Global Optimization with Differential-Algebraic Constraints

Joseph K. Scott and Paul I. Barton

Process Systems Engineering Laboratory
Department of Chemical Engineering
Massachusetts Institute of Technology
Cambridge MA 02139

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Outline

- Problem statement
  - Global Dynamic Optimization with DAEs
- Background and approach
  - Generalized McCormick’s Relaxations
- Relaxations for DAE solutions
- Interval bounds on DAE solutions
- Future directions

Problem Statement: Index 1

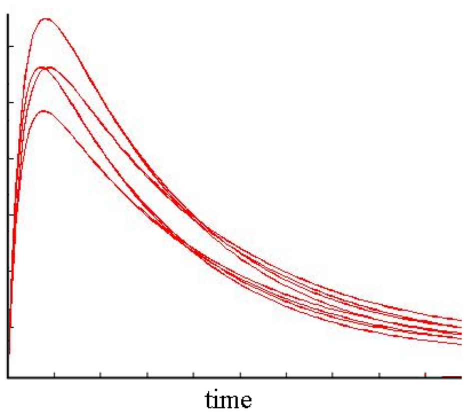
$$\min_{\mathbf{p}\in P} \; J(\mathbf{p}) \equiv \phi(\mathbf{p},\mathbf{x}(t_f,\mathbf{p}),\mathbf{y}(t_f,\mathbf{p})) + \int_{t_0}^{t_f} \ell(s,\mathbf{p},\mathbf{x}(s,\mathbf{p}),\mathbf{y}(s,\mathbf{p}))ds$$

$$\text{s.t.} \;\; \mathbf{G}(\mathbf{p}) \equiv \psi(\mathbf{p},\mathbf{x}(t_f,\mathbf{p}),\mathbf{y}(t_f,\mathbf{p})) + \int_{t_0}^{t_f} \xi(s,\mathbf{p},\mathbf{x}(s,\mathbf{p}),\mathbf{y}(s,\mathbf{p}))ds \leq \mathbf{0}$$

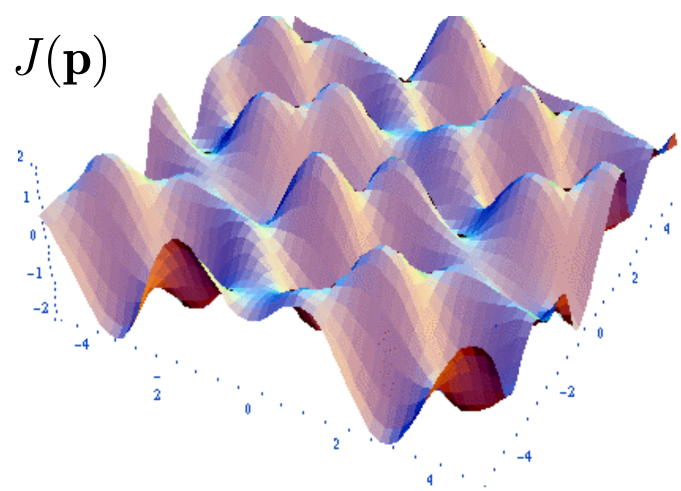
$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{x}(t_0,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}),$$

$$\mathbf{0} = \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{y}(t_0,\hat{\mathbf{p}}) = \mathbf{y}_0(\hat{\mathbf{p}}).$$

$\mathbf{x}(t,\mathbf{p})$



$J(\mathbf{p})$



Solution Strategy

$$\min_{\mathbf{p}\in P} \; J(\mathbf{p}) \equiv \phi(\mathbf{p}, \mathbf{x}(t_f, \mathbf{p}), \mathbf{y}(t_f, \mathbf{p})) + \int_{t_0}^{t_f} \ell(s, \mathbf{p}, \mathbf{x}(s, \mathbf{p}), \mathbf{y}(s, \mathbf{p}))ds$$

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$$\begin{aligned} \dot{\mathbf{x}}(t, \mathbf{p}) &= \mathbf{f}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p})), \quad & \mathbf{x}(t_0, \mathbf{p}) &= \mathbf{x}_0(\mathbf{p}), \\ \mathbf{0} &= \mathbf{g}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p})), \quad & \mathbf{y}(t_0, \hat{\mathbf{p}}) &= \mathbf{y}_0(\hat{\mathbf{p}}). \end{aligned}$$

- Sequential approach
  - Regard J and **G** as unknown (but computable) functions of **p**

$$\begin{aligned} &\min_{\mathbf{p}\in P} \; J(\mathbf{p}) \\ &\text{s.t.} \quad \mathbf{G}(\mathbf{p}) \le \mathbf{0} \end{aligned}$$

Solution Strategy

$$\min_{\mathbf{p}\in P} \; J(\mathbf{p}) \equiv \phi(\mathbf{p}, \mathbf{x}(t_f, \mathbf{p}), \mathbf{y}(t_f, \mathbf{p})) + \int_{t_0}^{t_f} \ell(s, \mathbf{p}, \mathbf{x}(s, \mathbf{p}), \mathbf{y}(s, \mathbf{p}))ds$$

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$$\dot{\mathbf{x}}(t, \mathbf{p}) = \mathbf{f}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p})), \quad \mathbf{x}(t_0, \mathbf{p}) = \mathbf{x}_0(\mathbf{p}),$$
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$$\min_{\mathbf{p}\in P} \; J(\mathbf{p}) \quad \text{s.t.} \quad \mathbf{G}(\mathbf{p}) \leq \mathbf{0}$$

$$\min_{\mathbf{p}\in P} \; J^c(\mathbf{p}) \quad \text{s.t.} \quad \mathbf{G}^c(\mathbf{p}) \leq \mathbf{0}$$

- Convex underestimating program requires:
  1. J^c a convex relaxation of J on P
  2. $\mathbf{G}^c$ a convex relaxation of $\mathbf{G}$ on P
- *P* a convex set

Solution Strategy

$$\min_{\mathbf{p}\in P} \; J(\mathbf{p}) \equiv \phi(\mathbf{p},\mathbf{x}(t_f,\mathbf{p}),\mathbf{y}(t_f,\mathbf{p})) + \int_{t_0}^{t_f} \ell(s,\mathbf{p},\mathbf{x}(s,\mathbf{p}),\mathbf{y}(s,\mathbf{p}))ds$$

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$$\min_{\mathbf{p}\in P} \; J(\mathbf{p}) \quad \text{s.t.} \;\; \mathbf{G}(\mathbf{p}) \leq \mathbf{0}$$

$$\min_{\mathbf{p}\in P} \; J^c(\mathbf{p}) \quad \text{s.t.} \;\; \mathbf{G}^c(\mathbf{p}) \leq \mathbf{0}$$

- How can J^c and $\mathbf{G}^c$ be computed when J and $\mathbf{G}$ are not known in closed form?

McCormick's Relaxations

- Uses known relaxations for
  - Binary addition
  - Binary multiplication
  - Composition with univariate functions:

$$-z,\ \frac{1}{z},\ cz,\ \sqrt{z},\ z^n,\ \exp(z),$$
$$\log(z),\ \sin(z),\ \cos(z),\ \text{etc.}$$

McCormick's Relaxations

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  - Binary addition
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  - Composition with univariate functions:

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$$\log(z), \ \sin(z), \ \cos(z), \ \text{etc.}$$

- Composes known relaxations to relax more complicated expressions

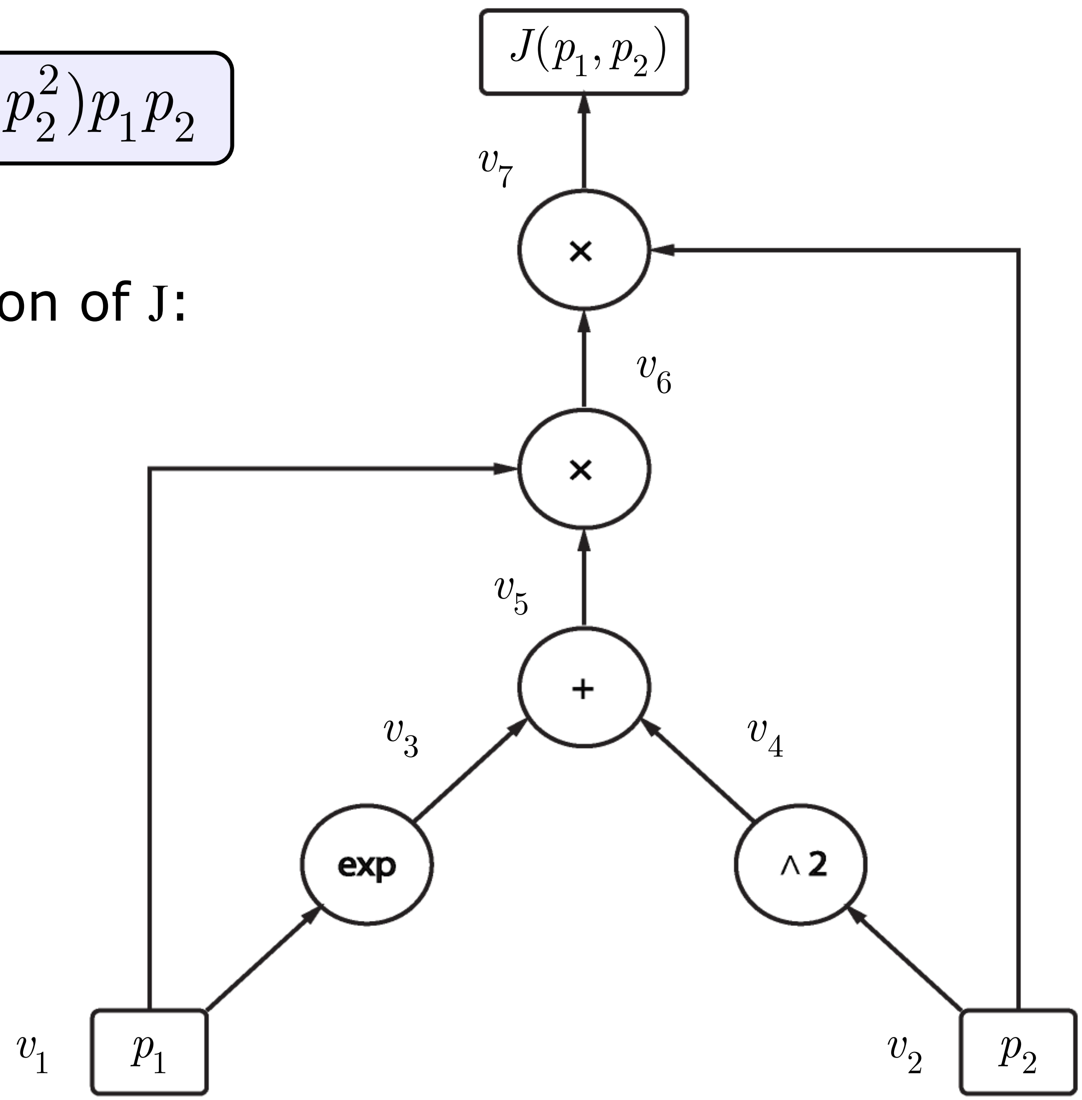
$$J(p_1, p_2) = (\exp(p_1) + p_2^2)p_1 p_2$$

McCormick's Relaxations

$$J(p_1, p_2) = (\exp(p_1) + p_2^2)p_1 p_2$$

Factorable representation of J:

$$\begin{aligned} v_1 &= p_1 \\ v_2 &= p_2 \\ v_3 &= \exp(v_1) \\ v_4 &= v_2^2 \\ v_5 &= v_3 + v_4 \\ v_6 &= v_5 v_1 \\ v_7 &= v_6 v_2 \\ J &= v_7 \end{aligned}$$



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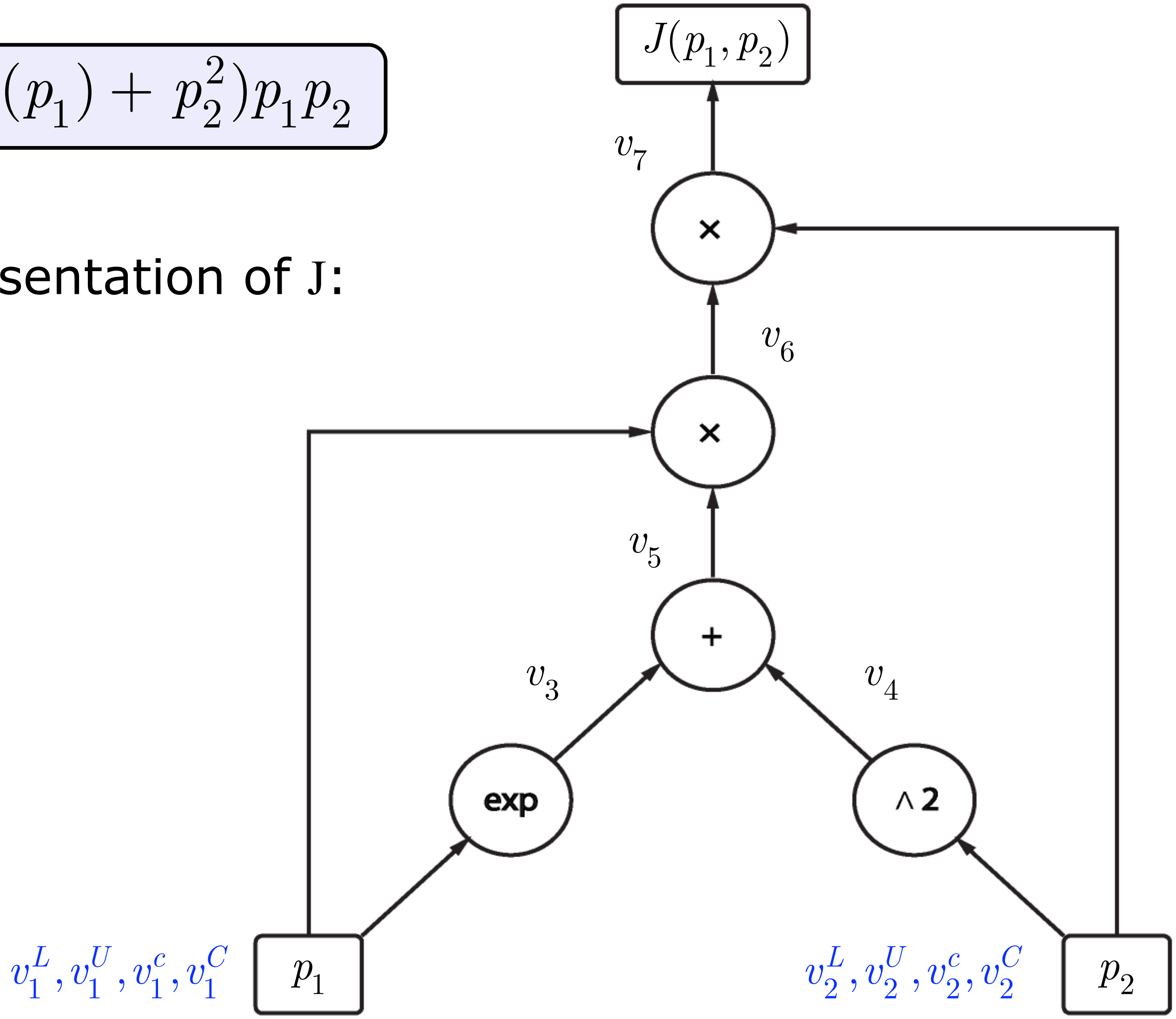

