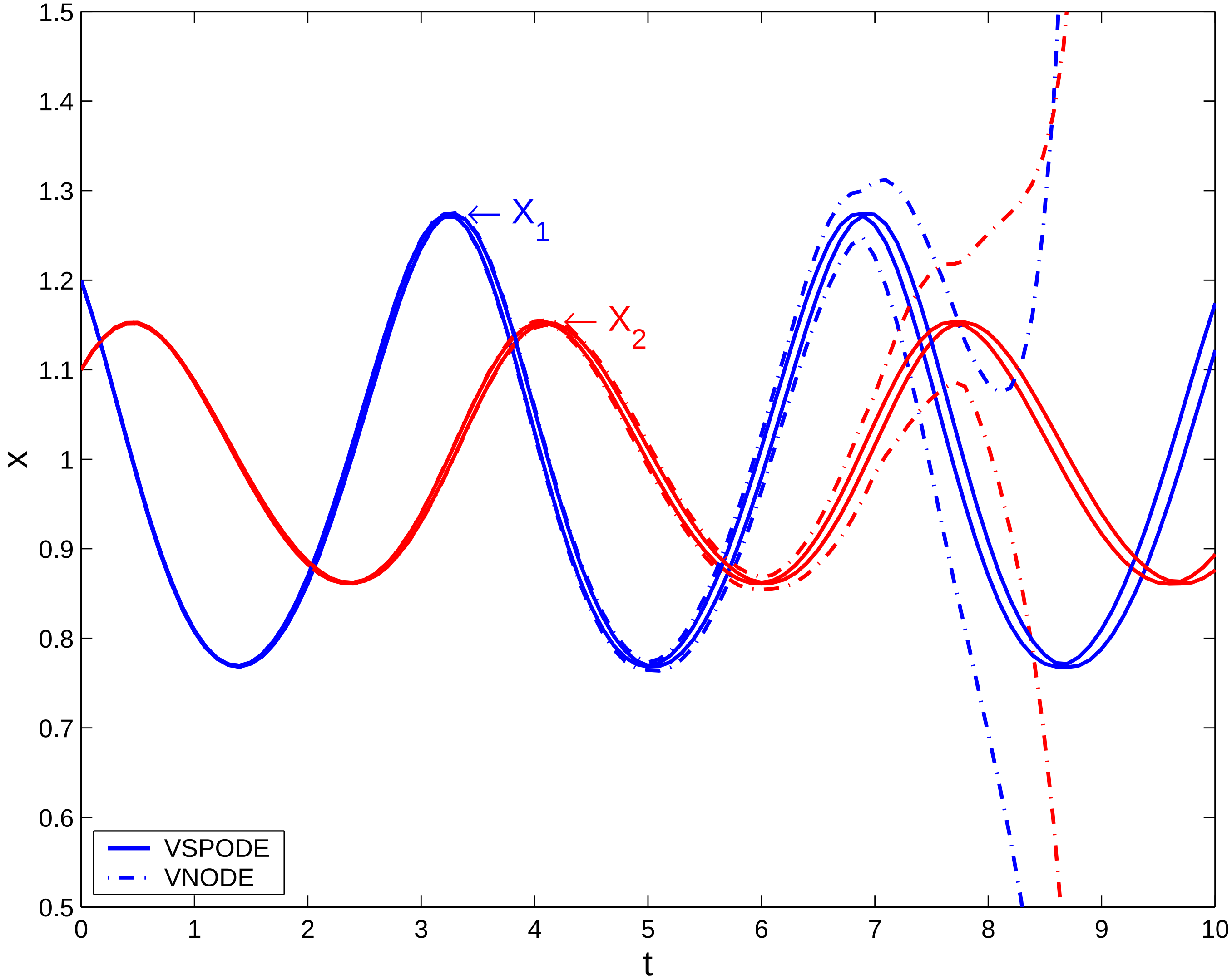
VSPODE Example

- Lotka-Volterra Problem

$$\dot{x}_1 = \theta_1 x_1 (1 - x_2)$$
$$\dot{x}_2 = \theta_2 x_2 (x_1 - 1)$$
$$\boldsymbol{x}_0 = (1.2, 1.1)^{\mathrm{T}}$$
$$\theta_1 \in [2.99, 3.01]$$
$$\theta_2 \in [0.99, 1.01]$$

- Integrate from $t_0 = 0$ to $t_N = 10$.
- VSPODE run using $q = 5$ (order of Taylor model), $k = 17$ (order of interval Taylor series) and QR for wrapping.
- For comparison, VNODE was used, with interval parameters treated as additional state variables, and run using $k = 17$ order interval Hermite-Obreschkoff and QR for wrapping.
- Constant step size of $h = 0.1$ used in both VSPODE and VNODE (step size may be reduced if necessary in Phase 1).

