Convexification Techniques for Stationary/Dynamic Global Optimization and Set-Based Computing

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in cooperation with

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ShanghaiTech University

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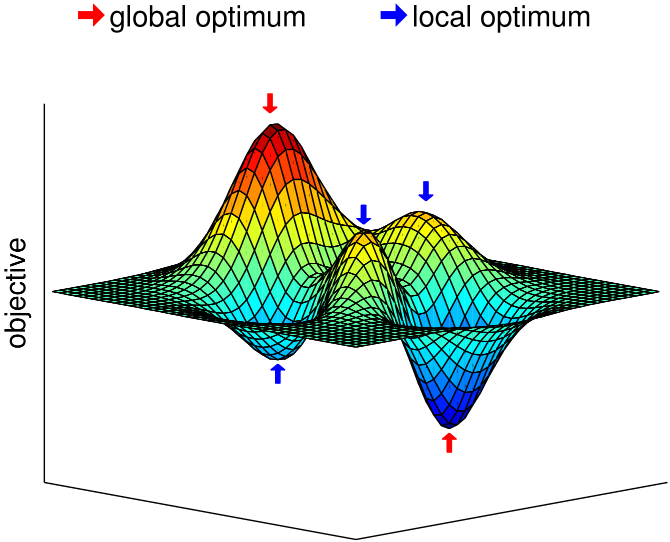
Why Global Optimization?



Outline

Spatial Branch-and-Bound (B&B) Algorithm

Convex Relaxation of Factorable Programs

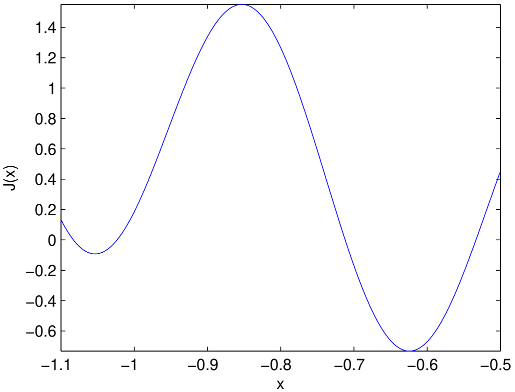
Bounding of Parametric ODEs

Guaranteed Parameter Estimation of Nonlinear Dynamic Systems

Spatial Branch-and-Bound (B&B) Algorithm

B&B algorithm steps

- **Initialization**
- Branching
- Finding upper bound
- Finding lower bound
- Fathoming
- Convergence check



Initialization

Initialize region of interest R.

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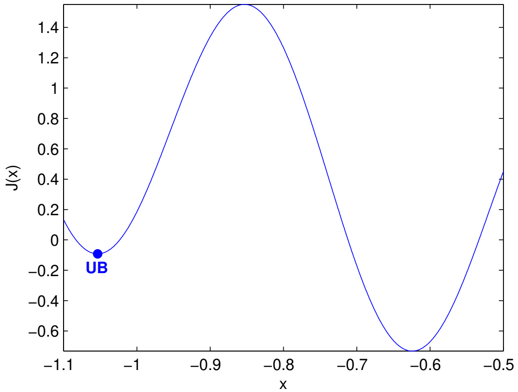

Finding upper bound

Solve original problem – find upper bound (UB).

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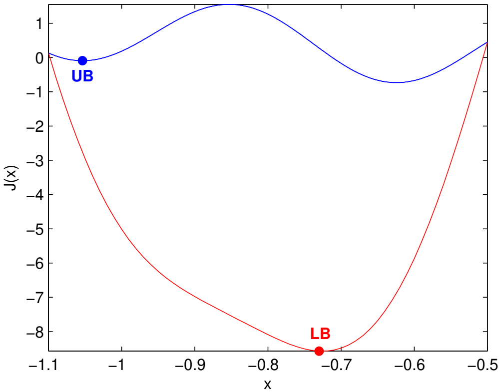

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Solve relaxed problem – find lower bound (LB).

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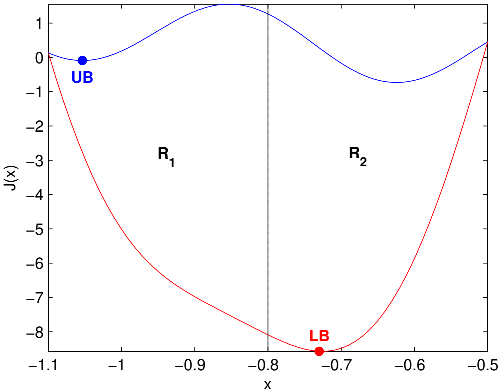

Branching

Partition R to new subregions R_1 and R_2.

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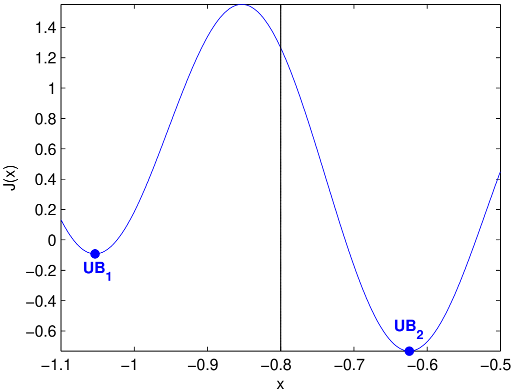

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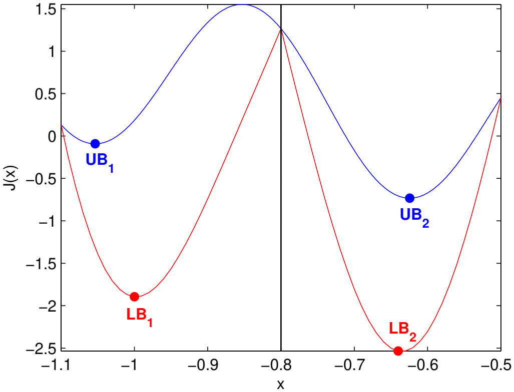

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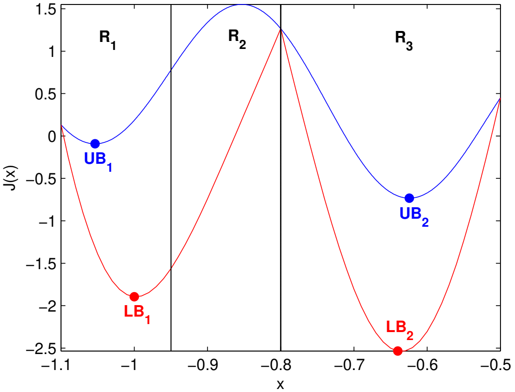

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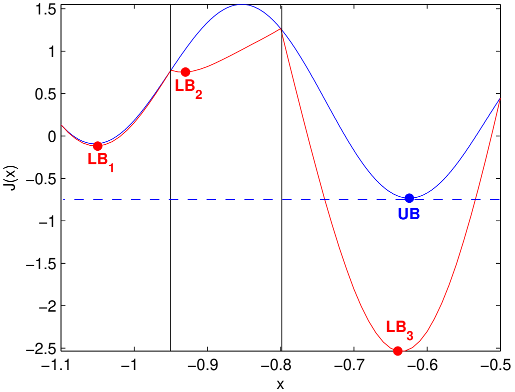

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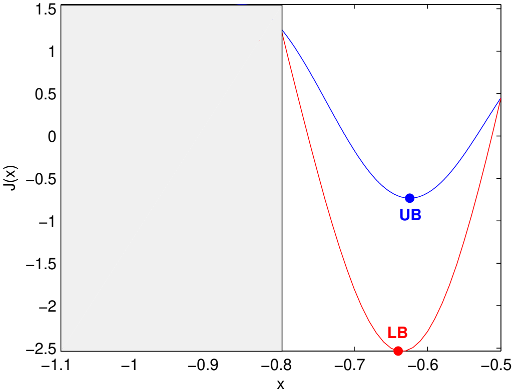

Fathoming

Remove subregions where solution cannot lie.