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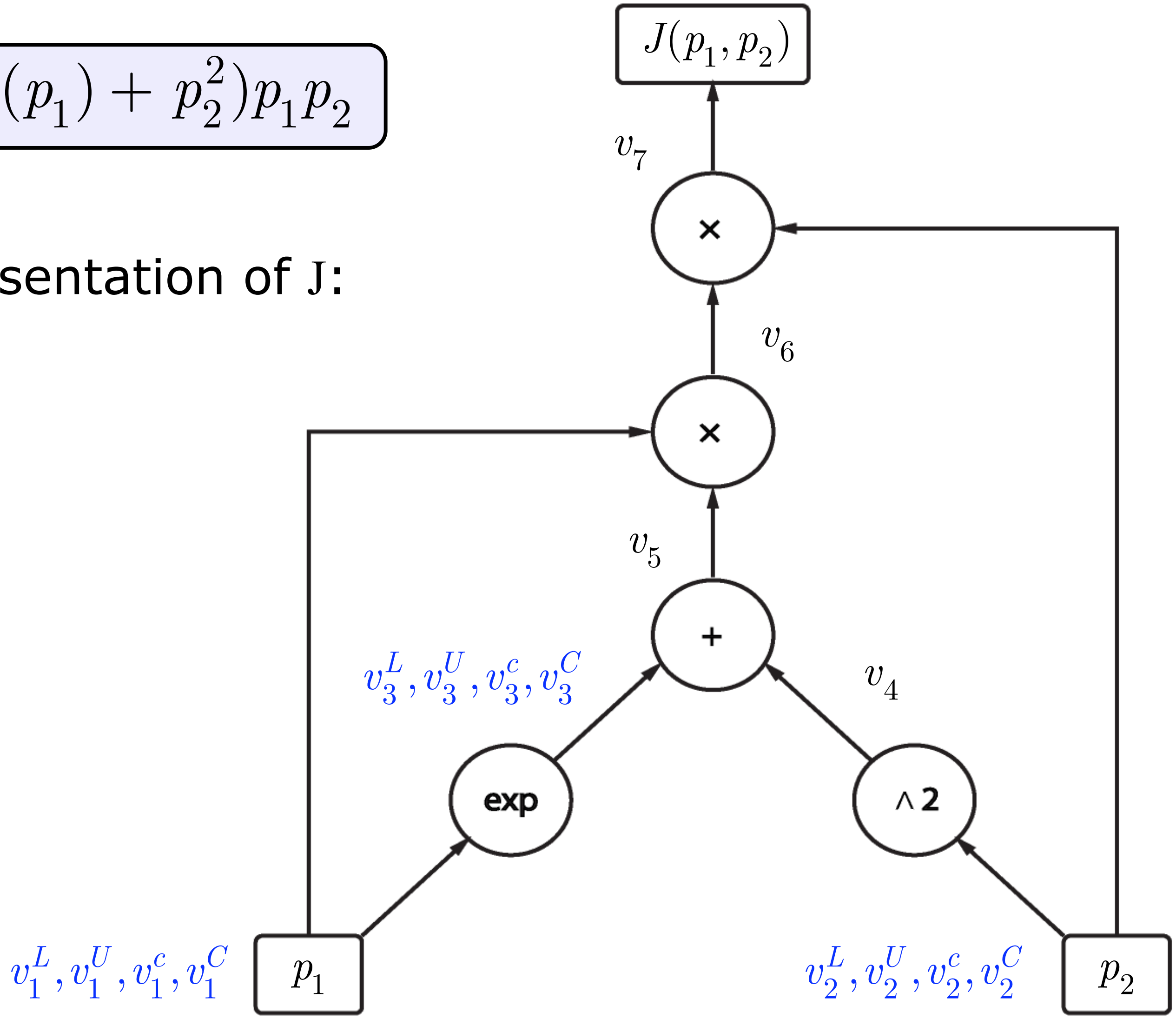

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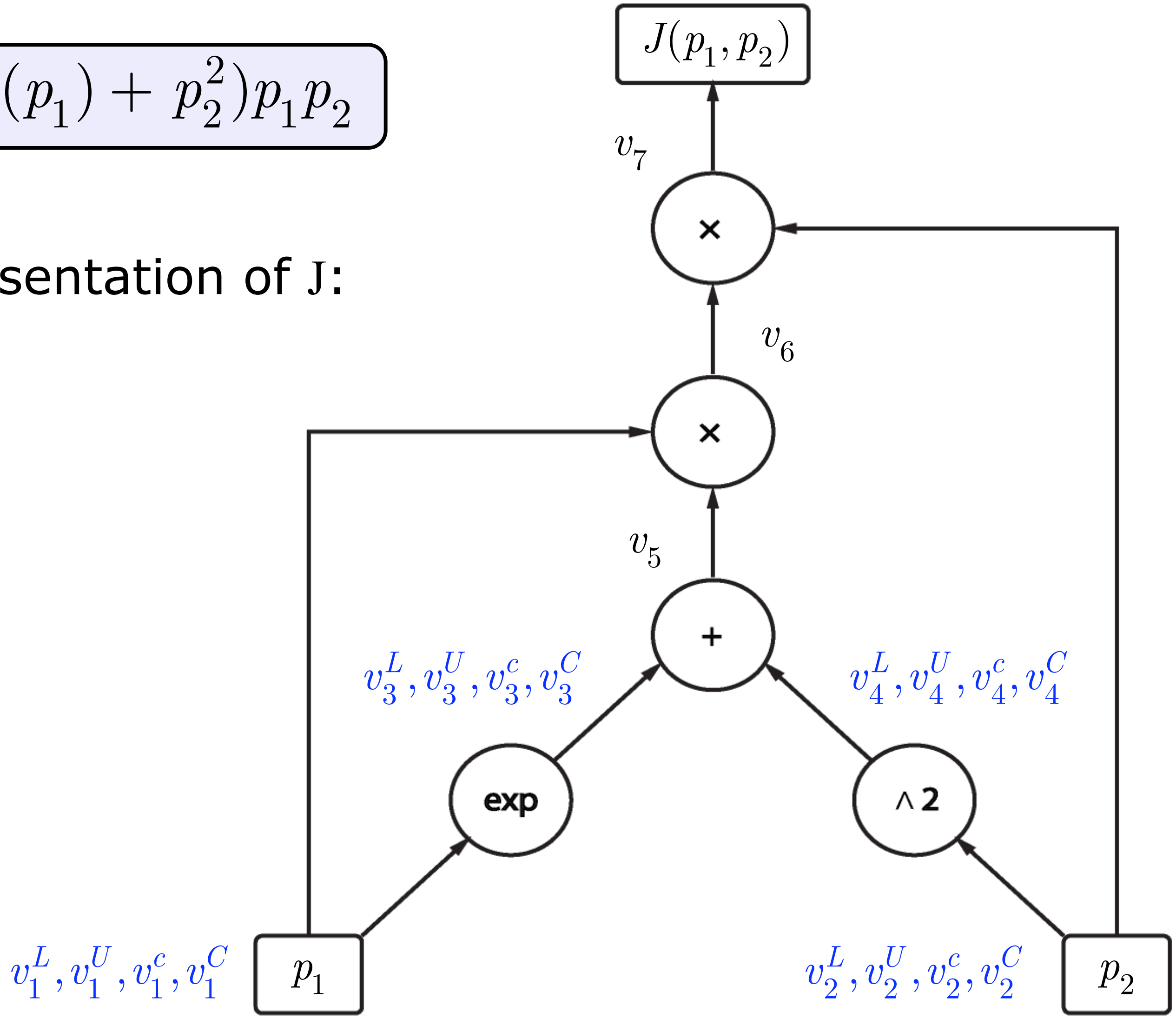

McCormick's Relaxations

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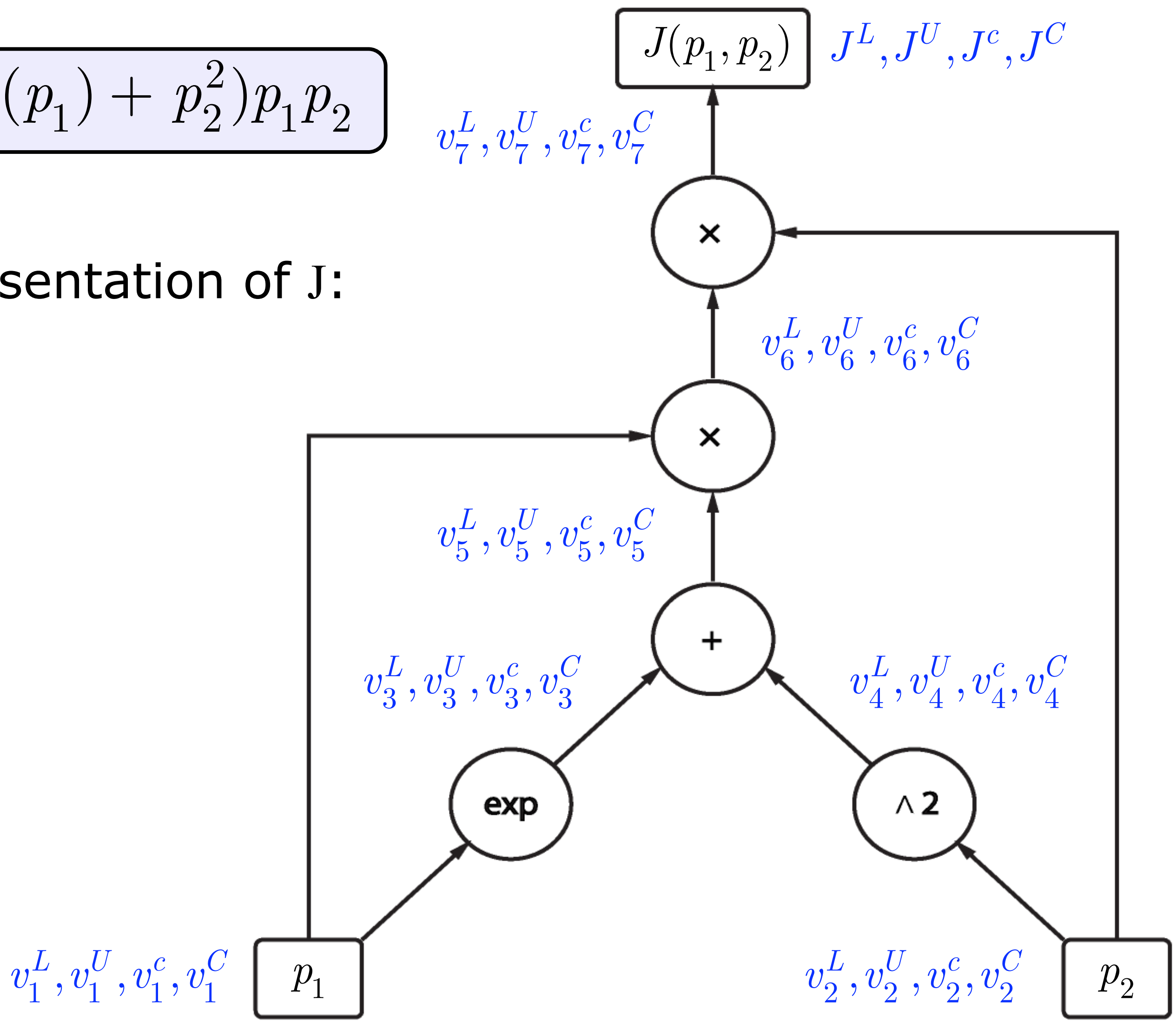
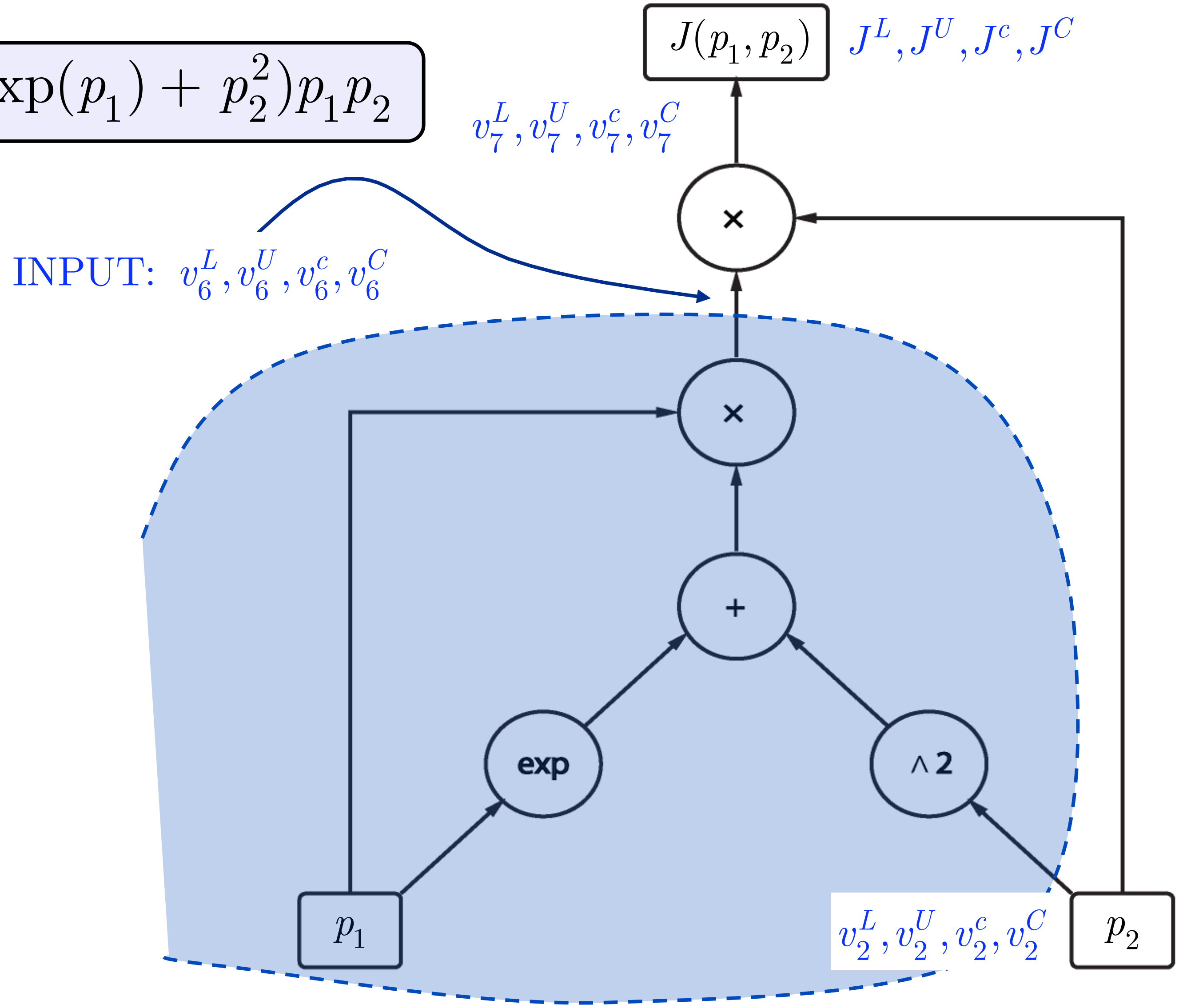