Lotka-Volterra Problem



(Eventual breakdown of VSPODE at $t = 31.8$)

Summary of Global Optimization Algorithm

Beginning with initial parameter interval $\mathbf{\Theta}^{(0)}$

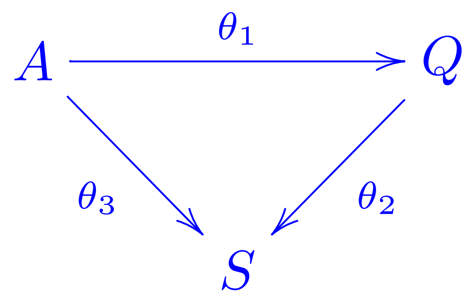
- Establish $\widehat{\phi}$, the upper bound on global minimum using p^2 local minimizations, where p is the number of parameters (decision variables)
- Iterate: for subinterval $\mathbf{\Theta}^{(k)}$
  1. Compute Taylor models of the states using VSPODE, and then obtain T_ϕ
  2. Perform constraint propagation using $T_\phi \leq \widehat{\phi}$ to reduce $\mathbf{\Theta}^{(k)}$
  3. If $\mathbf{\Theta}^{(k)} = \emptyset$, go to next subinterval
  4. If $(\widehat{\phi} - \underline{B(T_\phi)})/|\widehat{\phi}| \leq \epsilon^{\mathrm{rel}}$, or $\widehat{\phi} - \underline{B(T_\phi)} \leq \epsilon^{\mathrm{abs}}$, discard $\mathbf{\Theta}^{(k)}$ and go to next subinterval
  5. If $\overline{B(T_\phi)} < \widehat{\phi}$, update $\widehat{\phi}$ with local minimization, go to step 2
  6. If $\mathbf{\Theta}^{(k)}$ is sufficiently reduced, go to step 1
  7. Otherwise, bisect $\mathbf{\Theta}^{(k)}$ and go to next subinterval
- This finds an ϵ-global optimum with either a relative tolerance (ϵ^{rel}) or absolute tolerance (ϵ^{abs})

Global Optimization Algorithm (cont'd)

- By incorporating an interval-Newton approach, this can also be implemented as an exact algorithm ($\epsilon = 0$).
- This requires the validated integration of the first- and second-order sensitivity equations. VSPODE was used.
- Interval-Newton steps are applied only after reaching an appropriate depth in the branch-and-bound tree
- We have implemented the exact algorithm only for the case of parameter estimation problems with least squares objective
- The exact algorithm may require more or less computation time than the ϵ-global algorithm

Computational Studies – Example 1

- Parameter estimation – Catalytic cracking of gas oil (Tjoa and Biegler 1991)



- The problem is:

$$\min_{\boldsymbol{\theta}} \phi \quad = \quad \sum_{\mu=1}^{20} \sum_{i=1}^{2} \left(\widehat{x}_{\mu,i} - x_{\mu,i}\right)^2$$

$$\begin{aligned} \text{s.}t. \qquad \dot{x}_1 &= -(\theta_1 + \theta_3) x_1^2 \\ \dot{x}_2 &= \theta_1 x_1^2 - \theta_2 x_2 \\ \boldsymbol{x}_0 &= (1,0)^{\mathrm{T}}; \qquad \boldsymbol{x}_\mu = \boldsymbol{x}(t_\mu) \\ \boldsymbol{\theta} &\in [0,20] \times [0,20] \times [0,20] \end{aligned}$$

where $\widehat{\boldsymbol{x}}_\mu$ is given (experimental data).

Example 1 (Cont'd)

- Solution: $\boldsymbol{\theta}^* = (12.2139, 7.9798, 2.2217)^{\mathrm{T}}$ and $\phi^* = 2.6557 \times 10^{-3}$
- Comparisons:

Method	CPU time (s)	
	Reported	Adjusted*
This work (exact global optimum: $\epsilon = 0$) (Intel P4 3.2GHz)	11.5	11.5
This work ($\epsilon^{\mathrm{rel}} = 10^{-3}$) (Intel P4 3.2GHz)	14.3	14.3
Papamichail and Adjiman (2002) ($\epsilon^{\mathrm{rel}} = 10^{-3}$) (SUN UltraSPARC-II 360MHz)	35478	4541
Chachuat and Latifi (2003) ($\epsilon^{\mathrm{rel}} = 10^{-3}$) (Machine not reported)	10400	—
Singer and Barton (2006) ($\epsilon^{\mathrm{abs}} = 10^{-3}$) (AMD Athlon 2000XP+ 1.667GHz)	5.78	2.89

*Adjusted = Approximate CPU time after adjustment for machine used (based on SPEC benchmark)

Computational Studies – Example 2

- Singular control problem (Luus, 1990)
- The original problem is stated as:

$$\begin{aligned}
\min_{\theta(t)} \phi \quad &= \int_{t_0}^{t_f} \left[x_1^2 + x_2^2 + 0.0005(x_2 + 16t - 8 - 0.1x_3\theta^2)^2 dt\right] \\
s.t. \quad \dot{x}_1 &= x_2 \\
\dot{x}_2 &= -x_3\theta + 16t - 8 \\
\dot{x}_3 &= \theta \\
\boldsymbol{x}_0 &= (0, -1, -\sqrt{5})^{\mathrm{T}} \\
t &\in [t_0, t_f] = [0, 1] \\
\theta &\in [-4, 10]
\end{aligned}$$