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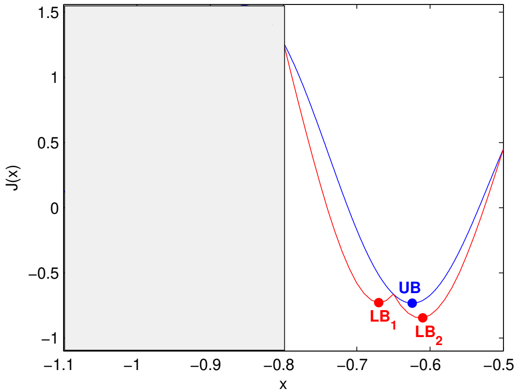

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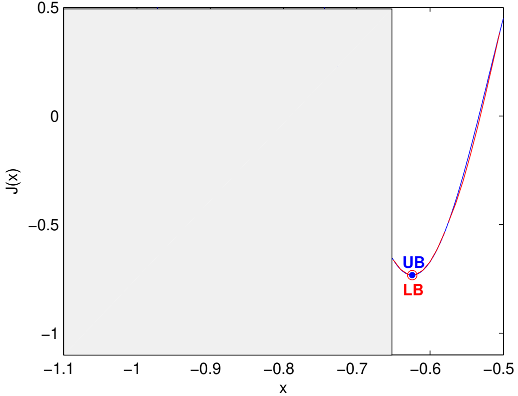

Convergence check

Evaluate convergence criterion $\mathbf{UB} - \mathbf{LB} \leq \varepsilon$.

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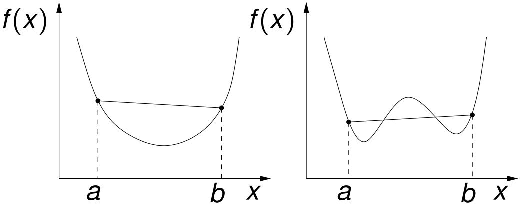
Convex Relaxation of an Optimization Problem

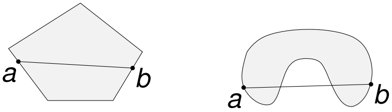
UB: $\min_x f(x)$ s.t. $g(x) \leq 0$

LB: $\min_x f^{\mathrm{cv}}(x)$ s.t. $g^{\mathrm{cv}}(x) \leq 0$

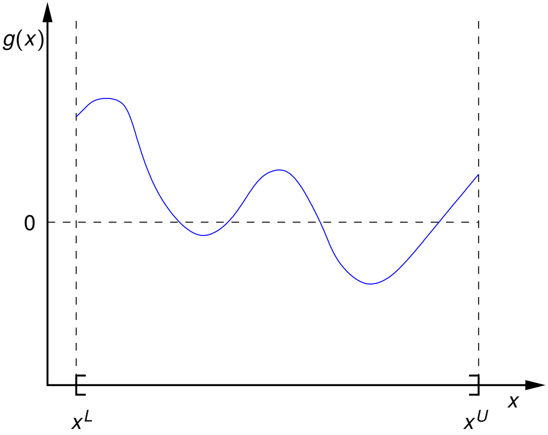
Lower bounding problem of spatial B&B consists of

- convex relaxation of objective function
- convex relaxation of the feasible set (constraint functions)





Convex Relaxation of the Feasible Set



Constraint:

$$g(x) \leq 0$$

Convex relaxation:

$$g^{\mathrm{cv}}(x) \leq 0$$

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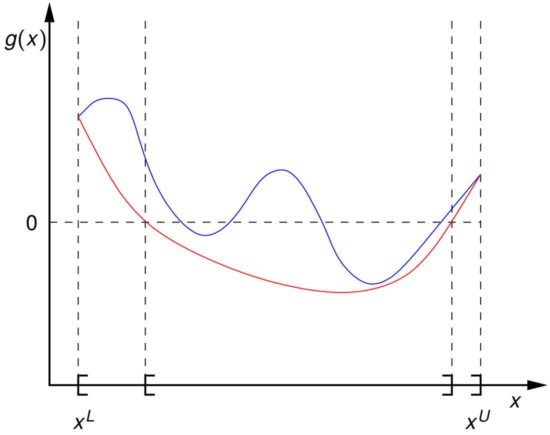

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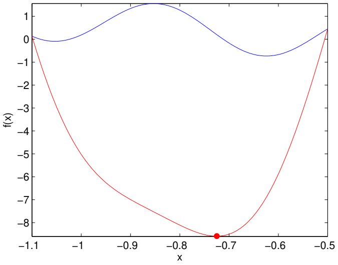
Convex Relaxation

Definition

Given a real-valued function $f(x)$ and interval $X = [x^L, x^U]$, identify $f^{\text{cv}}(x)$ such that:

a. $f^{\text{cv}}(x)$ underestimates $f(x)$ ($f^{\text{cv}}(x) \leq f(x),\ \forall x \in X$)
b. $f^{\text{cv}}(x)$ is convex ($\nabla^2 f^{\text{cv}}(x) \geq 0,\ \forall x \in X$)



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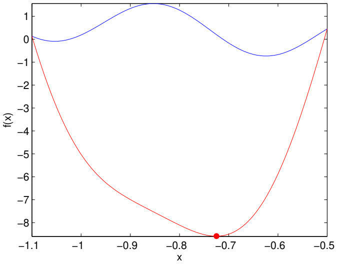
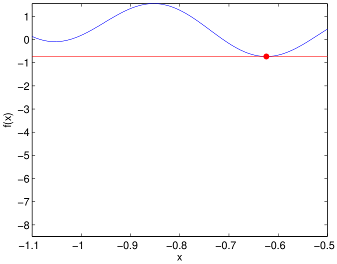
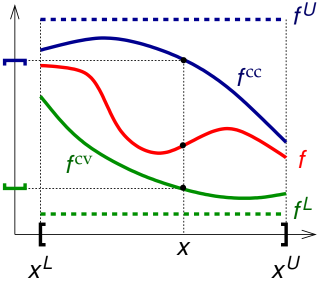




Convex/Concave Relaxations of Factorable Functions

Given a function f, construct functions f^{cv}, f^{cc} such that:

- $f^{\mathrm{cv}}(x) \leq f(x) \leq f^{\mathrm{cc}}(x), \forall x \in X$
- $f^{\mathrm{cv}} : X \to \mathbb{R}$ convex
- $f^{\mathrm{cc}} : X \to \mathbb{R}$ concave



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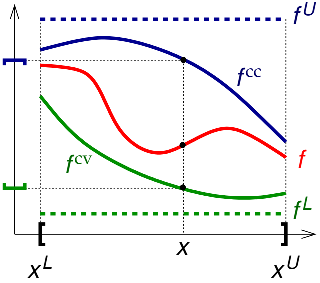

What are the sources of nonconvexity?

$$f(x) = \left(\exp(x_1) - x_2^2\right) x_1 x_2 \xrightarrow[\text{form}]{\text{factored}} \begin{cases} v_1(x) = x_1 \\ v_2(x) = x_2 \\ v_3(x) = \exp(v_1(x)) \\ v_4(x) = -v_2(x)^2 \\ v_5(x) = v_3(x) + v_4(x) \\ v_6(x) = v_5(x) v_1(x) \\ f(x) = v_6(x) v_2(x) \end{cases}$$

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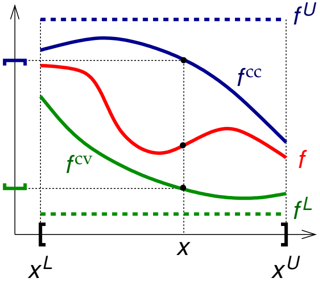