Generalized MC Relaxations

$$J(p_1, p_2) = (\exp(p_1) + p_2^2)p_1p_2$$



Generalized MC Relaxations

$$J(\mathbf{p}) = \phi(\mathbf{p}, x(t_f, \mathbf{p}))$$

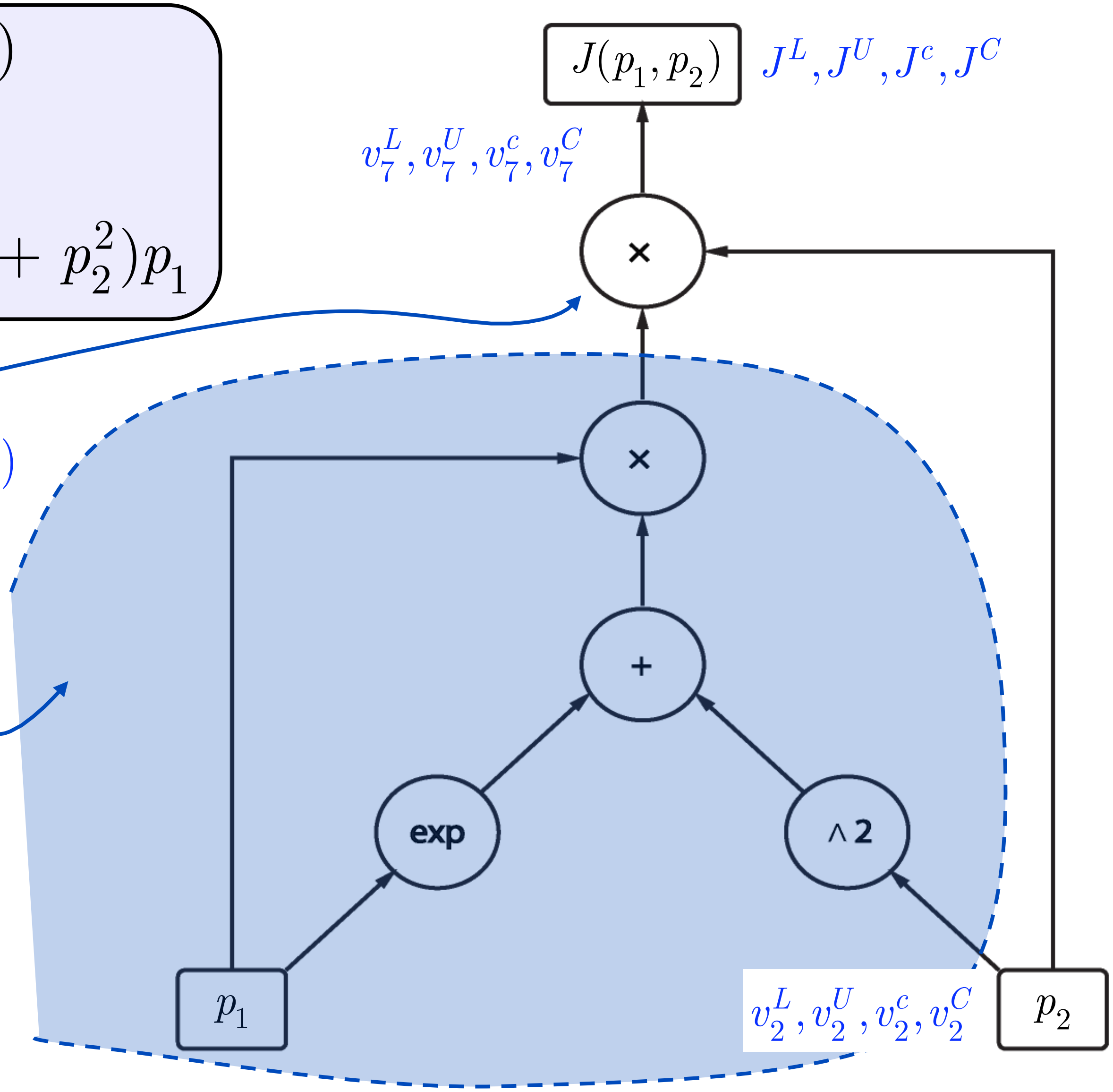
$$\phi(\mathbf{p}, z) = z p_2$$

$$x(t_f, \mathbf{p}) = (\exp(p_1) + p_2^2) p_1$$

INPUT:

$x^L(t_f), x^U(t_f), x^c(t_f, \mathbf{p}), x^C(t_f, \mathbf{p})$

$x(t_f, \mathbf{p})$

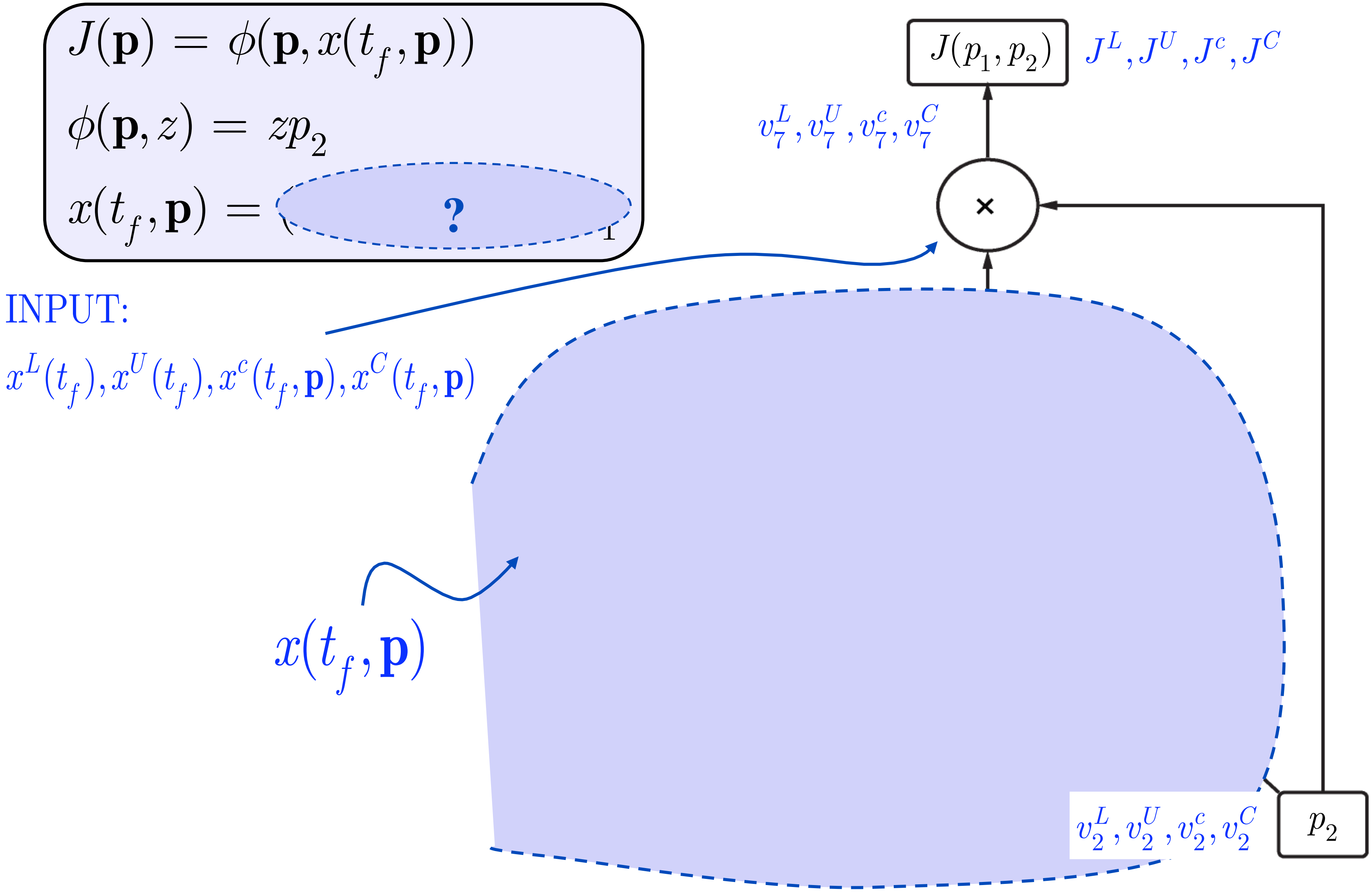


Generalized MC Relaxations

$$J(\mathbf{p}) = \phi(\mathbf{p}, x(t_f, \mathbf{p}))$$

$$\phi(\mathbf{p}, z) = z p_2$$

$$x(t_f, \mathbf{p}) = \ ?$$



Solution Strategy

$$\min_{\mathbf{p}\in P} \; J(\mathbf{p}) \equiv \phi(\mathbf{p},\mathbf{x}(t_f,\mathbf{p}),\mathbf{y}(t_f,\mathbf{p})) + \int_{t_0}^{t_f} \ell(s,\mathbf{p},\mathbf{x}(s,\mathbf{p}),\mathbf{y}(s,\mathbf{p}))ds$$

$$\text{s.t.} \quad \mathbf{G}(\mathbf{p}) \equiv \psi(\mathbf{p},\mathbf{x}(t_f,\mathbf{p}),\mathbf{y}(t_f,\mathbf{p})) + \int_{t_0}^{t_f} \xi(s,\mathbf{p},\mathbf{x}(s,\mathbf{p}),\mathbf{y}(s,\mathbf{p}))ds \leq \mathbf{0}$$

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{x}(t_0,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}),$$
$$\mathbf{0} = \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{y}(t_0,\hat{\mathbf{p}}) = \mathbf{y}_0(\hat{\mathbf{p}}).$$

- Computing J^c and $\mathbf{G}^c$ reduces to computing:
  - Interval bounds for $\mathbf{x}(t,\cdot)$ and $\mathbf{y}(t,\cdot)$ on P
  - Convex/concave relaxations of $\mathbf{x}(t,\cdot)$ and $\mathbf{y}(t,\cdot)$ on P

$$\min_{\mathbf{p}\in P} \; J(\mathbf{p}) \qquad \text{s.t.} \quad \mathbf{G}(\mathbf{p}) \leq \mathbf{0}$$

$$\min_{\mathbf{p}\in P} \; J^c(\mathbf{p}) \qquad \text{s.t.} \quad \mathbf{G}^c(\mathbf{p}) \leq \mathbf{0}$$

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Relaxations for DAEs

$$\begin{aligned}\dot{\mathbf{x}}(t,\mathbf{p}) &= \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{x}(t_0,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}),\\ \mathbf{0} &= \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{y}(t_0,\hat{\mathbf{p}}) = \mathbf{y}_0(\hat{\mathbf{p}}).\end{aligned}$$

- State Relaxations:

$$\left.\begin{aligned}\mathbf{x}^c(t,\mathbf{p}) \le \mathbf{x}(t,\mathbf{p}) \le \mathbf{x}^C(t,\mathbf{p})\\ \mathbf{y}^c(t,\mathbf{p}) \le \mathbf{y}(t,\mathbf{p}) \le \mathbf{y}^C(t,\mathbf{p})\end{aligned}\right\} \quad \forall (t,\mathbf{p}) \in [t_0,t_f] \times P$$

Relaxations for DAEs

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{x}(t_0,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}),$$
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- State Relaxations:

$$\left.\begin{array}{l}\mathbf{x}^c(t,\mathbf{p}) \le \mathbf{x}(t,\mathbf{p}) \le \mathbf{x}^C(t,\mathbf{p}) \\ \mathbf{y}^c(t,\mathbf{p}) \le \mathbf{y}(t,\mathbf{p}) \le \mathbf{y}^C(t,\mathbf{p})\end{array}\right\} \quad \forall (t,\mathbf{p}) \in [t_0,t_f] \times P$$

Convex on P for each t

Concave on P for each t

Relaxations for DAEs

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{x}(t_0,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}),$$
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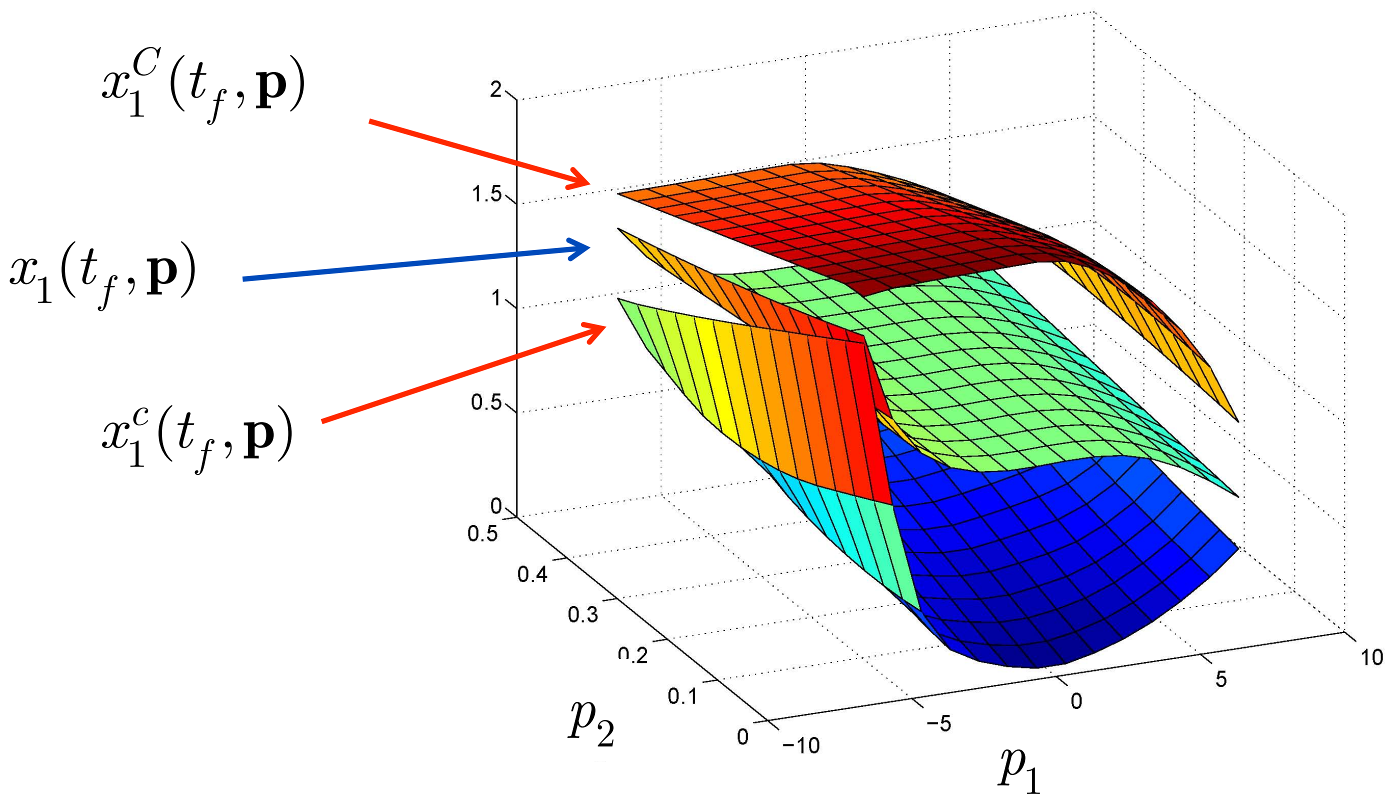

Relaxations for DAEs

$$\begin{aligned}\dot{\mathbf{x}}(t,\mathbf{p}) &= \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{x}(t_0,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}),\\ \mathbf{0} &= \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{y}(t_0,\hat{\mathbf{p}}) = \mathbf{y}_0(\hat{\mathbf{p}}).\end{aligned}$$

