Global Optimization for Parameter Estimation of Dynamic Systems

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Outline

- Background
- Interval Analysis
- Taylor Models
- Validated Solutions for Parametric ODEs
- Algorithm Summary
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Background

- Parameter estimation is a key step in development of mathematical models
- Models of interest may be ODEs/DAEs
- Minimization of a weighted squared error

$$\min_{\boldsymbol{\theta}, \boldsymbol{z}_\mu} \phi = \sum_{m \in M} \sum_{\mu=1}^{r} (z_{\mu,m} - \bar{z}_{\mu,m})^2$$

$$\text{s.}t. \quad \dot{\boldsymbol{z}} = \boldsymbol{f}(\boldsymbol{z}, \boldsymbol{\theta}, t), \quad \boldsymbol{z}(t_0) = \boldsymbol{z}_0$$

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

$$\boldsymbol{z}_\mu = \boldsymbol{z}(t_\mu), \quad t_\mu \in [t_0, t_f]$$

- Sequential approach – eliminate $\boldsymbol{z}_\mu$ using parametric ODE solver
- Multiple local solutions – a need for global optimization

Deterministic Global Optimization with Dynamic Systems

- Much recent interest, e.g.
  - Esposito and Floudas (2000)
  - Chachuat and Latifi (2003)
  - Papamichail and Adjiman (2002, 2004)
  - Singer and Barton (2004)
- New approach: branch and reduce algorithm based on interval analysis
  - Construct Taylor models of the states using a new validated solver for parametric ODEs (VSPODE) (Lin and Stadtherr, 2005)
  - Compute the Taylor model T_ϕ of the objective function
  - Perform constraint propagation procedure using $T_\phi \leq \hat{\phi}$, to reduce the parameter domain

Interval Analysis

- A real interval

$$X = [\underline{X}, \overline{X}] = \{x \in \Re \mid \underline{X} \leq x \leq \overline{X}\}$$

- A real interval vector – a box

$$\boldsymbol{X} = (X_1, X_2, \cdots, X_n)^T$$

- Interval arithmetic – basic operations and elementary functions
- An interval extension of a function $f(\boldsymbol{x})$ over $\boldsymbol{X}$

$$F(\boldsymbol{X}) \supseteq \{f(\boldsymbol{x}) \mid \boldsymbol{x} \in \boldsymbol{X}\}$$

- Natural interval extension – leads to overestimation (dependence problem)

Taylor Models

- Taylor Model T_f – an interval extension of a function over $\boldsymbol{X}$

$$T_f = (p_f, R_f)$$

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

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

where,

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

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

- p_f is a polynomial function; store and operate on its coefficients only

Taylor Models - Remainder Differential Algebra (RDA)

- Basic operations

$$T_{f\pm g} = (p_f, R_f) \pm (p_g, R_g) = (p_f \pm p_g, R_f \pm R_g)$$

$$\begin{aligned} T_{f\times g} &= (p_f, R_f) \times (p_g, R_g) \\ &= p_f \times p_g + p_f \times R_g + p_g \times R_f + R_f \times R_g \\ &= (p_{f\times g}, R_{f\times g}) \end{aligned}$$

where,

$$p_{f\times g} = p_f \times p_g - p_e$$

$$R_{f\times g} = B(p_e) + B(p_f) \times R_g + B(p_g) \times R_f + R_f \times R_g$$

- $B(p)$ indicates an interval bound on the function p.
- Reciprocal operation and intrinsic functions can also be defined.
- It is possible to compute Taylor models of complex functions.