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Interval Arithmetics

Set of simple rules:

$$
\begin{aligned}
[a,b]+[c,d] &= [a+c, b+d] \\
-[a,b] &= [-b,-a] \\
[a,b][c,d] &= [\min\{ac,ad,bc,bd\}, \\
&\quad \max\{ac,ad,bc,bd\}] \\
f([a,b]) &= [\min_{[a,b]} f, \max_{[a,b]} f]
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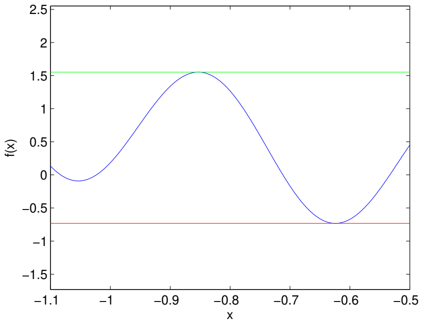

But...let's consider the following example

$$f(x) = x^2 - x = \left(x - \frac{1}{2}\right)^2 - \frac{1}{4}$$

$$x \in X = [0,1]$$

$$f(X) = ?$$

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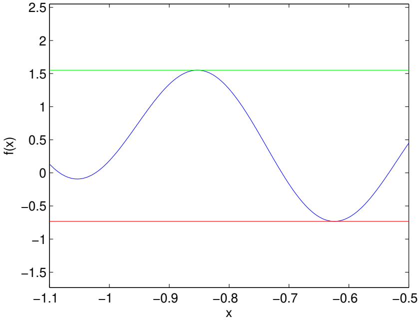

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Convex Relaxation using αBB Method

Find $f^{\text{cv}}(x)$ by subtracting a 'convex-enough' function from $f(x)$:

$$f^{\text{cv}}(x) = f(x) - \alpha(x - x^L)(x - x^U)$$

if $\alpha \geq 0$ then $f^{\text{cv}}(x) \leq f(x),\ \forall x \in X$

if $\alpha = -\min(0, (1/2)\lambda_{\text{min}}([\nabla^2 f(X)]))$

then $\nabla^2 f^{\text{cv}}(x) = \nabla^2 f(x) + 2I\alpha \geq 0,\ \forall x \in X$

Illustrative example:

$$f(x) = x\sin(x),\ \forall x \in [0, 2\pi]$$

$$[\nabla_x^2 f(X)] = 2\cos(X) - X\sin(X)$$

(interval arithmetics)

Adjiman, et al. *Computers & Chemical Engineering* 22 (9), 1998.

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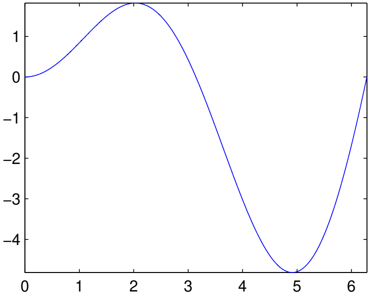

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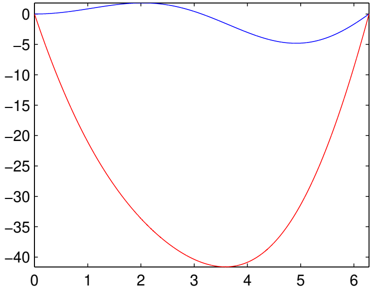

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Convex Relaxation of Special Functions

McCormick relaxations for bilinear functions

$$(x - x^L)(y - y^L) = xy - x^L y - y^L x + x^L y^L \geq 0$$

$$(x - x^U)(y - y^U) = xy - x^U y - y^U x + x^U y^U \geq 0$$

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Relaxation:

$$w = xy$$

$$\begin{cases} w \geq x^L y + y^L x - x^L y^L \\ w \geq x^U y + y^U x - x^U y^U \\ w \leq x^U y + y^L x - x^U y^L \\ w \leq x^L y + y^U x - x^L y^U \end{cases}$$

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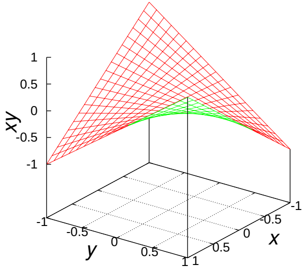

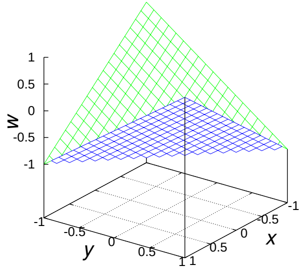

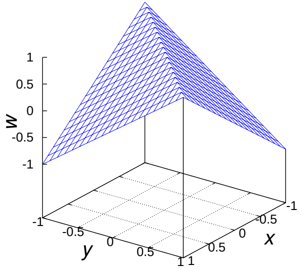

McCormick Relaxations...

...work similarly for bilinear, trilinear, fractional terms. Even...

Theorem [1]

- $f, g : X \to \mathbb{R}$, with $X \subset \mathbb{R}^n$ convex
- $[f^L, f^U]$ and $[g^L, g^U]$ interval bounds for f and g on X
- $[f^{\mathrm{cv}}, f^{\mathrm{cc}}]$ and $[g^{\mathrm{cv}}, g^{\mathrm{cc}}]$ cvx/ccve relaxations for f and g on X

Convex/concave bounds for $h = f \times g$ on X:

$$\begin{aligned}
h^{\mathrm{cv}}(x) = \max\{ & \min\{g^L f^{\mathrm{cv}}(x), g^L f^{\mathrm{cc}}(x)\} + \min\{f^L g^{\mathrm{cv}}(x), f^L g^{\mathrm{cc}}(x)\} - f^L g^L, \\
& \min\{g^U f^{\mathrm{cv}}(x), g^U f^{\mathrm{cc}}(x)\} + \min\{f^U g^{\mathrm{cv}}(x), f^U g^{\mathrm{cc}}(x)\} - f^U g^U\} \\
h^{\mathrm{cc}}(x) = \min\{ & \max\{g^L f^{\mathrm{cv}}(x), g^L f^{\mathrm{cc}}(x)\} + \max\{f^U g^{\mathrm{cv}}(x), f^U g^{\mathrm{cc}}(x)\} - f^U g^L, \\
& \max\{g^U f^{\mathrm{cv}}(x), g^U f^{\mathrm{cc}}(x)\} + \max\{f^L g^{\mathrm{cv}}(x), f^L g^{\mathrm{cc}}(x)\} - f^L g^U\}
\end{aligned}$$

---

[1] McCormick, G.P., *Mathematical Programming*, **10**:147-175, 1976

Relaxation of Special Univariate Terms

Univariate Terms: $w = \varphi(x)$, $x^L \leq x \leq x^U$

- Convex Case: e.g., $\varphi : v \mapsto v^{2n}$, $\varphi : v \mapsto \exp(v)$

$$w = \varphi(x) \quad \xrightarrow{\text{relax}} \quad \begin{cases} w \geq \varphi(x) \\ w \leq \varphi(x^L) + \frac{\varphi(x^U)-\varphi(x^L)}{x^U-x^L}(x - x^L) \end{cases}$$

- Concave Case: e.g., $\varphi : v \mapsto \sqrt{v}$, $\varphi : v \mapsto \log(v)$

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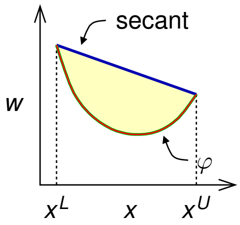

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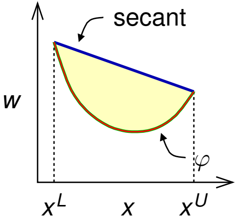
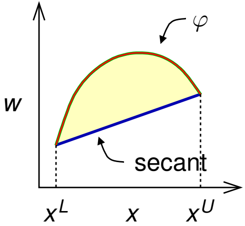