- Deriving relaxations requires interval bounds
  - Suppose for now:

$$\mathbf{x}^L(t) \leq \mathbf{x}(t,\mathbf{p}) \leq \mathbf{x}^U(t)$$
$$\mathbf{y}^L(t) \leq \mathbf{y}(t,\mathbf{p}) \leq \mathbf{y}^U(t)$$
$$\forall \mathbf{p} \in P, \quad \forall t \in [t_0, t_f]$$

Relaxations for DAEs

- Use generalized McCormick technique to derive:

$$\mathbf{u}_f, \mathbf{o}_f : [t_0, t_f] \times P \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_y} \longrightarrow \mathbb{R}^{n_x}$$

Convex / **Concave**

$$\varphi^c(t,\mathbf{p}) \le \mathbf{x}(t,\mathbf{p}) \le \varphi^C(t,\mathbf{p})$$

$$\psi^c(t,\mathbf{p}) \le \mathbf{y}(t,\mathbf{p}) \le \psi^C(t,\mathbf{p})$$

$$\mathbf{u}_f(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p}),\psi^c(t,\mathbf{p}),\psi^C(t,\mathbf{p}))$$

$$\le \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})) \le$$

$$\mathbf{o}_f(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p}),\psi^c(t,\mathbf{p}),\psi^C(t,\mathbf{p}))$$

Relaxations for DAEs

- Suppose that $\mathbf{g}$ has the form

$$\mathbf{y}(t,\mathbf{p}) = \mathbf{h}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$

Relaxations for DAEs

- Suppose that $\mathbf{g}$ has the form

$$\mathbf{y}(t,\mathbf{p}) = \mathbf{h}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$

Convex | Concave

$$\varphi^c(t,\mathbf{p}) \leq \mathbf{x}(t,\mathbf{p}) \leq \varphi^C(t,\mathbf{p})$$

$$\psi^c(t,\mathbf{p}) \leq \mathbf{y}(t,\mathbf{p}) \leq \psi^C(t,\mathbf{p})$$

$$\mathbf{u}_h(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p}),\psi^c(t,\mathbf{p}),\psi^C(t,\mathbf{p}))$$

$$\leq \mathbf{h}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})) \leq$$

$$\mathbf{o}_h(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p}),\psi^c(t,\mathbf{p}),\psi^C(t,\mathbf{p}))$$

Relaxations for DAEs

- Suppose that $\mathbf{g}$ has the form

$$\mathbf{y}(t,\mathbf{p}) = \mathbf{h}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$

- Interval bounds are trivially relaxations
  - Define:

$$\bar{\mathbf{y}}^c(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p})) = \mathbf{u}_h(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p}),\mathbf{y}^L(t),\mathbf{y}^U(t))$$

$$\bar{\mathbf{y}}^C(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p})) = \mathbf{o}_h(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p}),\mathbf{y}^L(t),\mathbf{y}^U(t))$$

- Can be refined iteratively for tighter relaxations

Relaxations for DAEs

- Suppose that $\mathbf{g}$ has the form

$$\mathbf{y}(t,\mathbf{p}) = \mathbf{h}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$

Convex **Concave**

$$\varphi^c(t,\mathbf{p}) \leq \mathbf{x}(t,\mathbf{p}) \leq \varphi^C(t,\mathbf{p})$$

$$\psi^c(t,\mathbf{p}) \leq \mathbf{y}(t,\mathbf{p}) \leq \psi^C(t,\mathbf{p})$$

$$\overline{\mathbf{y}}^c(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p})) \leq \mathbf{y}(t,\mathbf{p})) \leq \overline{\mathbf{y}}^C(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p}))$$

Relaxations for DAEs

- Suppose that $\mathbf{g}$ has the form

$$\mathbf{y}(t,\mathbf{p}) = \mathbf{h}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$

Convex **Concave**

$$\varphi^c(t,\mathbf{p}) \leq \mathbf{x}(t,\mathbf{p}) \leq \varphi^C(t,\mathbf{p})$$

$$\psi^c(t,\mathbf{p}) \leq \mathbf{y}(t,\mathbf{p}) \leq \psi^C(t,\mathbf{p})$$

$$\bar{\mathbf{y}}^c(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p})) \leq \mathbf{y}(t,\mathbf{p})) \leq \bar{\mathbf{y}}^C(t,\mathbf{p},\varphi^c(t,\mathbf{p}),\varphi^C(t,\mathbf{p}))$$

- Analogous functions can be derived in the general case
  - McCormick extensions of interval Newton-type methods

Relaxations for DAEs

- Use $\mathbf{u}_{\mathrm{f}}$ and $\mathbf{o}_{\mathrm{f}}$ to inductively define a sequence of relaxations

Convex — Concave

$$\mathbf{x}^{c,k}(t,\mathbf{p}) \leq \mathbf{x}(t,\mathbf{p}) \leq \mathbf{x}^{C,k}(t,\mathbf{p})$$

$$\mathbf{y}(t,\mathbf{p}) = \mathbf{h}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$

$$\mathbf{y}^{c,k}(t,\mathbf{p}) =$$

$$\mathbf{y}^{C,k}(t,\mathbf{p}) =$$

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$$\mathbf{y}(t,\mathbf{p}) = \mathbf{h}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$

$$\mathbf{y}^{c,k}(t,\mathbf{p}) = \bar{\mathbf{y}}^{c}(t,\mathbf{p},\mathbf{x}^{c,k}(t,\mathbf{p}),\mathbf{x}^{C,k}(t,\mathbf{p}))$$

$$\mathbf{y}^{C,k}(t,\mathbf{p}) = \bar{\mathbf{y}}^{C}(t,\mathbf{p},\mathbf{x}^{c,k}(t,\mathbf{p}),\mathbf{x}^{C,k}(t,\mathbf{p}))$$

Relaxations for DAEs

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Convex | Concave

$$\mathbf{x}^{c,k}(t,\mathbf{p}) \leq \mathbf{x}(t,\mathbf{p}) \leq \mathbf{x}^{C,k}(t,\mathbf{p})$$

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$$\mathbf{x}(t,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}) + \int_{t_0}^{t} \mathbf{f}(s,\mathbf{p},\mathbf{x}(s,\mathbf{p}),\mathbf{y}(s,\mathbf{p}))ds$$

$$\mathbf{x}^{c,k+1}(t,\mathbf{p}) =$$

$$\mathbf{x}^{C,k+1}(t,\mathbf{p}) =$$

Relaxations for DAEs

- Use $\mathbf{u}_f$ and $\mathbf{o}_f$ to inductively define a sequence of relaxations

Convex | Concave

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$$\mathbf{x}^{c,k+1}(t,\mathbf{p}) = \mathbf{x}_0^c(\mathbf{p})$$

$$\mathbf{x}^{C,k+1}(t,\mathbf{p}) = \mathbf{x}_0^C(\mathbf{p})$$

McCormick relaxations of $\mathbf{x}_0$ on P

Relaxations for DAEs

- Use $\mathbf{u}_f$ and $\mathbf{o}_f$ to inductively define a sequence of relaxations

Convex | | Concave

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Relaxations for DAEs

Theorem : If $\ell(t,\mathbf{p})$ is convex w.r.t. $\mathbf{p}$ for each fixed $t \in [t_0, t_f]$, then

$$L(t,\mathbf{p}) = \int_{t_0}^{t} \ell(s,\mathbf{p})ds$$

is convex w.r.t. $\mathbf{p}$ for each fixed $t \in [t_0, t_f]$.

$$\mathbf{x}(t,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}) + \int_{t_0}^{t} \mathbf{f}(s,\mathbf{p},\mathbf{x}(s,\mathbf{p}),\mathbf{y}(s,\mathbf{p}))ds$$

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Relaxations for DAEs

- Initialize sequence with interval bounds

$$\mathbf{x}^{c,0}(t,\mathbf{p}) = \mathbf{x}^L(t)$$
$$\mathbf{x}^{C,0}(t,\mathbf{p}) = \mathbf{x}^U(t)$$

- Induction shows:

Convex | Concave

$$\underbrace{\mathbf{x}^{c,k}(t,\mathbf{p})}_{\text{Convex}} \leq \mathbf{x}(t,\mathbf{p}) \leq \underbrace{\mathbf{x}^{C,k}(t,\mathbf{p})}_{\text{Concave}} \qquad \forall k \in \mathbb{N}$$

Relaxations for DAEs

- Sequences converge to solutions of

$$\mathbf{x}^c(t,\mathbf{p}) = \mathbf{x}_0^c(\mathbf{p}) + \int_{t_0}^{t} \mathbf{u}_f(s,\mathbf{p},\mathbf{x}^c(s,\mathbf{p}),\mathbf{x}^C(s,\mathbf{p}),\mathbf{y}^c(s,\mathbf{p}),\mathbf{y}^C(s,\mathbf{p}))ds$$

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DAE Example

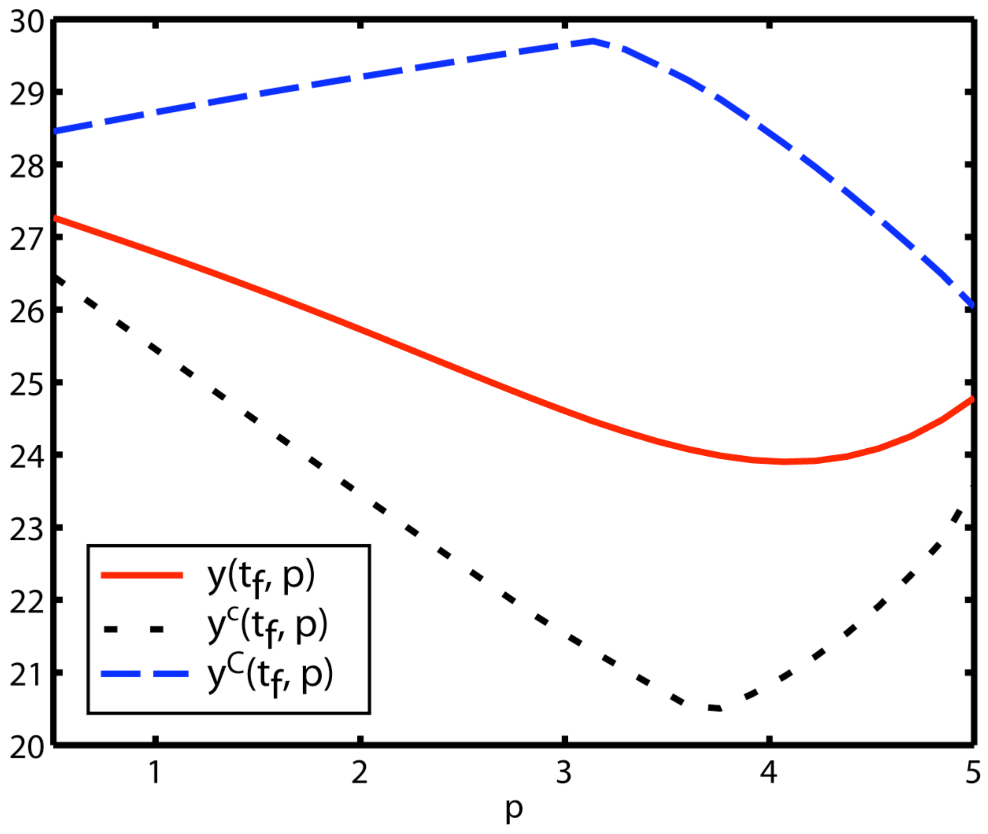
$$\dot{x}(t,p) = -px(t,p) + 0.01y(t,p), \quad x_0 = 1,$$

$$0 = y(t,p) - (y(t,p))^{-1/2}(p - p^3 / 6 + p^5 / 120) - 25x(t,p)$$

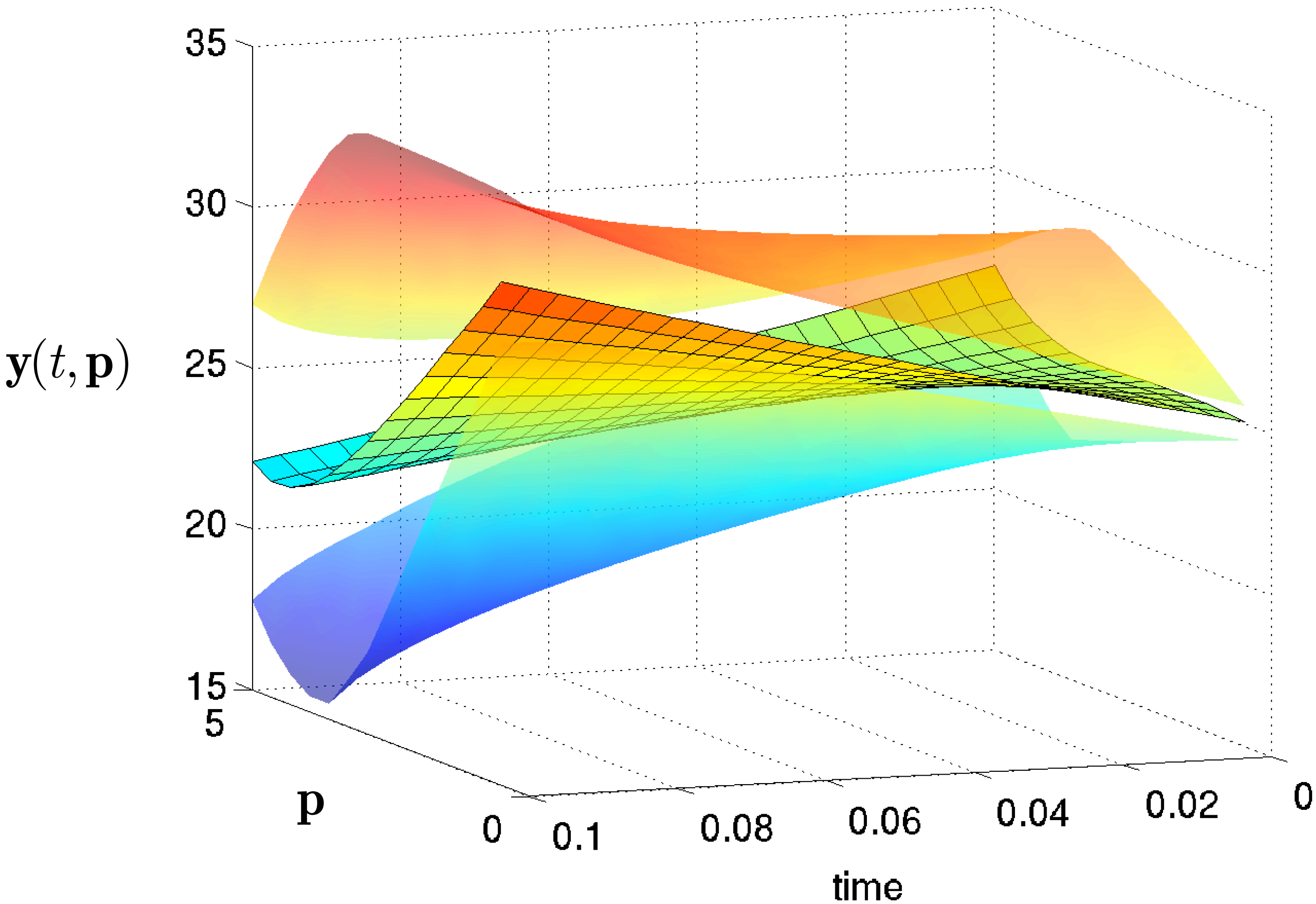
$$P = [0.5, 5.0], \quad I = [0, 0.1].$$

- Compute $\mathbf{u}_{\mathrm{f}}$, $\mathbf{o}_{\mathrm{f}}$, $\mathbf{u}_{\mathrm{h}}$ and $\mathbf{o}_{\mathrm{h}}$ automatically
  - Chachuat, B. libMC, 2007. http://yoric.mit.edu/libMC/