Taylor Models - Range Bounding

- Exact range bounding of the interval polynomials – NP hard
- Direct evaluation of the interval polynomials – inefficient
- Focus on bounding the dominant part (1st and 2nd order terms)
- Exact range bounding of a general interval quadratic - computationally expensive
- A compromise approach – 1st order and diagonal elements of 2nd order

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

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

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

Taylor Models - Constraint Propagation

- Goal – to reduce part of domain not satisfying $c(\boldsymbol{x}) \leq 0$
- For some $i = 1, 2 \cdots, m$

$$
\begin{aligned}
B(T_c) &= B(p_c) + R_c = a_i \left(X_i - x_{i0} + \frac{b_i}{2a_i} \right)^2 - \frac{b_i^2}{4a_i} + S_i \leq 0 \\
\Longrightarrow \quad & a_i U_i^2 \leq V_i, \quad \text{with } U_i = X_i - x_{i0} + \frac{b_i}{2a_i} \text{ and } V_i = \frac{b_i^2}{4a_i} - S_i \\
\Longrightarrow \quad & U_i = \begin{cases} \emptyset & \text{if } a_i > 0 \text{ and } \overline{V_i} < 0 \\ \left[-\sqrt{\frac{\overline{V_i}}{a_i}}, \sqrt{\frac{\overline{V_i}}{a_i}} \right] & \text{if } a_i > 0 \text{ and } \overline{V_i} \geq 0 \\ [-\infty, \infty] & \text{if } a_i < 0 \text{ and } \overline{V_i} \geq 0 \\ \left[-\infty, -\sqrt{\frac{\overline{V_i}}{a_i}} \right] \cup \left[\sqrt{\frac{\overline{V_i}}{a_i}}, \infty \right] & \text{if } a_i < 0 \text{ and } \overline{V_i} < 0 \end{cases} \\
\Longrightarrow \quad & X_i = X_i \cap \left(U_i + x_{i0} - \frac{b_i}{2a_i} \right)
\end{aligned}
$$

Validated Solutions for Parametric ODEs

- Consider the IVP for the parametric ODEs

$$\dot{\boldsymbol{y}} = \boldsymbol{f}(\boldsymbol{y}, \boldsymbol{\theta}), \quad \boldsymbol{y}(t_0) = \boldsymbol{y}_0, \quad \boldsymbol{\theta} \in \boldsymbol{\Theta}$$

- Validated methods:
  - Guarantee there exists a unique solution $\boldsymbol{y}$ in the interval $[t_0, t_f]$, for each $\boldsymbol{\theta} \in \boldsymbol{\Theta}$
  - Compute the interval $\boldsymbol{Y}_{t_f}$ that encloses all solutions of the ODEs at t_f.
- Tools – AWA, VNODE, COSY VI, VSPODE, etc.

Validated Solutions for Parametric ODEs (Cont'd)

- VSPODE (Lin and Stadtherr, 2005) – novel use of Taylor model approach for dependency problem in solving ODEs with interval valued parameters
- Phase 1 – Validate existence and uniqueness (h_j and $\tilde{\boldsymbol{Y}}_j$) – like in VNODE