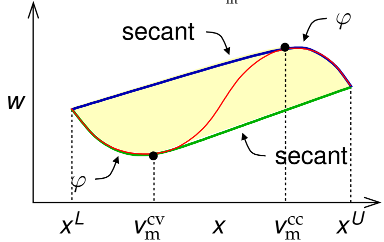
Relaxation of Special Univariate Terms

Univariate Terms: $w = \varphi(x)$, $x^L \leq x \leq x^U$

- Concavoconvex Case: e.g., $\varphi : v \mapsto v^{2n+1}$

$$w = \varphi(x) \quad \xrightarrow{\text{relax}} \quad \begin{cases} w \geq \begin{cases} \varphi(x), & \text{if } x \leq v_{\rm m}^{\rm cv} \\ \varphi(x^U) + \frac{\varphi(x^U)-\varphi(v_{\rm m}^{\rm cv})}{x^U - v_{\rm m}^{\rm cv}}(x - x^U), & \text{otherwise} \end{cases} \\ w \leq \begin{cases} \varphi(x), & \text{if } x \geq v_{\rm m}^{\rm cc} \\ \varphi(x^L) + \frac{\varphi(x^L)-\varphi(v_{\rm m}^{\rm cc})}{x^L - v_{\rm m}^{\rm cc}}(x - x^L), & \text{otherwise} \end{cases} \end{cases}$$

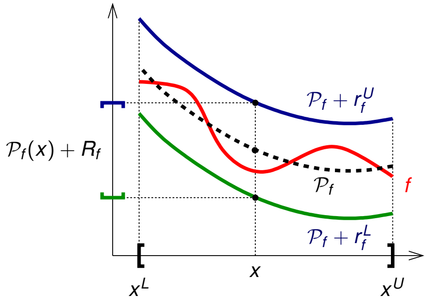
$$v_{\rm m}^{\rm cv}, v_{\rm m}^{\rm cc} \in [x^L, x^U] : \ \varphi'(v_{\rm m}^{\rm cv}) = \frac{\varphi(x^U)-\varphi(v_{\rm m}^{\rm cv})}{x^U - v_{\rm m}^{\rm cv}} \text{ and } \varphi'(v_{\rm m}^{\rm cc}) = \frac{\varphi(x^L)-\varphi(v_{\rm m}^{\rm cc})}{x^L - v_{\rm m}^{\rm cc}}$$



Taylor Model Estimators

Taylor Models:

- $f(x) \in \mathcal{T}_f(x) := \mathcal{P}_f(x) + R_f, \forall x \in X$
- $\mathcal{P}_f$ polynomial of order q
- R_f remainder interval term
- Use of recursive arithmetic rules
- Range: $f(X) \subseteq \mathcal{P}_f(X) + R_f$



TM of algebraic function

$$\mathcal{T}_f^q = f(\text{mid}(X)) + \left.\frac{\partial f}{\partial x}\right|_{\text{mid}(X)} (x - \text{mid}(X)) + \cdots + r_f^q \qquad \forall x \in X$$

- remainder can be evaluated using interval arithmetics

$$r_f^q = \left.\frac{\partial^{(q+1)} f}{\partial x^{(q+1)}}\right|_X (X - \text{mid}(X))^{(q+1)}$$

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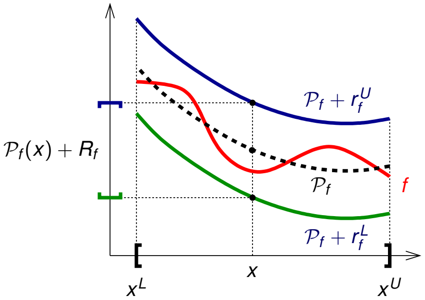

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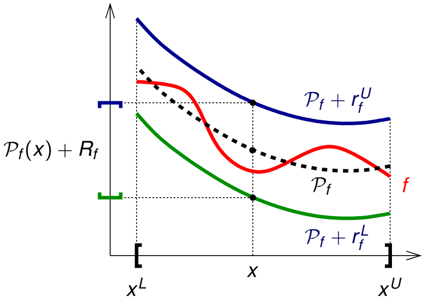

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Outline

Spatial Branch-and-Bound (B&B) Algorithm

Convex Relaxation of Factorable Programs

Bounding of Parametric ODEs

Guaranteed Parameter Estimation of Nonlinear Dynamic Systems

Bounding of Parametric ODEs

Problem Definition

Given a parameter box $P = [p^L, p^U]$ and a set of parametric ODEs $\dot{x} = f(x, p)$ and $x(t_0) = g(p)$, identify $X(t) = [x^L(t), x^U(t)]$ such that

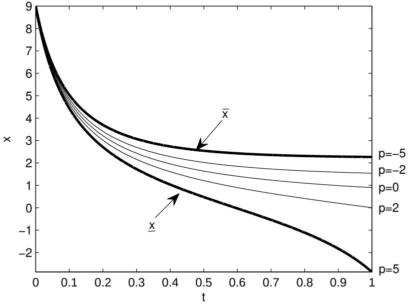
$$x(t, p) \in X(t), \ \forall t \in [t_0, t_N], \ \forall p \in P$$

ODE

$$\dot{x} = -x^2 - p$$
$$p \in [-5, 5]$$

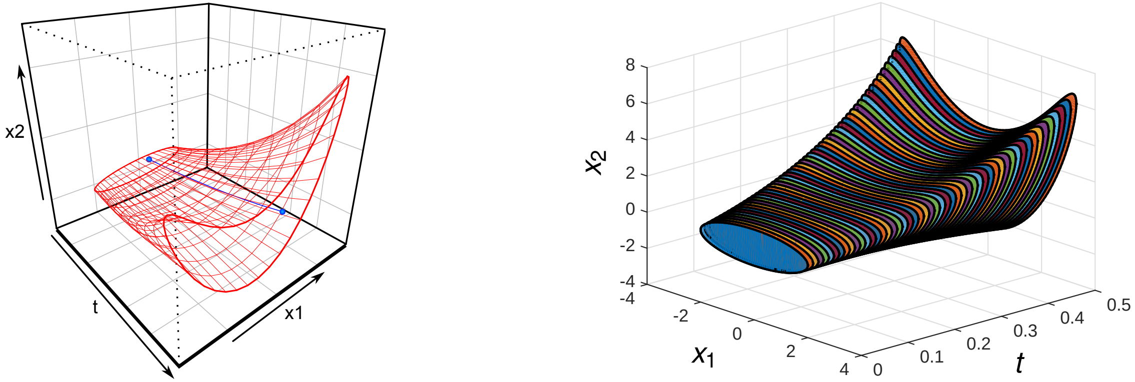
ODE Bounds

$$\dot{x}^U = -(x^U)^2 + 5$$
$$\dot{x}^L = -(x^L)^2 - 5$$



Bounding of Parametric ODEs

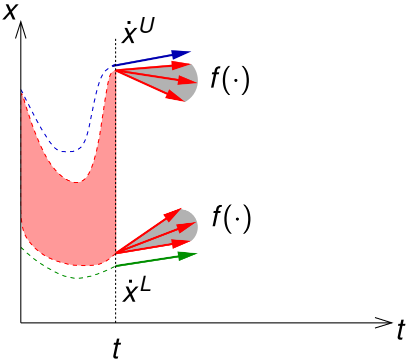
$$\dot{x}_1 = x_1$$
$$\dot{x}_2 = 2x_2 + x_1^2 + (1/8)x_2^2$$
$$x_1(0,p) = p_1, \quad x_2(0,p) = p_2, \quad p = (p_1, p_2)^{\mathrm{T}}$$