- $\theta(t)$ is parameterized as a piecewise constant control profile with n pieces (equal time intervals)

Example 2 (Cont'd)

- Reformulate problem to be autonomous, and introduce quadrature variable:

$$
\begin{aligned}
\min_{\theta(t)} \phi \quad &= \quad x_5(t_f) \\
s.t. \quad \dot{x}_1 \quad &= x_2 \\
\dot{x}_2 \quad &= -x_3\theta + 16x_4 - 8 \\
\dot{x}_3 \quad &= \theta \\
\dot{x}_4 \quad &= 1 \\
\dot{x}_5 \quad &= x_1^2 + x_2^2 + 0.0005(x_2 + 16x_4 - 8 - 0.1x_3\theta^2)^2 \\
\boldsymbol{x}_0 \quad &= (0, -1, -\sqrt{5}, 0, 0)^{\mathrm{T}} \\
t \quad &\in [t_0, t_f] = [0, 1] \\
\theta \quad &\in [-4, 10]
\end{aligned}
$$

- Do ϵ-global optimization with $\epsilon^{\mathrm{abs}} = 10^{-3}$

Example 2 (Cont'd)

			CPU time (s)	
n	ϕ^*	$\boldsymbol{\theta}^*$	This work	Singer and Barton (2006)*
1	0.4965	(4.071)	0.02	0.9
2	0.2771	(5.575, -4.000)	0.32	11.3
3	0.1475	(8.001, -1.944, 6.042)	10.88	270.3
4	0.1237	(9.789, -1.200, 1.257, 6.256)	369.0	—
5	0.1236	(10.00, 1.494, -0.814, 3.354, 6.151)	8580.6	—

* Approximate CPU time after adjustment for machine used

Computational Studies – Example 3

- Oil shale pyrolysis problem (Luus, 1990)
- The original problem is stated as:

$$
\begin{aligned}
\min_{\theta(t)} \quad & \phi && = -x_2(t_f) \\
s.t. \quad & \dot{x}_1 && = -k_1 x_1 - (k_3 + k_4 + k_5) x_1 x_2 \\
& \dot{x}_2 && = k_1 x_1 - k_2 x_2 + k_3 x_1 x_2 \\
& k_i && = a_i \exp\left(\frac{-b_i/R}{\theta}\right), i = 1, \ldots, 5 \\
& \boldsymbol{x}_0 && = (1, 0)^{\mathrm{T}} \\
& t && \in [t_0, t_f] = [0, 10] \\
& \theta && \in [698.15, 748.15].
\end{aligned}
$$

- $\theta(t)$ is paramaterized as a piecewise constant control profile with n pieces (equal time intervals)

Example 3 (Cont'd)

- Transformation of control variable

$$\bar{\theta} = \frac{698.15}{\theta}$$

- The reformulated problem is stated as:

$$\begin{aligned}
\min_{\bar{\theta}(t)} \quad & \phi && = -x_2(t_f) \\
s.t. \quad & \dot{x}_1 && = -k_1 x_1 - (k_3 + k_4 + k_5) x_1 x_2 \\
& \dot{x}_2 && = k_1 x_1 - k_2 x_2 + k_3 x_1 x_2 \\
& k_i && = a_i \exp\left(-\bar{\theta} b_i / R\right), i = 1, \cdots, 5 \\
& \boldsymbol{x}_0 && = (1, 0)^{\mathrm{T}} \\
& t && \in [t_0, t_f] = [0, 10] \\
& \bar{\theta} && \in [698.15/748.15,\ 1].
\end{aligned}$$

- Do ϵ-global optimization with $\epsilon^{\text{abs}} = 10^{-3}$

Example 3 (Cont'd)

			CPU time (s)	
n	ϕ^*	$\bar{\boldsymbol{\theta}}^*$	This work	Singer and Barton (2006)*
1	-0.3479	(0.984)	3.2	13.1
2	-0.3510	(0.970, 1.000)	26.8	798.7
3	-0.3517	(1.000, 0.963, 1.000)	251.6	-
4	-0.3523	(1.000, 0.955, 1.000, 1.000)	2443.5	-

* Approximate CPU time after adjustment for machine used

Concluding Remarks

- An approach has been described for deterministic global optimization of dynamic systems using interval analysis and Taylor models
  - A validated solver for parametric ODEs is used to construct bounds on the states of dynamic systems
  - An efficient constraint propagation procedure is used to reduce the incompatible parameter domain
- Can be combined with the interval-Newton method (Lin and Stadtherr, 2006)
  - True global optimum instead of ϵ-convergence
  - May or may not reduce CPU time required

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