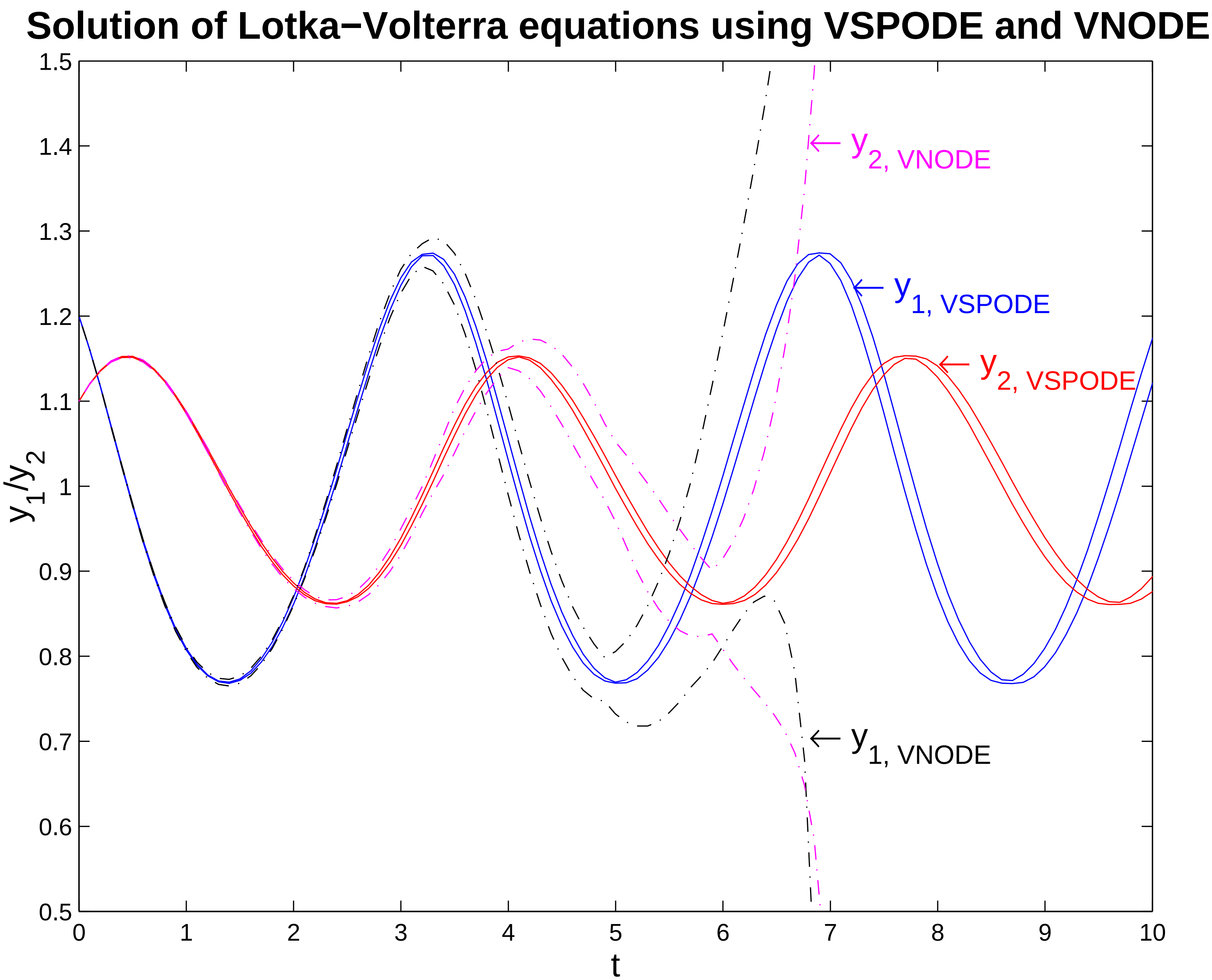
$$\tilde{\boldsymbol{Y}}_j = \sum_{i=0}^{k-1} [0, h_j]^i \boldsymbol{F}^{[i]}(\boldsymbol{Y}_j, \boldsymbol{\Theta}) + [0, h_j]^k \boldsymbol{F}^{[k]}(\tilde{\boldsymbol{Y}}_j^0, \boldsymbol{\Theta}) \subseteq \tilde{\boldsymbol{Y}}_j^0$$

- Phase 2 – Compute tighter enclosure
  - Dependence problem – Taylor model
  - Wrapping effect – QR factorization
  - Solutions: $\boldsymbol{T}_{y_{j+1}} = p_{y_{j+1}} + A_{j+1}\boldsymbol{V}_{j+1}$

Validated Solutions for Parametric ODEs (Cont'd)

- Example – Lotka-Volterra equations

$$\dot{y}_1 = \theta_1 y_1 (1 - y_2)$$
$$\dot{y}_2 = \theta_2 y_2 (y_1 - 1)$$
$$t \in [0, 10]$$
$$y_1(0) = 1.2$$
$$y_2(0) = 1.1$$
$$\theta_1 \in 3 + [-0.01, 0.01]$$
$$\theta_2 \in 1 + [-0.01, 0.01]$$