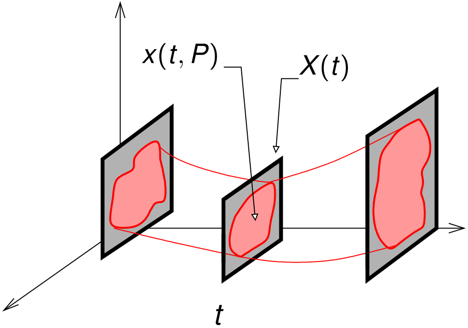


Techniques for Bounding of Parametric ODEs

1. interval methods (differential inequalities) (Walter, 1970)
2. Taylor models methods (Berz, 1997; Chachuat et al., 2012)

$$\dot{x}^U \geq \sup\{f(x,p) : p \in P, x \in [x^L, x^U]\}$$
$$\dot{x}^L \leq \inf\{f(x,p) : p \in P, x \in [x^L, x^U]\}$$





Techniques for Bounding of Parametric ODEs

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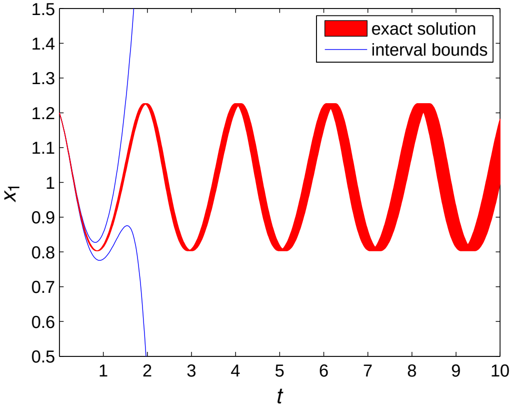
Lotka-Volterra system

$$\dot{x}_1 = p x_1 (1 - x_2), \; x_1(0) = 1.2,$$
$$\dot{x}_2 = p x_2 (x_1 - 1), \; x_2(0) = 1.1,$$
$$p \in [2.95, 3.05]$$



Order of convergence is linear: $\Delta X = a \Delta P$

Techniques for Bounding of Parametric ODEs

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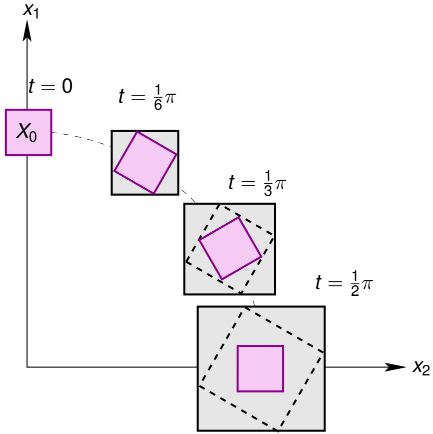
Wrapping effect

$$\dot{x}_1 = x_2$$
$$\dot{x}_2 = -x_1$$
$$x(0) \in X_0;$$

$$x(t) = \begin{pmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{pmatrix} X_0$$



Techniques for Bounding of Parametric ODEs

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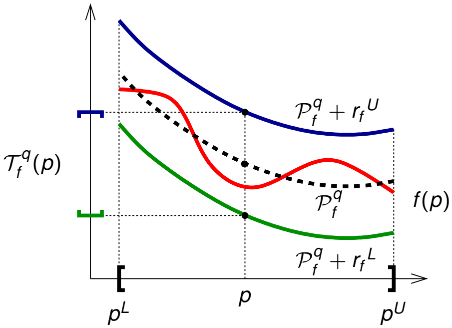
Idea: Enclose the image of solution to ODE using

$$\mathcal{T}^q_{x(t)}(p) = \mathcal{P}^q_{x(t)} + r^q_{x(t)}$$

where $\mathcal{P}^q_{x(t)}(p)$ is qth order Taylor expansion of $x(t)$ and

$$\mathcal{P}^q_{x(t)} - x(t,p) \in r^q_{x(t)}, \ \forall p \in P$$



TM of ODE solution

$$\mathcal{T}^q_{x(t)} = x(t)(\mathrm{mid}(P)) + \left.\frac{\partial x(t)}{\partial p}\right|_{\mathrm{mid}(P)} (p - \mathrm{mid}(P)) + \cdots + r^q_f \qquad \forall p \in P$$

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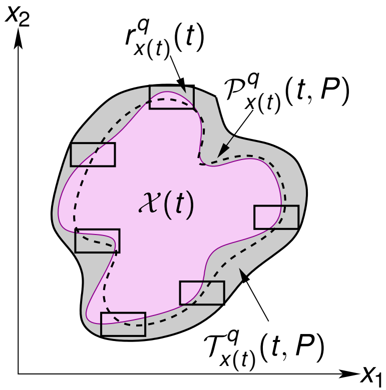

Enclosure of solution to parametric ODE found by:

- coefficients of $\mathcal{P}^q_{x(t)}$ – parametric sensitivities $\left(\frac{\partial^q x(t)}{\partial p^q}\Big|_{\mathrm{mid}(P)}\right)$

Techniques for Bounding of Parametric ODEs

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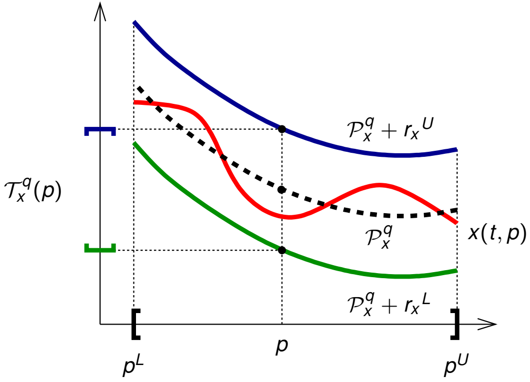

$$\dot{x} = f(x, p)$$

$$\mathcal{T}_x^q = \mathcal{P}_x^q + r_x, \quad r_x \in [{r_x}^L, {r_x}^U]$$

$$\Downarrow$$

$$\dot{\mathcal{T}}_x^q = f(\mathcal{T}_x^q, p)$$

$$\Downarrow$$

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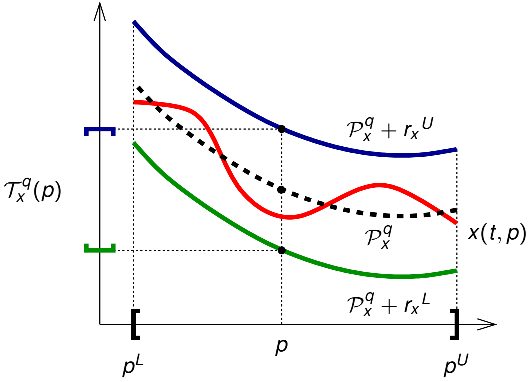

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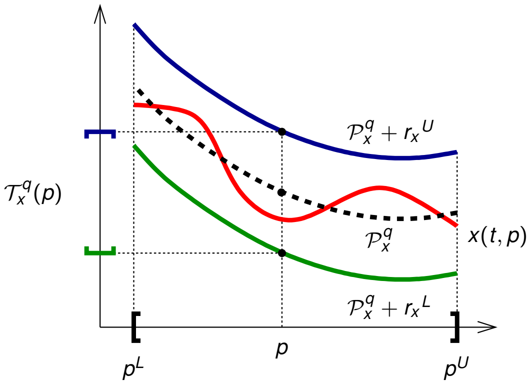

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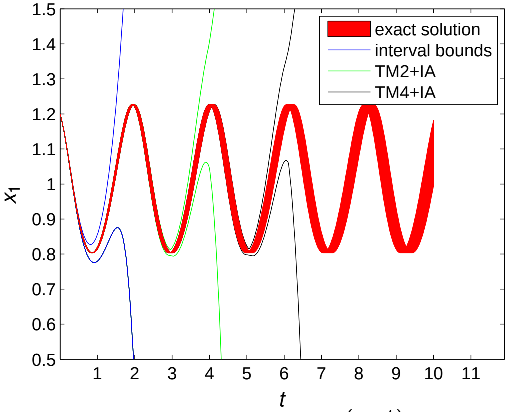