DAE Example

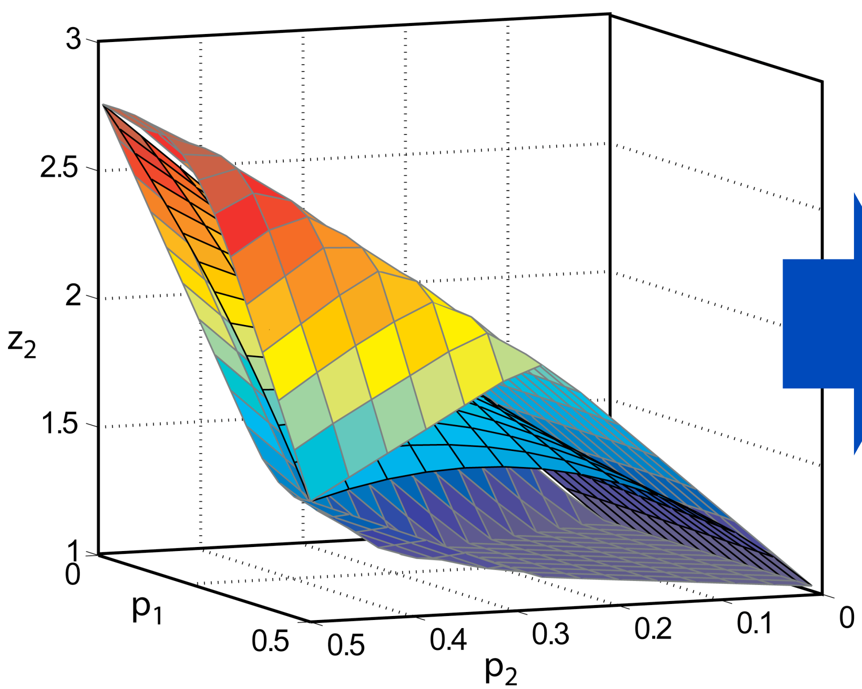


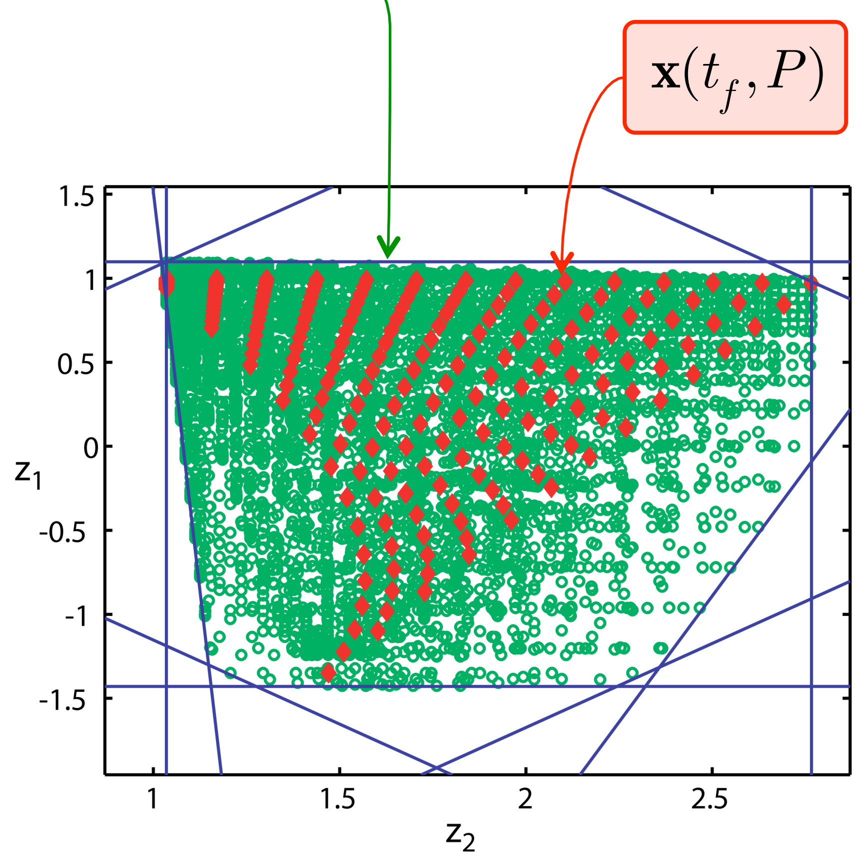
DAE Example


35
30
25
20
15
$\mathbf{y}(t,\mathbf{p})$
5
$\mathbf{p}$
0
0.1
0.08
0.06
0.04
0.02
0
time

Convex Enclosures of Reachable Sets

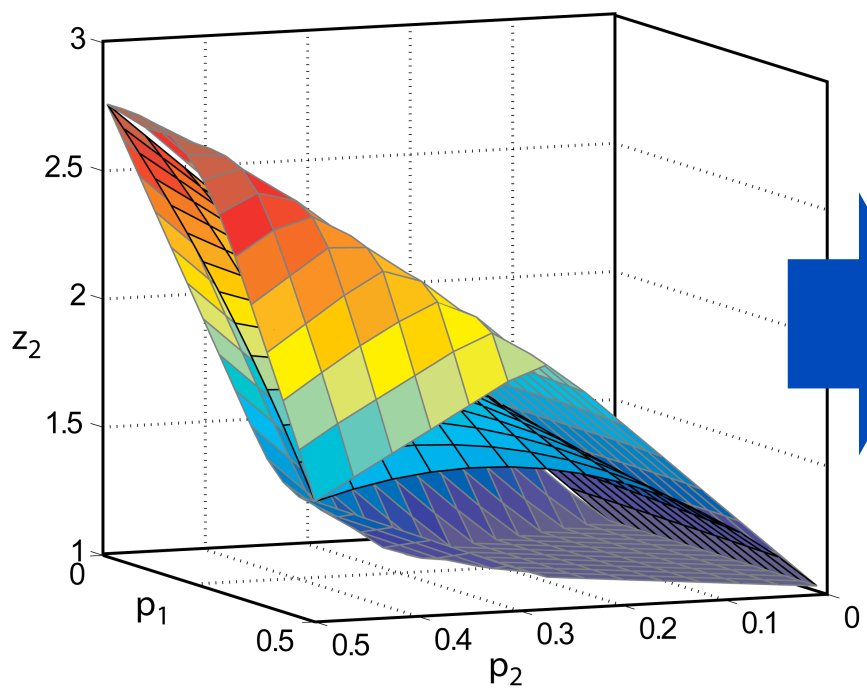
$$A \equiv \bigcup_{\mathbf{p} \in P} [\mathbf{x}^c(t_f, \mathbf{p}), \mathbf{x}^C(t_f, \mathbf{p})]$$

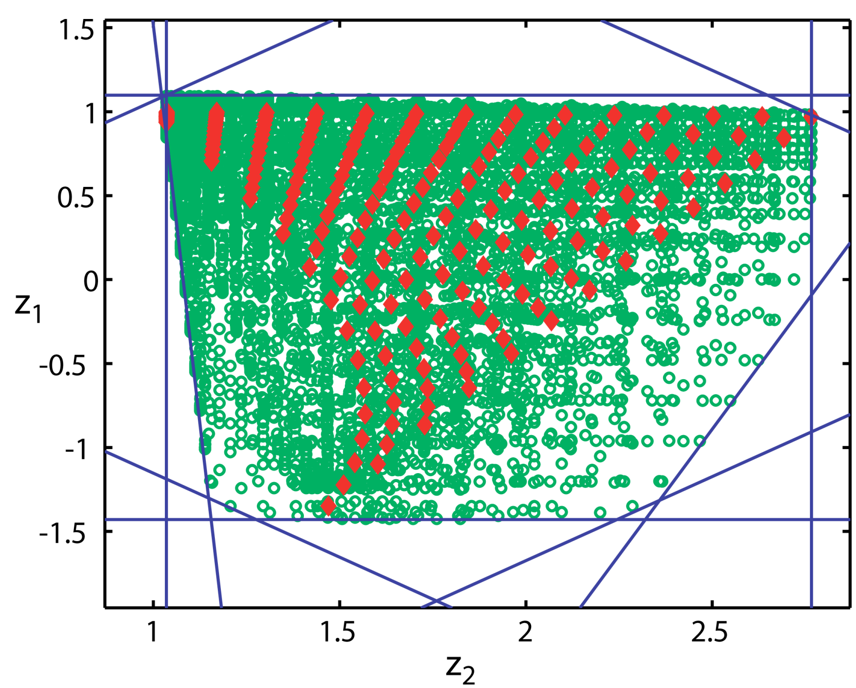




Convex Enclosures of Reachable Sets

$$A \equiv \bigcup_{\mathbf{p}\in P} [\mathbf{x}^c(t_f,\mathbf{p}), \mathbf{x}^C(t_f,\mathbf{p})] \Longleftrightarrow A^* \equiv \bigcap_{\mu\in B(0,1)} H^+(\mu)$$





Convex Enclosures of Reachable Sets

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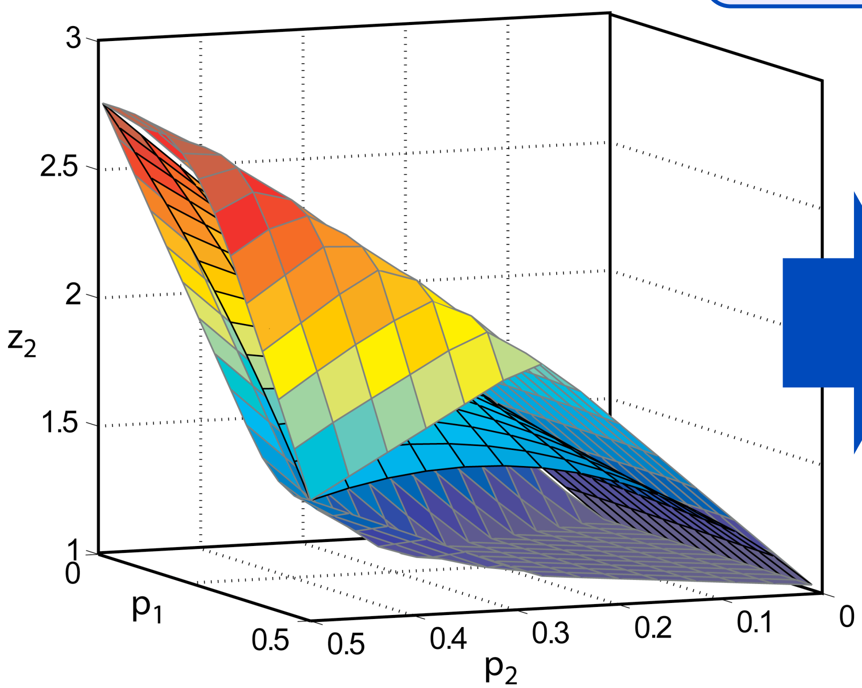
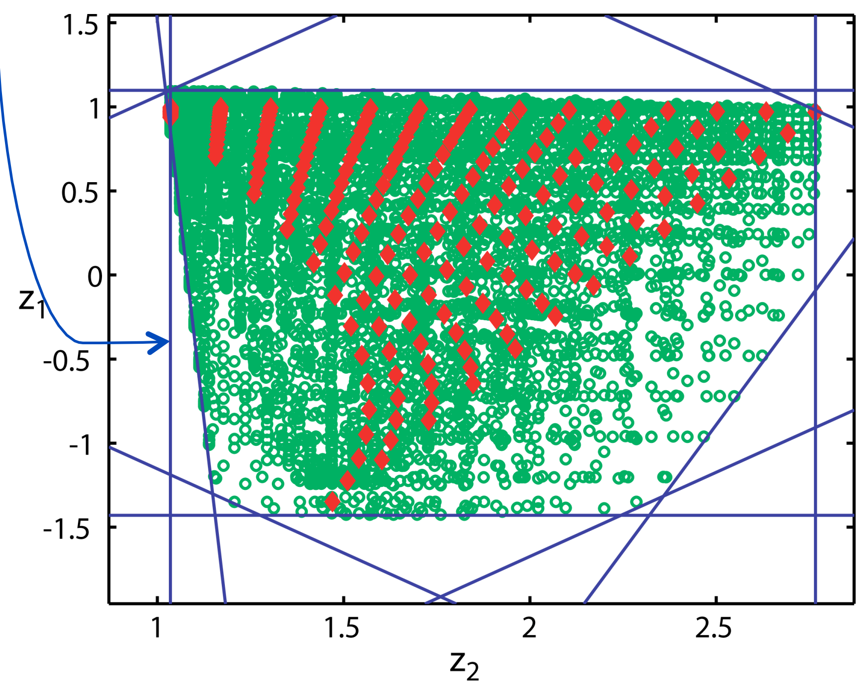
$$H^+(\mu) = \left\{ \mathbf{z} : \mu^T \mathbf{z} \geq d^*(\mu) \right\}$$

$$d^*(\mu) \equiv \min_{\mathbf{p}\in P} \sum_{i=1}^{n_x} \min\left(\mu_i^T x_i^c(t_f,\mathbf{p}), \mu_i^T x_i^C(t_f,\mathbf{p}) \right)$$





DAE Relaxations: Conclusions

- Can construct tight, non-affine relaxations for the parametric solutions of DAEs
  - Enables convex relaxations for general dynamic optimization problems
- No discretization is required
  - No additional optimization variables
- Computational cost is comparable to numerical integration of original model

Outline

- Problem statement
  - Global Dynamic Optimization with DAEs
- Background and approach
  - Generalized McCormick's Relaxations
- Relaxations for DAE solutions
- Interval bounds on DAE solutions
- Future directions

Interval bounds for DAEs

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{x}(t_0,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}),$$
$$\mathbf{0} = \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{y}(t_0,\hat{\mathbf{p}}) = \mathbf{y}_0(\hat{\mathbf{p}}).$$

- State Bounds:

$$\mathbf{x}^L(t) \leq \mathbf{x}(t,\mathbf{p}) \leq \mathbf{x}^U(t)$$
$$\mathbf{y}^L(t) \leq \mathbf{y}(t,\mathbf{p}) \leq \mathbf{y}^U(t)$$
$$\forall \mathbf{p} \in P, \quad \forall t \in [t_0, t_f]$$

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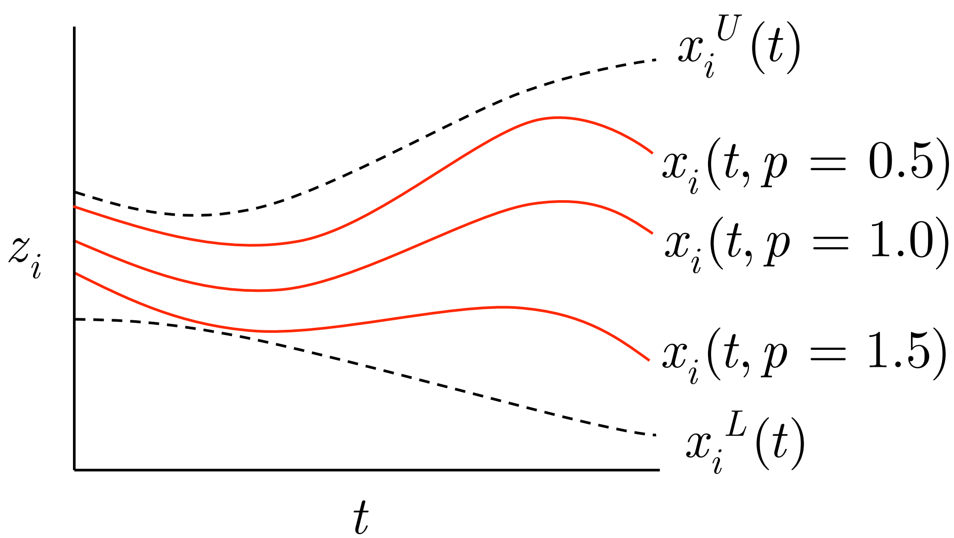