Solution of Lotka−Volterra equations using VSPODE and VNODE
y_1/y_2
t
0
1
2
3
4
5
6
7
8
9
10
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
$y_{2,\ \mathrm{VNODE}}$
$y_{1,\ \mathrm{VSPODE}}$
$y_{2,\ \mathrm{VSPODE}}$
$y_{1,\ \mathrm{VNODE}}$

Branch and Reduce Algorithm Summary

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

- Establish $\hat{\phi}$, the upper bound on global minimum using p^2 local minimizations
- 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 $T_\phi \leq \hat{\phi}$ to reduce $\mathbf{\Theta}^{(k)}$
  3. If $\mathbf{\Theta}^{(k)} = \emptyset$, go to next subinterval
  4. If $(\hat{\phi} - \underline{B(T_\phi)})/|\hat{\phi}| \leq \epsilon$, discard $\mathbf{\Theta}^{(k)}$ and go to next subinterval
  5. If $\overline{B(T_\phi)} < \hat{\phi}$, update $\hat{\phi}$ 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

Computational Studies - Example 1

- First-order irreversible series reaction (Esposito and Floudas, 2000)

$$A \xrightarrow{\theta_1} B \xrightarrow{\theta_2} C$$

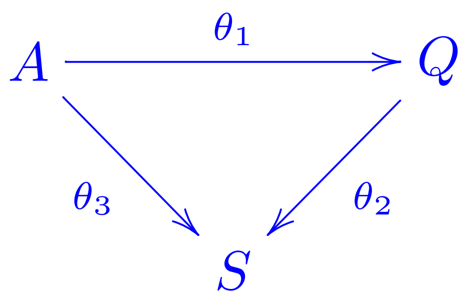
- The differential equation model

$$\begin{aligned} \dot{z}_A &= -\theta_1 z_A \\ \dot{z}_B &= \theta_1 z_A - \theta_2 z_B \\ \boldsymbol{z}_0 &= [1, 0] \\ \boldsymbol{\theta} &\in [0, 10] \times [0, 10] \end{aligned}$$

- Solution: $\boldsymbol{\theta}^* = (5.0035, 1.0000)$ and $\phi^* = 1.1858 \times 10^{-6}$
- Results: 4 iterations and < 0.1 CPU seconds

Computational Studies - Example 2

- Catalytic Cracking of Gas Oil (Esposito and Floudas, 2000)



- The differential equation model

$$
\begin{aligned}
\dot{z}_A &= -(\theta_1 + \theta_3) z_A^2 \\
\dot{z}_Q &= \theta_1 z_A^2 - \theta_2 z_Q \\
\boldsymbol{z}_0 &= [1, 0] \\
\boldsymbol{\theta} &\in [0, 20] \times [0, 20] \times [0, 20]
\end{aligned}
$$

- Solution: $\boldsymbol{\theta}^* = (12.2139, 7.9798, 2.2217)$ and $\phi^* = 2.6557 \times 10^{-3}$
- Results: 359 iterations and 14.3 CPU seconds

Computational Performance Comparison (CPU seconds)

	Example 1		Example 2	
Method	Reported	Adjusted	Reported	Adjusted
This work (Intel P4 3.2GHz)	< 0.1	< 0.1	14.3	14.3
Papamichail and Adjiman (SUN UltraSPARC-II 360MHz)	801	102.5	35478	4541
Chachuat and Latifi (Machine not reported)	280	-	10400	-
Esposito and Floudas* (HP 9000 model J2240)	13.30	1.53	100.21	11.5

Adjusted = Approximate CPU time adjusted for machine used based on SPEC benchmarks

* Does not provide rigorous guarantee of global optimality.

Concluding Remarks and Acknowledgments

- A deterministic global optimization approach based on interval analysis can be used to estimate the parameters of dynamic systems
- 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
- This approach can be combined with the interval-Newton method (Lin and Stadtherr, 2005)
  - True global optimum instead of ϵ-convergence
  - May or may not reduce CPU time required
- Acknowledgments

  - Indiana 21st Century Research & Technology Fund
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