Order of convergence is much higher than linear: $\Delta X = a(\Delta P)^{(q+1)}$

Outline

Spatial Branch-and-Bound (B&B) Algorithm

Convex Relaxation of Factorable Programs

Bounding of Parametric ODEs

Guaranteed Parameter Estimation of Nonlinear Dynamic Systems

Classical Parameter Estimation

$$\text{model: } \hat{y} = F(p) \begin{cases} \text{dynamic system:} & \dot{x} = f(x, p),\ x(0) = g(p) \\ \text{output equation:} & \hat{y} = h(x, p) \end{cases}$$

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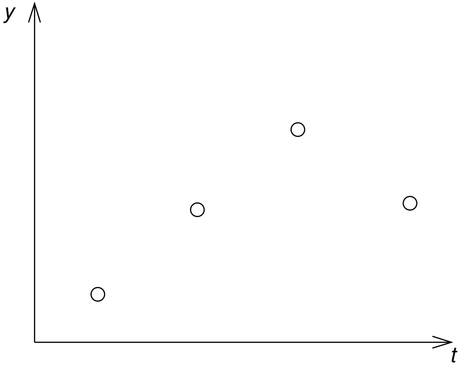

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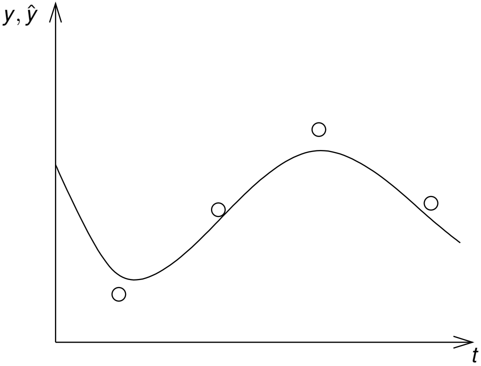

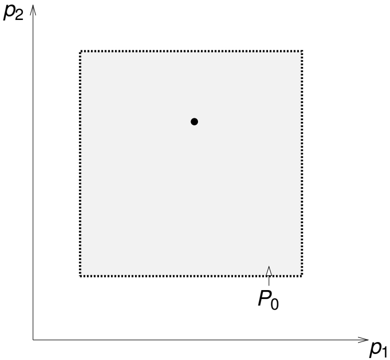

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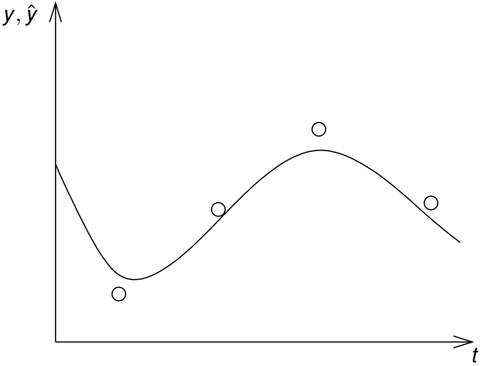
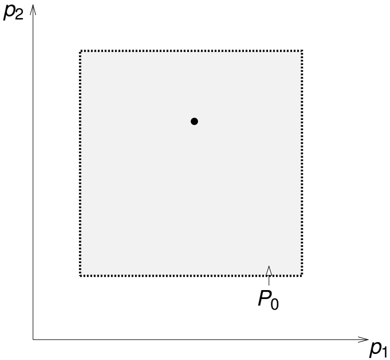
$$\min_{p \in P_0} \|\hat{y} - y\|_2^2$$
$$\text{s.t. } \hat{y} = F(p)$$





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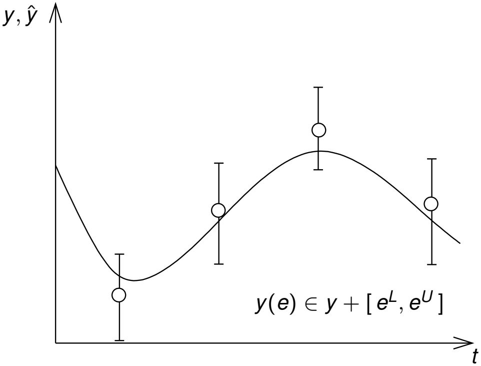
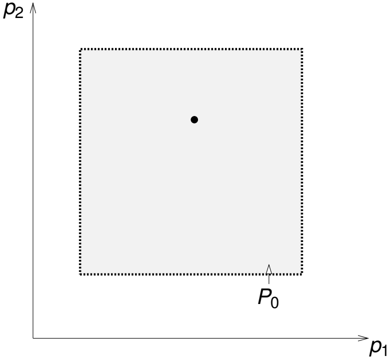
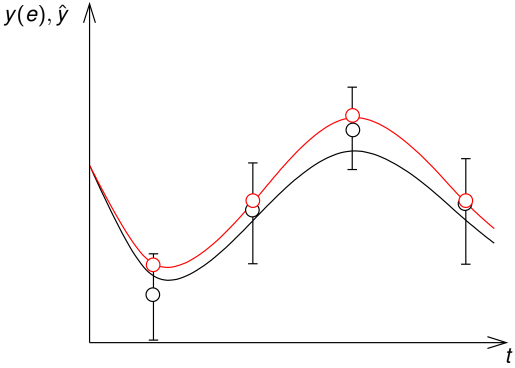


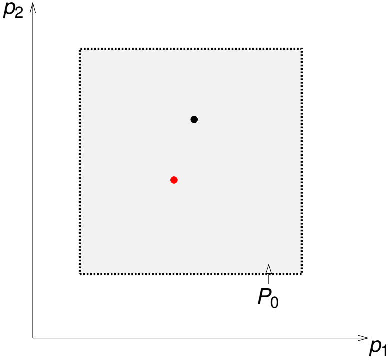


Guaranteed Parameter Estimation

$$e \in [e^L, e^U] : \min_{p \in P_0} \|\hat{y} - y + e\|_2^2$$

$$\text{s.t. } \hat{y} = F(p)$$





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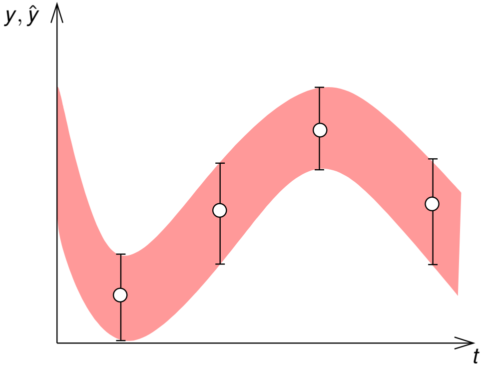
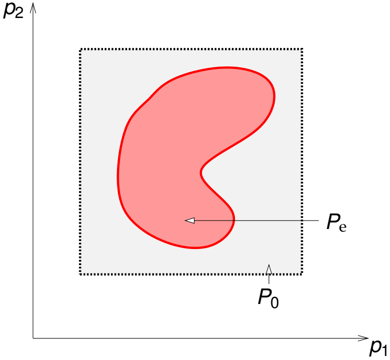