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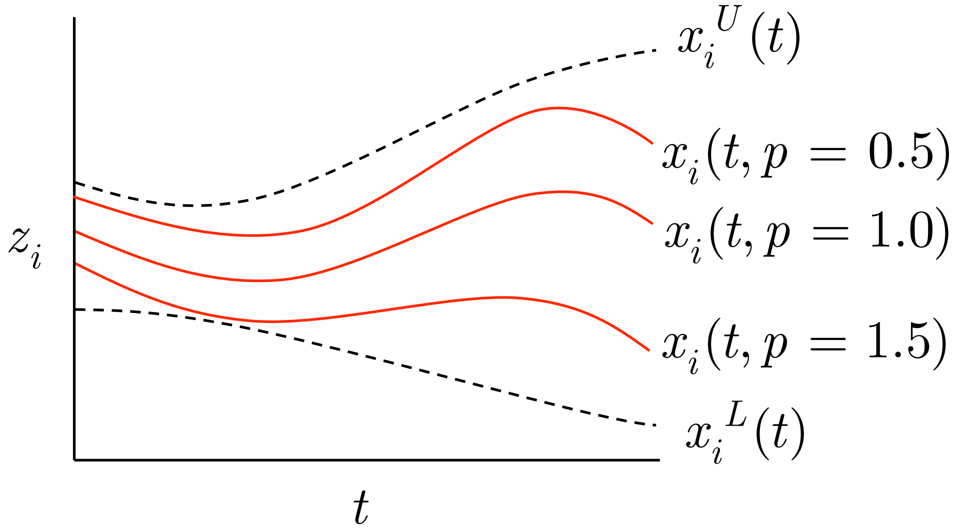

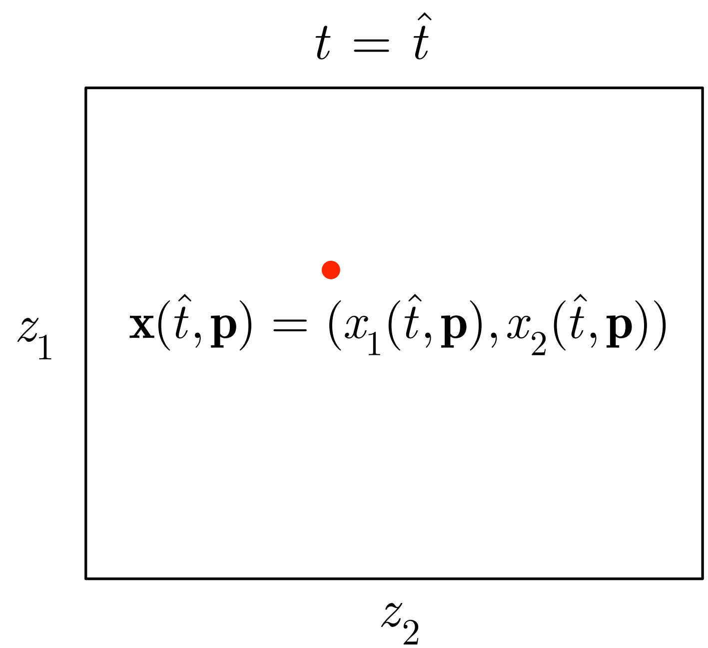

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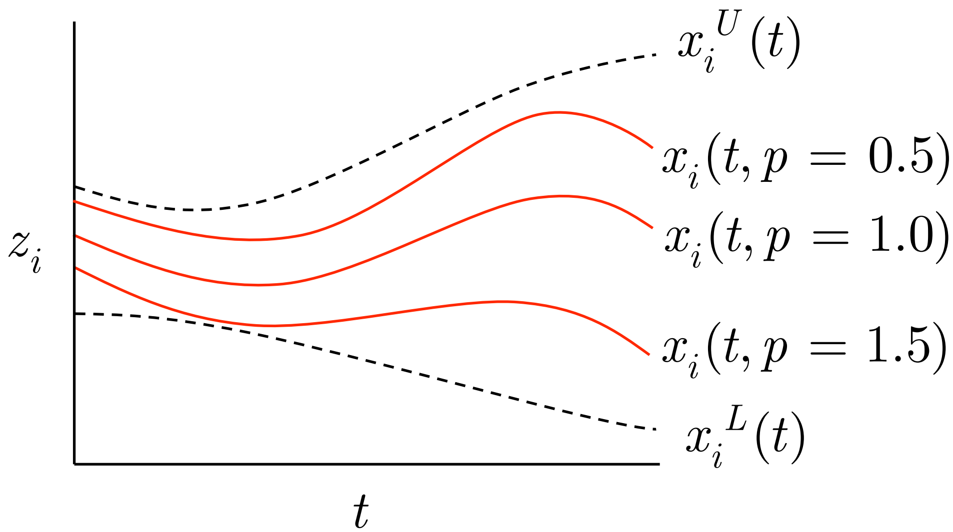

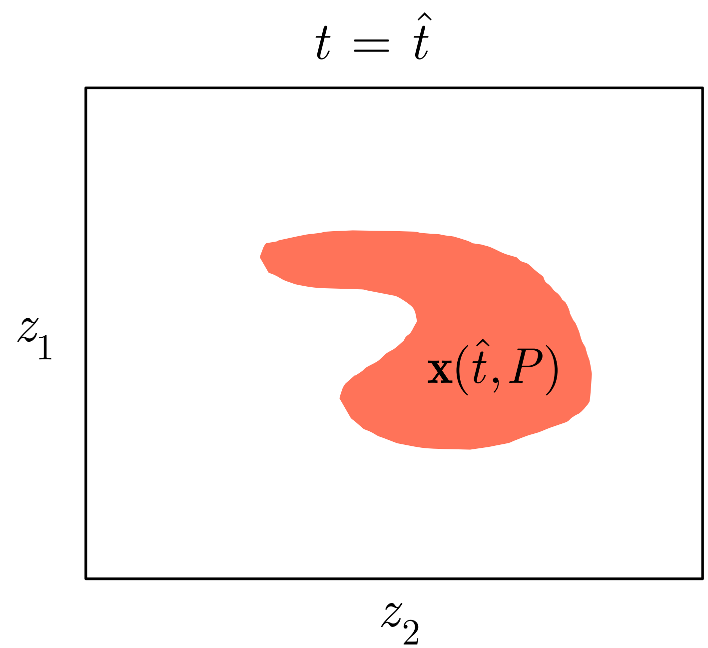

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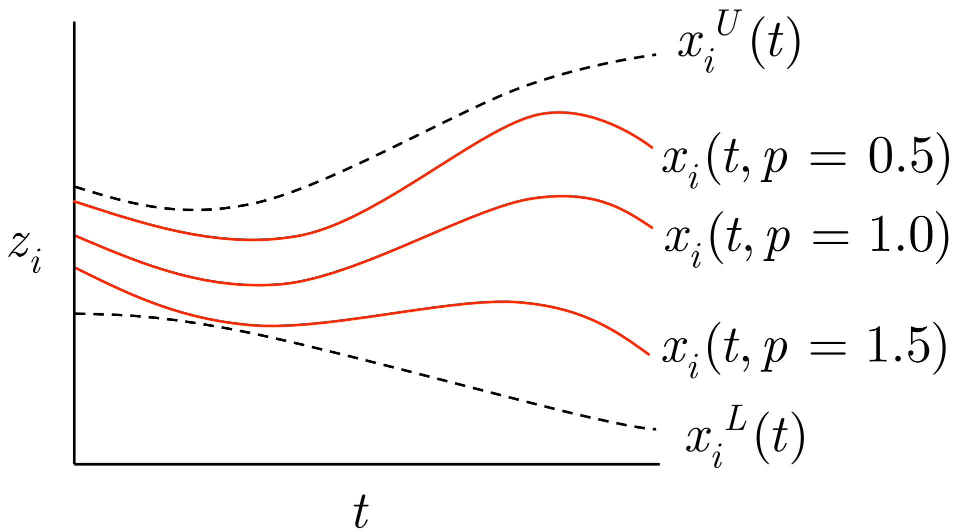

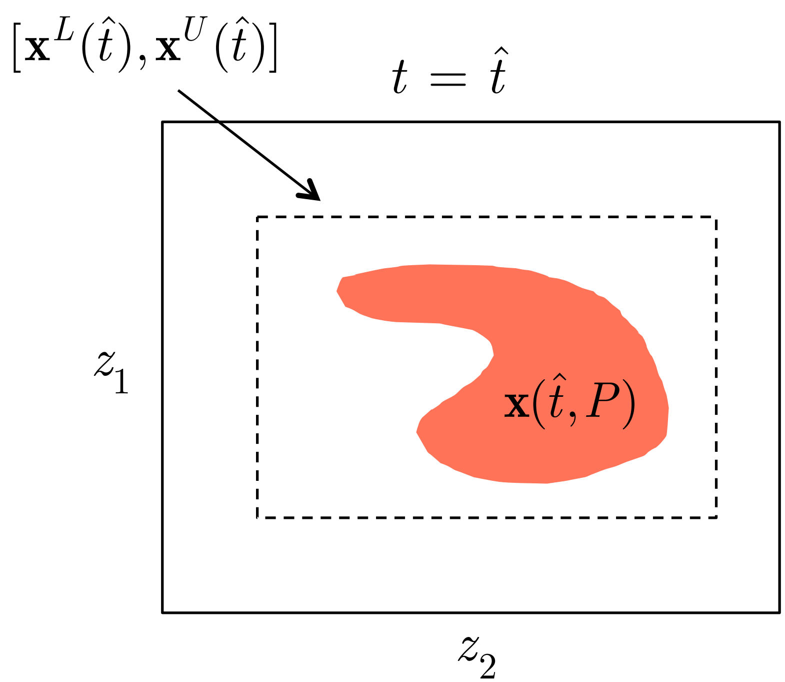

Deriving State Bounds

- Differential Inequalities

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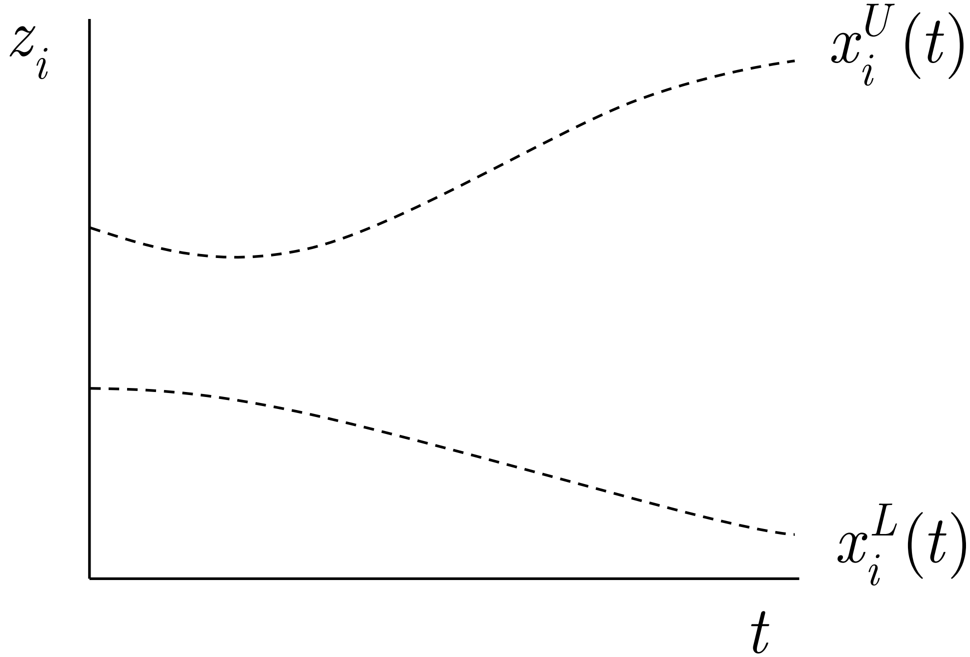

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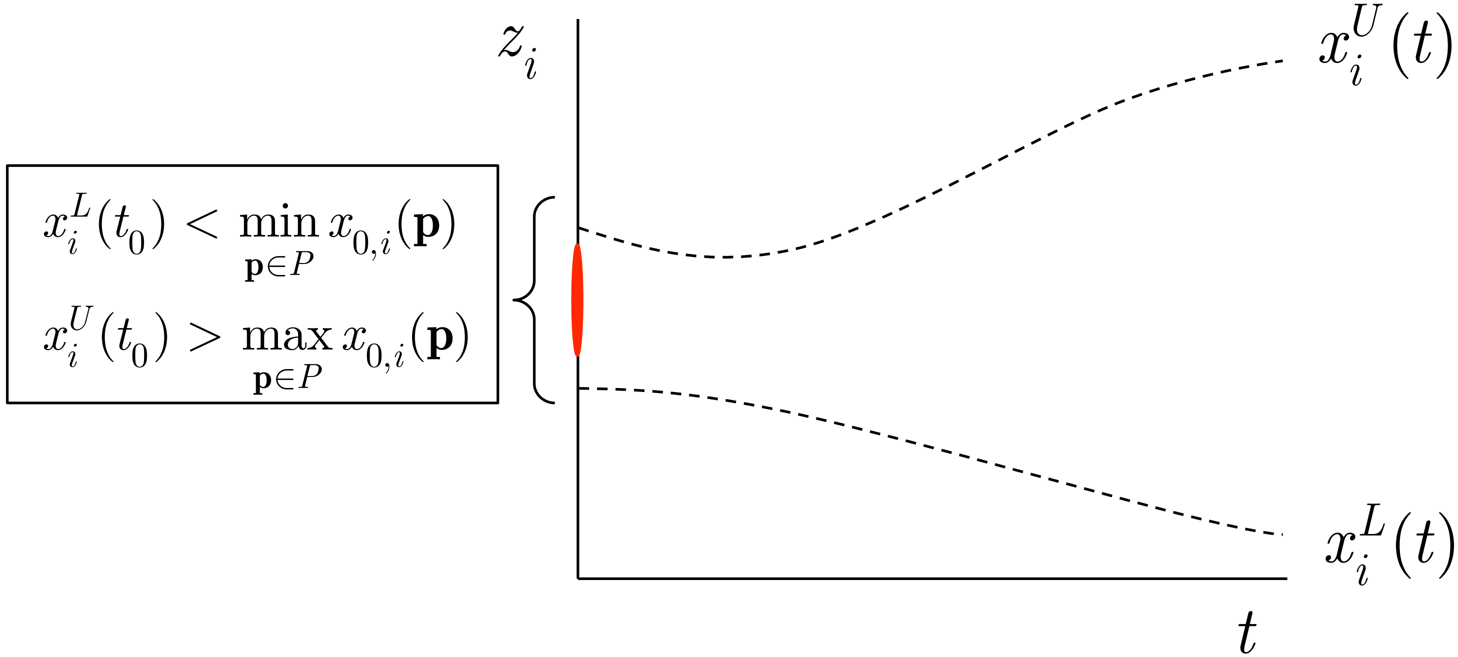