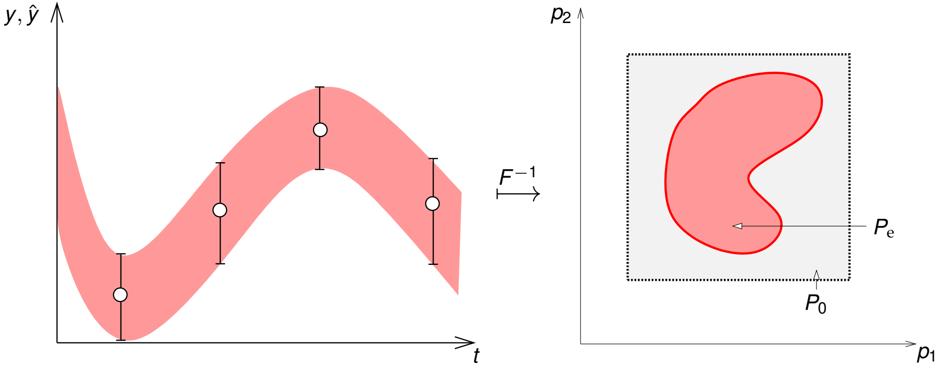


Finding Solution to Guaranteed PE Problem

- Find a set

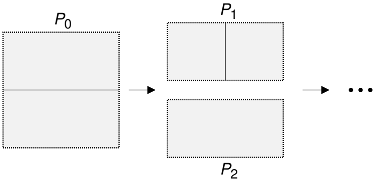
$$P_e := \left\{ p \in P_0 \,\middle|\, \begin{array}{l} \hat{y} = F(p), \\ e^L \le \hat{y} - y \le e^U \end{array} \right\} \equiv \{p \in P_0 | g(p) \le 0\}$$

- Apply set inversion via interval analysis (Jaulin, 1993)

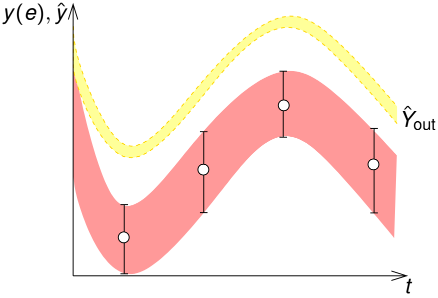


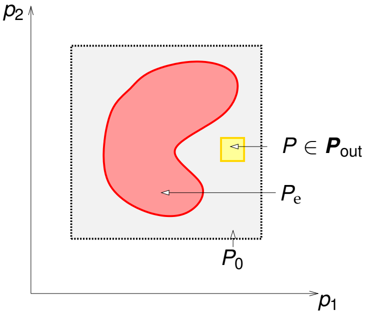
Finding Solution via Set Inversion

1. Apply branching on parameter space



2. Employ exclusion tests on parameter space partitions





Finding Solution via Set Inversion

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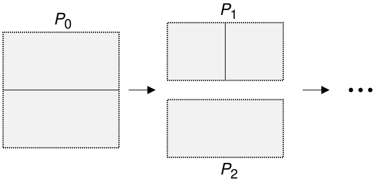

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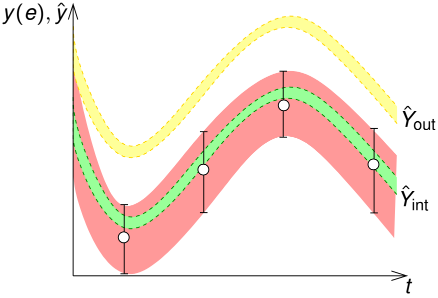

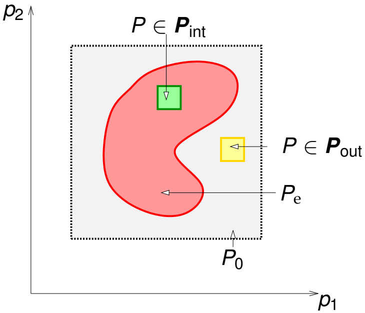

Finding Solution via Set Inversion

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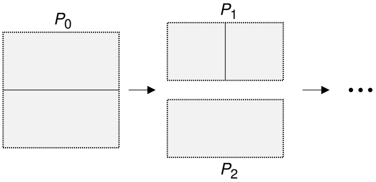

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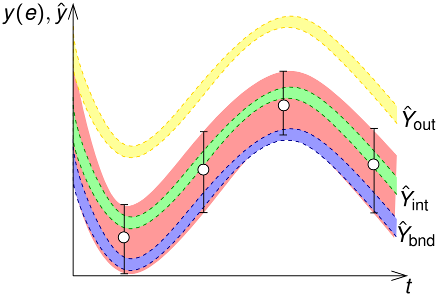

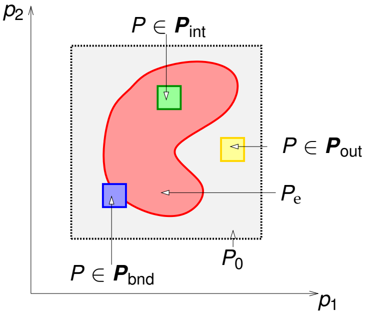

Finding Solution via Set Inversion

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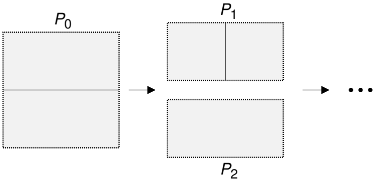

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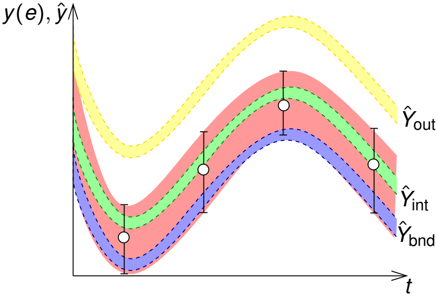
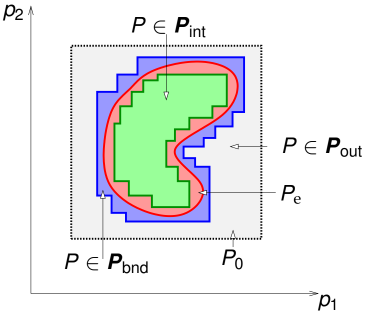
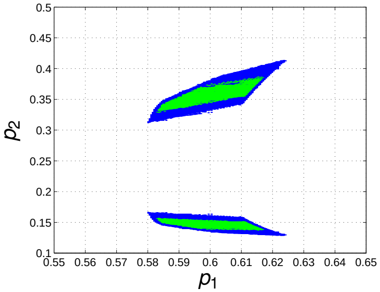


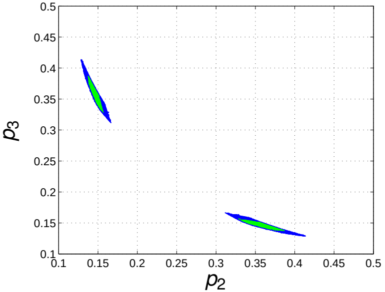


Case Study

$$\dot{x}_1 = -(p_1 + p_3)x_1 + p_2 x_2, \qquad x_1(0) = 1,$$
$$\dot{x}_2 = p_1 x_1 - p_2 x_2, \qquad x_2(0) = 0.$$

$$(p_1, p_2, p_3) = (0.6, 0.15, 0.35) \rightarrow y = x_2 + [-0.05, 0.05]$$





$V_{\text{bnd}} = 5 \times 10^{-6}$ (2nd-order TM, $>$70,000 boxes, 900s CPU time)

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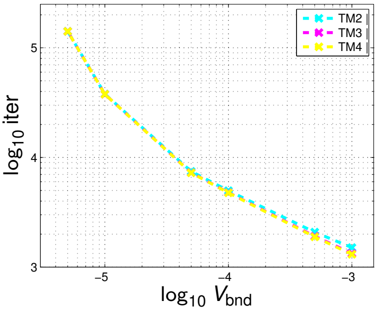
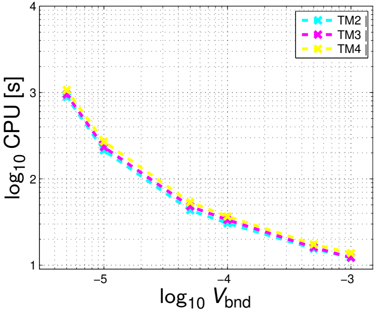
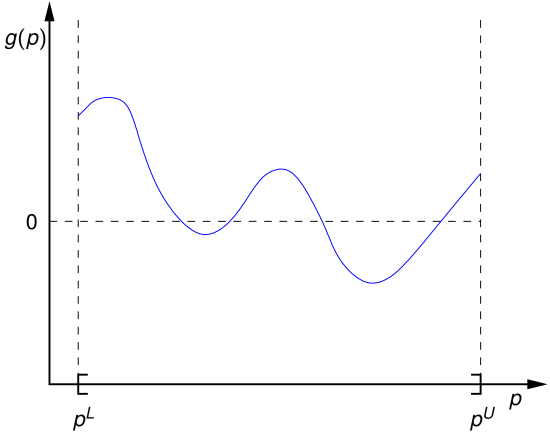




Implementation in C++ libraries MC++ and CRONOS (Chachuat et al.)

Optimization-based Domain Reduction



Constraint:

$$g(x) \leq 0$$

Convex relaxation:

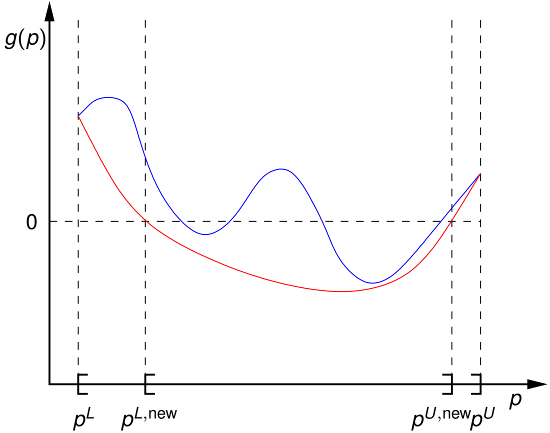
$$g^{\mathrm{cv}}(p) \leq 0$$

$$p^{L,\mathrm{new}} / p^{U,\mathrm{new}} =$$

$$\min_{p \in P} / \max_{p \in P} p$$

$$\text{s.t. } g^{\mathrm{cv}}(p) \leq 0$$

Optimization-based Domain Reduction



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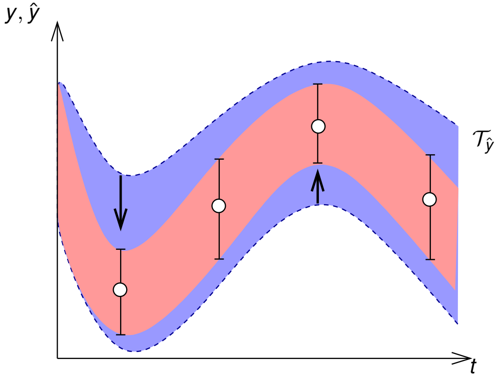
$$p^{L,\text{new}} / p^{U,\text{new}} = \min_{p \in P} / \max_{p \in P} p \quad \text{s.t. } g^{\text{cv}}(p) \leq 0$$

Domain Reduction for Guaranteed PE

$$p^{L,\text{new}} / p^{U,\text{new}} = \min_{p \in P} / \max_{p \in P} p$$

$$\text{s.t.} \ \left(\mathcal{P}^q_{\hat{y}}(p)\right)^{\text{cv}} + r_{\hat{y}}{}^L \leq y + e^L$$

$$\left(-\mathcal{P}^q_{\hat{y}}(p)\right)^{\text{cv}} - r_{\hat{y}}{}^U \leq -y - e^U$$



Convex relaxation of $\mathcal{P}^q_{\hat{y}}(p)$ by polyhedral relaxation $\Rightarrow$ LP

Domain Reduction for Guaranteed PE

$$p^{L,\text{new}} / p^{U,\text{new}} = \min_{p \in P} / \max_{p \in P} p$$

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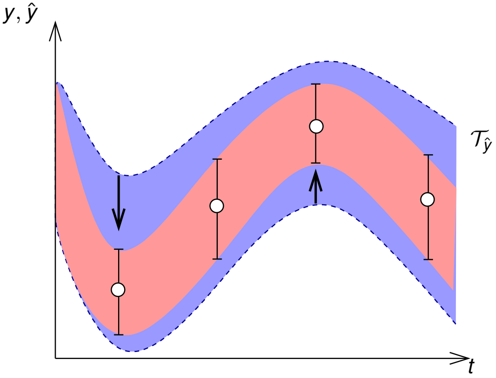

Convex relaxation of $\mathcal{P}^q_{\hat{y}}(p)$ by polyhedral relaxation $\Rightarrow$ LP

Polyhedral Relaxation of Polynomial Functions

1. Decomposition

$$\mathcal{P}(p) = a_1 p_1 + a_2 p_2 + a_3 p_2^2 + a_4 p_1 p_2^2$$

$$\mathcal{P}(v) = a_1 v_1 + a_2 v_2 + a_3 v_3 + a_4 v_4$$
$$v_1 = p_1,\ v_2 = p_2,\ v_3 = v_2^2,\ v_4 = v_1 v_3$$

2. Affine relaxation of bilinear terms (McCormick, 1976)
3. Outer-approximation

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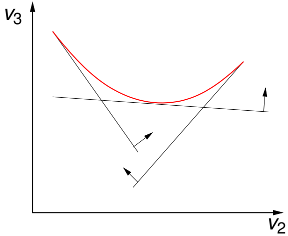

Case Study (Continued)

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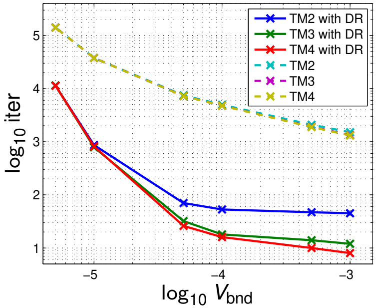

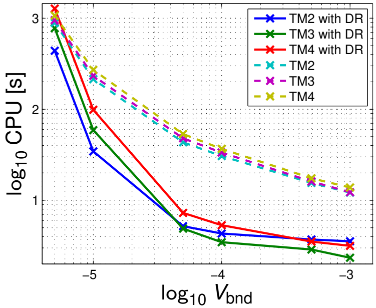

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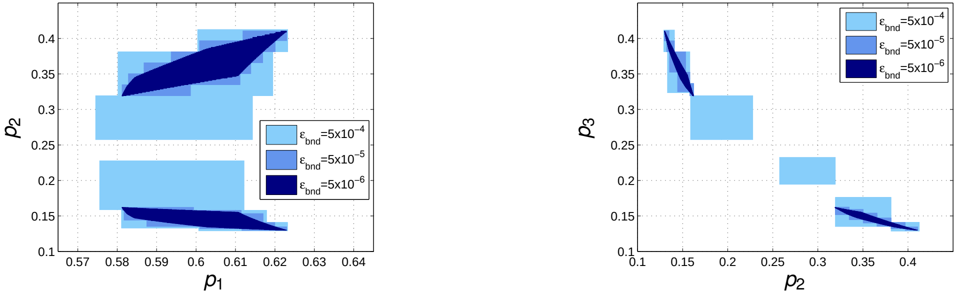

$$V_{bnd} = 5 \times 10^{-6} \text{ (2nd-order TM, 11,250 boxes, 350s CPU time)}$$
$$V_{bnd} = 5 \times 10^{-5} \text{ (2nd-order TM, 34 boxes, 5s CPU time)}$$

Conclusions

- effective convexification techniques are vital for solution of static/dynamic optimization and set-based problems
- efficient bounding techniques for parametric ODEs are essential ingredients
- optimization-based domain-reduction techniques can further enhance the convergence and properties of the obtained solutions

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