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$$\text{s.t.} \quad \mathbf{p} \in P, \quad \mathbf{z} \in [\mathbf{x}^L(t), \mathbf{x}^U(t)], \quad z_i = x_i^U(t)$$

$$x_i^L(t_0) < \min_{\mathbf{p} \in P} x_{0,i}(\mathbf{p})$$
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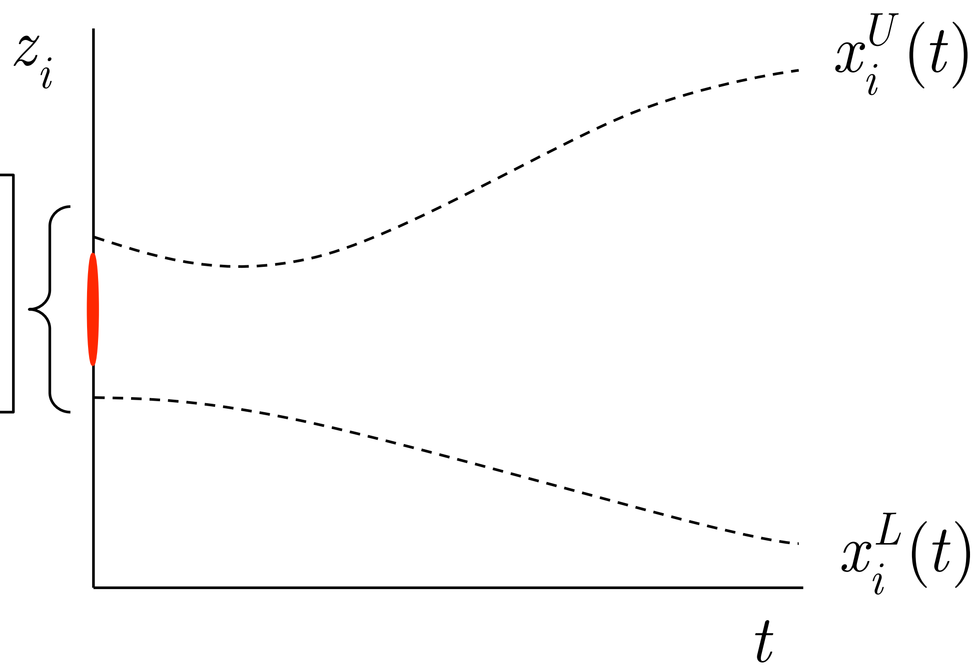

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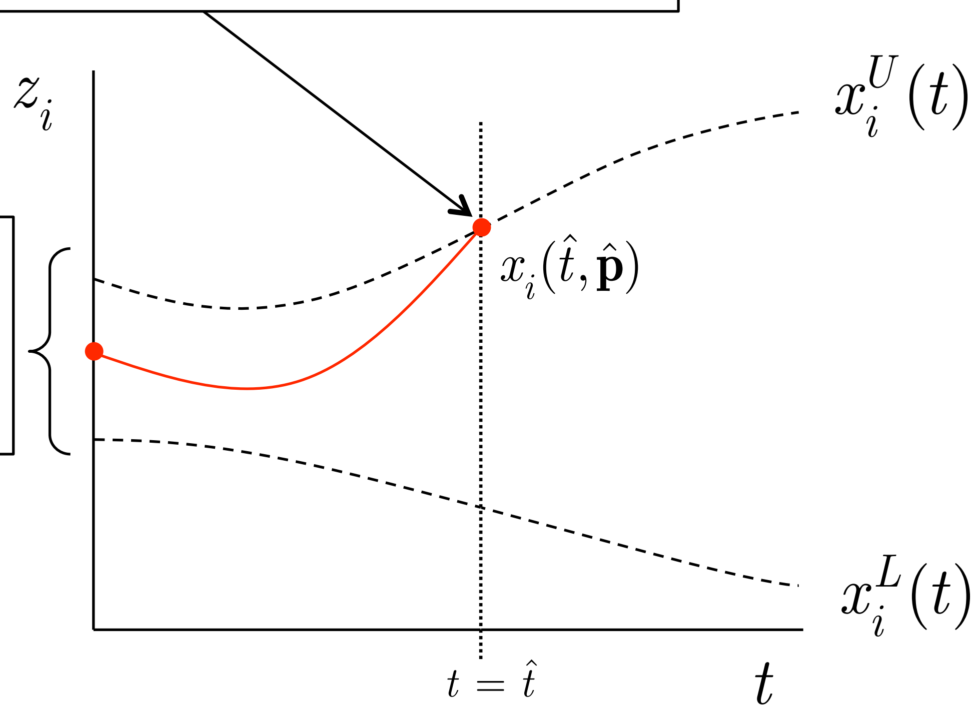

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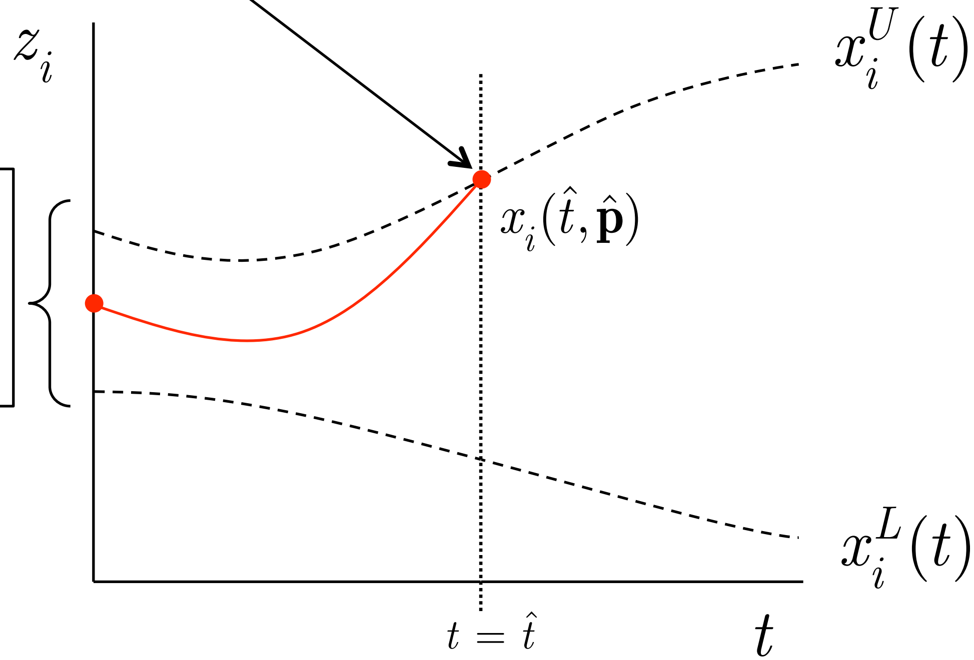

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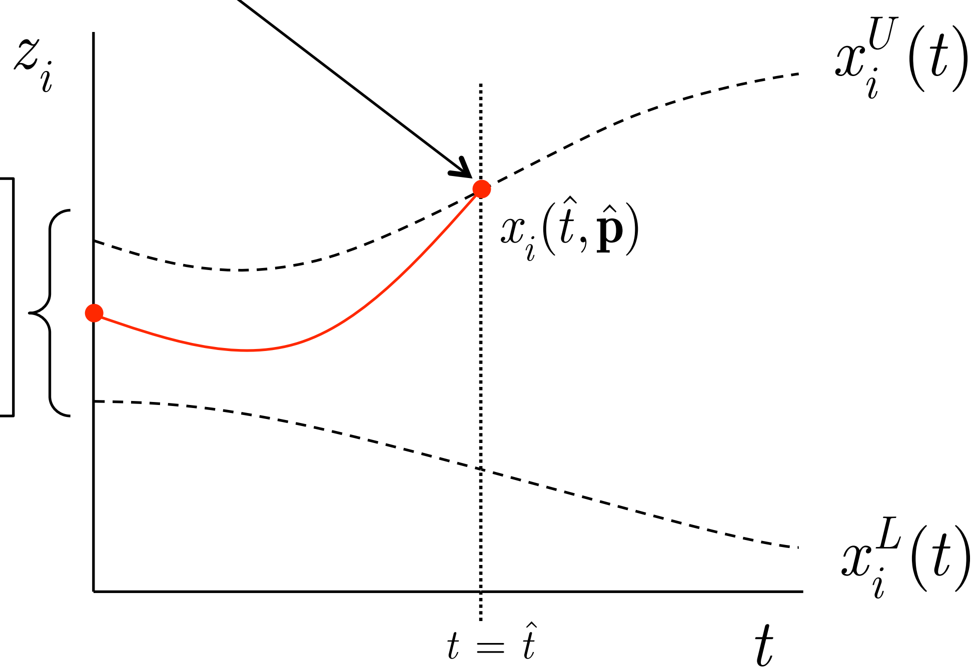

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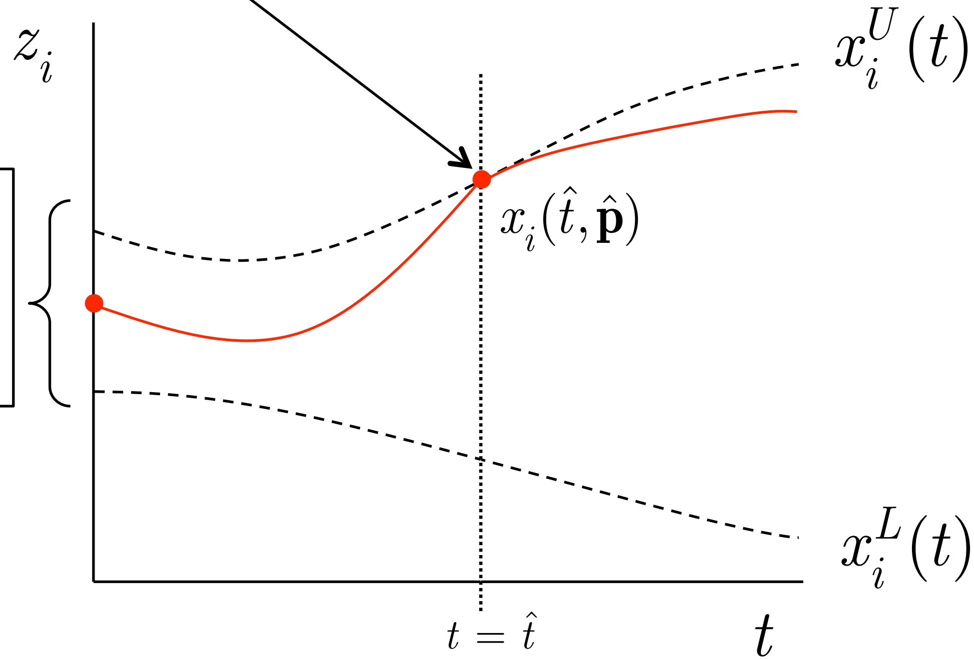

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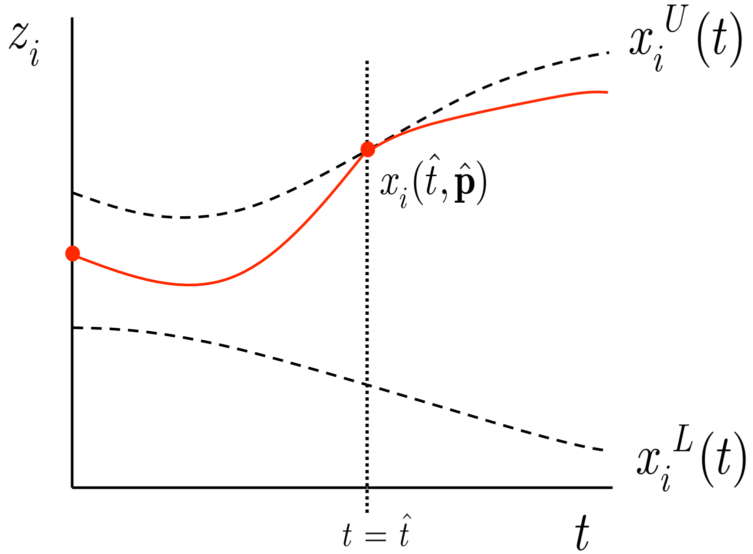
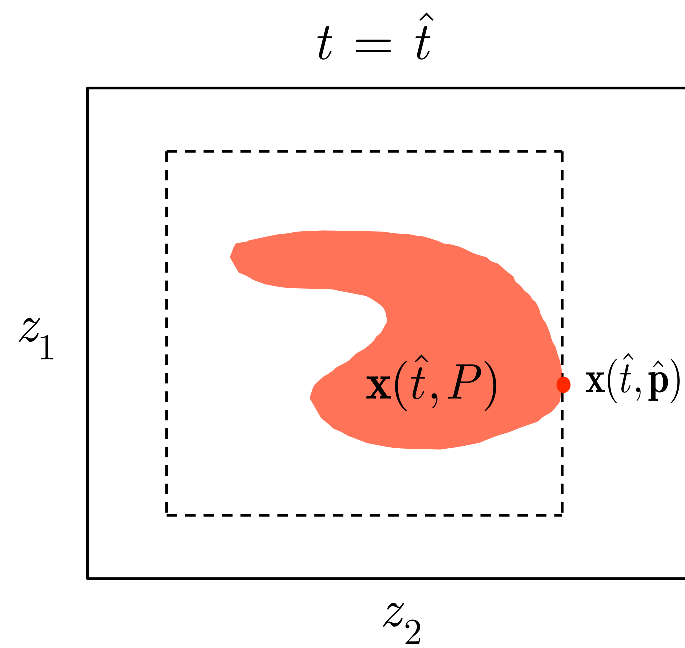
- Differential Inequalities

$$\dot{x}_i^U(t) > \max f_i(t,\mathbf{p},\mathbf{z}) \quad \text{s.t.} \quad \mathbf{p} \in P, \quad \mathbf{z} \in [\mathbf{x}^L(t),\mathbf{x}^U(t)], \quad z_i = x_i^U(t)$$



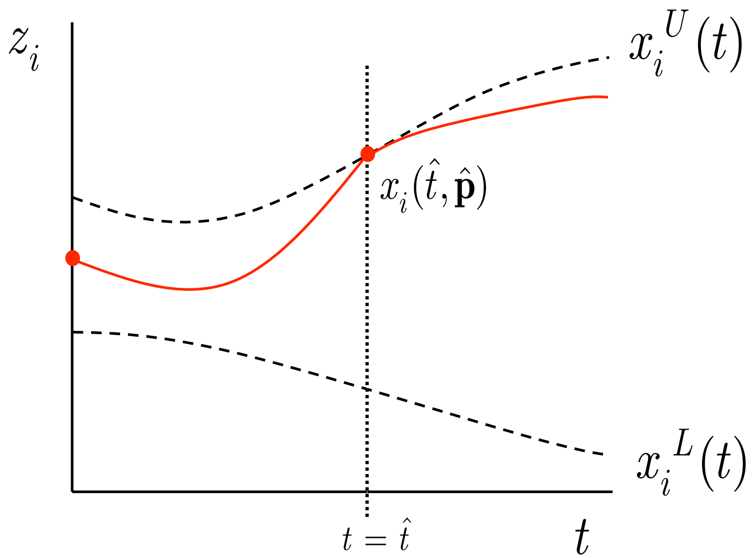


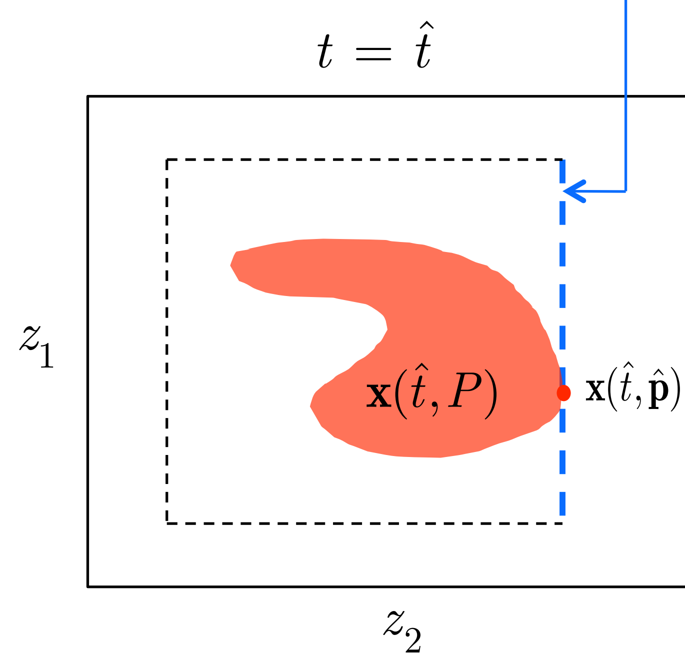
Deriving State Bounds

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}))$$
$$\mathbf{x}(t_0,\mathbf{p}) = \mathbf{x}_0(\mathbf{p})$$

- Differential Inequalities

$$\dot{x}_i^U(t) > \max f_i(t,\mathbf{p},\mathbf{z})$$
$$\text{s.t.} \quad \mathbf{p} \in P, \quad \mathbf{z} \in [\mathbf{x}^L(t),\mathbf{x}^U(t)], \quad z_i = x_i^U(t)$$





Deriving State Bounds

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{x}(t_0,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}),$$
$$\mathbf{0} = \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{y}(t_0,\hat{\mathbf{p}}) = \mathbf{y}_0(\hat{\mathbf{p}}).$$

- Bound the underlying ODE:

$$\frac{\partial \mathbf{g}}{\partial \mathbf{y}}\dot{\mathbf{y}} + \frac{\partial \mathbf{g}}{\partial \mathbf{x}}\dot{\mathbf{x}} + \frac{\partial \mathbf{g}}{\partial t} = \mathbf{0}$$

$$\mathbf{f}_x \equiv \mathbf{f}, \quad \mathbf{f}_y \equiv -\left(\frac{\partial \mathbf{g}}{\partial \mathbf{y}}\right)^{-1}\left(\frac{\partial \mathbf{g}}{\partial \mathbf{x}}\mathbf{f} + \frac{\partial \mathbf{g}}{\partial t}\right)$$

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}_x(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$
$$\dot{\mathbf{y}}(t,\mathbf{p}) = \mathbf{f}_y(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$

Deriving State Bounds

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{x}(t_0,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}),$$
$$\mathbf{0} = \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad \mathbf{y}(t_0,\hat{\mathbf{p}}) = \mathbf{y}_0(\hat{\mathbf{p}}).$$

- Bound the underlying ODE:

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}_x(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$
$$\dot{\mathbf{y}}(t,\mathbf{p}) = \mathbf{f}_y(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$

- Tighten bounds based on:

$$\mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})) = \mathbf{0}$$

Differential Inequalities Result

- Notation:

Let $\mathcal{B}_i^L, \mathcal{B}_i^U : \mathbb{IR}^{n_x} \to \mathbb{IR}^{n_x}$ be defined by

$$\mathcal{B}_i^L([\mathbf{z}^L, \mathbf{z}^U]) \equiv \{\mathbf{z} : \mathbf{z}^L \leq \mathbf{z} \leq \mathbf{z}^U,\ z_i = z_i^L\},$$

$$\mathcal{B}_i^U([\mathbf{z}^L, \mathbf{z}^U]) \equiv \{\mathbf{z} : \mathbf{z}^L \leq \mathbf{z} \leq \mathbf{z}^U,\ z_i = z_i^U\},$$

for every $[\mathbf{z}^L, \mathbf{z}^U] \in \mathbb{IR}^{n_x}$.

Differential Inequalities Result

Let $\mathbf{x}^L, \mathbf{x}^U : [t_0, t_f] \to \mathbb{R}^{n_x}$ and $\mathbf{y}^L, \mathbf{y}^U : [t_0, t_f] \to \mathbb{R}^{n_y}$ be differentiable on (t_0, t_f) and satisfy

(IC): 1. $\mathbf{x}^L(t_0) < \mathbf{x}(t_0, \mathbf{p}) < \mathbf{x}^U(t_0)$.

2. $\mathbf{y}^L(t_0) < \mathbf{y}(t_0, \mathbf{p}) < \mathbf{y}^U(t_0)$.

(RHS): For every $t \in (t_0, t_f]$ and each i, letting $X(t) \equiv [\mathbf{x}^L(t), \mathbf{x}^U(t)]$ and $Y(t) \equiv [\mathbf{y}^L(t), \mathbf{y}^U(t)]$:

1. $\dot{x}_i^L(t) < f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in \mathcal{B}_i^L(X(t)) \cap D_x$, $\mathbf{z}_y \in Y(t) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$
2. $\dot{x}_i^U(t) > f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in \mathcal{B}_i^U(X(t)) \cap D_x$, $\mathbf{z}_y \in Y(t) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$
3. $\dot{\mathrm{y}}_i^L(t) < f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^L(Y(t)) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$
4. $\dot{\mathrm{y}}_i^U(t) > f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^U(Y(t)) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$

Then $\mathbf{x}^L(t) < \mathbf{x}(t, \mathbf{p}) < \mathbf{x}^U(t)$ and $\mathbf{y}^L(t) < \mathbf{y}(t, \mathbf{p}) < \mathbf{y}^U(t)$, $\forall (t, \mathbf{p}) \in [t_0, t_f] \times P$.

Differential Inequalities Result

Let $\mathbf{x}^L, \mathbf{x}^U : [t_0, t_f] \to \mathbb{R}^{n_x}$ and $\mathbf{y}^L, \mathbf{y}^U : [t_0, t_f] \to \mathbb{R}^{n_y}$ be differentiable on (t_0, t_f) and satisfy

(IC):
1. $\mathbf{x}^L(t_0) < \mathbf{x}(t_0, \mathbf{p}) < \mathbf{x}^U(t_0)$.
2. $\mathbf{y}^L(t_0) < \mathbf{y}(t_0, \mathbf{p}) < \mathbf{y}^U(t_0)$.

(RHS): For every $t \in (t_0, t_f]$ and each i, letting $X(t) \equiv [\mathbf{x}^L(t), \mathbf{x}^U(t)]$ and $Y(t) \equiv [\mathbf{y}^L(t), \mathbf{y}^U(t)]$:

1. $\dot{x}_i^L(t) < f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in \mathcal{B}_i^L(X(t)) \cap D_x$, $\mathbf{z}_y \in Y(t) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$
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3. $\dot{y}_i^L(t) < f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^L(Y(t)) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$
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Then $\mathbf{x}^L(t) < \mathbf{x}(t, \mathbf{p}) < \mathbf{x}^U(t)$ and $\mathbf{y}^L(t) < \mathbf{y}(t, \mathbf{p}) < \mathbf{y}^U(t)$, $\forall (t, \mathbf{p}) \in [t_0, t_f] \times P$.

Differential Inequalities Result

Let $\mathbf{x}^L, \mathbf{x}^U : [t_0, t_f] \to \mathbb{R}^{n_x}$ and $\mathbf{y}^L, \mathbf{y}^U : [t_0, t_f] \to \mathbb{R}^{n_y}$ be differentiable on (t_0, t_f) and satisfy

(IC): 1. $\mathbf{x}^L(t_0) < \mathbf{x}(t_0, \mathbf{p}) < \mathbf{x}^U(t_0)$.

2. $\mathbf{y}^L(t_0) < \mathbf{y}(t_0, \mathbf{p}) < \mathbf{y}^U(t_0)$.

(RHS): For every $t \in (t_0, t_f]$ and each i, letting $X(t) \equiv [\mathbf{x}^L(t), \mathbf{x}^U(t)]$ and $Y(t) \equiv [\mathbf{y}^L(t), \mathbf{y}^U(t)]$:

1. $\dot{x}_i^L(t) < f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in \mathcal{B}_i^L(X(t)) \cap D_x$, $\mathbf{z}_y \in Y(t) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$
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3. $\dot{y}_i^L(t) < f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^L(Y(t)) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$
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Then $\mathbf{x}^L(t) < \mathbf{x}(t, \mathbf{p}) < \mathbf{x}^U(t)$ and $\mathbf{y}^L(t) < \mathbf{y}(t, \mathbf{p}) < \mathbf{y}^U(t)$, $\forall (t, \mathbf{p}) \in [t_0, t_f] \times P$.

Differential Inequalities Result

Let $\mathbf{x}^L, \mathbf{x}^U : [t_0, t_f] \to \mathbb{R}^{n_x}$ and $\mathbf{y}^L, \mathbf{y}^U : [t_0, t_f] \to \mathbb{R}^{n_y}$ be differentiable on (t_0, t_f) and satisfy

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3. $\dot{y}_i^L(t) < f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^L(Y(t)) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$
4. $\dot{y}_i^U(t) > f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^U(Y(t)) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$

Then $\mathbf{x}^L(t) < \mathbf{x}(t, \mathbf{p}) < \mathbf{x}^U(t)$ and $\mathbf{y}^L(t) < \mathbf{y}(t, \mathbf{p}) < \mathbf{y}^U(t)$, $\forall (t, \mathbf{p}) \in [t_0, t_f] \times P$.

Differential Inequalities Result

Let $\mathbf{x}^L, \mathbf{x}^U : [t_0, t_f] \to \mathbb{R}^{n_x}$ and $\mathbf{y}^L, \mathbf{y}^U : [t_0, t_f] \to \mathbb{R}^{n_y}$ be differentiable on (t_0, t_f) and satisfy

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2. $\mathbf{y}^L(t_0) < \mathbf{y}(t_0, \mathbf{p}) < \mathbf{y}^U(t_0)$.

(RHS): For every $t \in (t_0, t_f]$ and each i, letting $X(t) \equiv [\mathbf{x}^L(t), \mathbf{x}^U(t)]$ and $Y(t) \equiv [\mathbf{y}^L(t), \mathbf{y}^U(t)]$:

1. $\dot{x}_i^L(t) < f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in \mathcal{B}_i^L(X(t)) \cap D_x$, $\mathbf{z}_y \in Y(t) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$
2. $\dot{x}_i^U(t) > f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in \mathcal{B}_i^U(X(t)) \cap D_x$, $\mathbf{z}_y \in Y(t) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$
3. $\dot{y}_i^L(t) < f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^L(Y(t)) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$
4. $\dot{y}_i^U(t) > f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^U(Y(t)) \cap D_y$, and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$

Then $\mathbf{x}^L(t) < \mathbf{x}(t, \mathbf{p}) < \mathbf{x}^U(t)$ and $\mathbf{y}^L(t) < \mathbf{y}(t, \mathbf{p}) < \mathbf{y}^U(t)$, $\forall (t, \mathbf{p}) \in [t_0, t_f] \times P$.

Differential Inequalities Result

Let $\mathbf{x}^L, \mathbf{x}^U : [t_0, t_f] \to \mathbb{R}^{n_x}$ and $\mathbf{y}^L, \mathbf{y}^U : [t_0, t_f] \to \mathbb{R}^{n_y}$ be differentiable on (t_0, t_f) and satisfy

(IC): 1. $\mathbf{x}^L(t_0) < \mathbf{x}(t_0, \mathbf{p}) < \mathbf{x}^U(t_0)$.

2. $\mathbf{y}^L(t_0) < \mathbf{y}(t_0, \mathbf{p}) < \mathbf{y}^U(t_0)$.

(RHS): For every $t \in (t_0, t_f]$ and each i, letting $X(t) \equiv [\mathbf{x}^L(t), \mathbf{x}^U(t)]$ and $Y(t) \equiv [\mathbf{y}^L(t), \mathbf{y}^U(t)]$:

1. $\dot{x}_i^L(t) < f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}$ … $\cap D_x,\ \mathbf{z}_y \in Y(t) \cap D_y,$

2. $\dot{x}_i^U(t) > f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}$ … $\cap D_x,\ \mathbf{z}_y \in Y(t) \cap D_y,$

and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ …

Cannot Compute these bounds cheaply

3. $\dot{\mathrm{y}}_i^L(t) < f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P,\ \mathbf{z}_x \in X(t) \cap D_x,\ \mathbf{z}_y \in \mathcal{B}_i^L(Y(t)) \cap D_y,$ and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$

4. $\dot{\mathrm{y}}_i^U(t) > f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P,\ \mathbf{z}_x \in X(t) \cap D_x,\ \mathbf{z}_y \in \mathcal{B}_i^U(Y(t)) \cap D_y,$ and $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$

Then $\mathbf{x}^L(t) < \mathbf{x}(t, \mathbf{p}) < \mathbf{x}^U(t)$ and $\mathbf{y}^L(t) < \mathbf{y}(t, \mathbf{p}) < \mathbf{y}^U(t),\ \forall (t, \mathbf{p}) \in [t_0, t_f] \times P.$

Computing State Bounds

$$\mathbf{0} = \mathbf{g}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p}))$$

- Interval Newton-type methods
  - Can derive an interval map

$$\mathcal{N} : [t_0, t_f] \times \mathbb{IR}^{n_p} \times \mathbb{IR}^{n_x} \times \mathbb{IR}^{n_y} \rightarrow \mathbb{IR}^{n_y}$$

  - with the properties:

1. $\mathcal{N}(t, P, Z_x, Z_y) \subset Z_y$
2. If $(\mathbf{z}_x, \mathbf{z}_y) \in Z_x \times Z_y$ and $\mathbf{z}_y \notin \mathcal{N}(t, P, Z_x, Z_y)$,

   then $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) \neq \mathbf{0}, \ \forall \mathbf{p} \in P$
3. $\mathcal{N}$ is locally Lipschitz

Computing State Bounds

Let $\mathbf{x}^L, \mathbf{x}^U : [t_0, t_f] \to \mathbb{R}^{n_x}$ and $\mathbf{y}^L, \mathbf{y}^U : [t_0, t_f] \to \mathbb{R}^{n_y}$ be differentiable on (t_0, t_f) and satisfy

(IC): 1. $\mathbf{x}^L(t_0) \le \mathbf{x}(t_0, \mathbf{p}) \le \mathbf{x}^U(t_0)$.

2. $\mathbf{y}^L(t_0) \le \mathbf{y}(t_0, \mathbf{p}) \le \mathbf{y}^U(t_0)$.

(RHS): For every $t \in (t_0, t_f]$ and each i, letting $X(t) \equiv [\mathbf{x}^L(t), \mathbf{x}^U(t)]$ and $Y(t) \equiv \mathcal{N}(t, [\mathbf{x}^L(t), \mathbf{x}^U(t)], [\mathbf{y}^L(t), \mathbf{y}^U(t)])$:

1. $\dot{x}_i^L(t) \le f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in \mathcal{B}_i^L(X(t)) \cap D_x$, $\mathbf{z}_y \in Y(t) \cap D_y$
2. $\dot{x}_i^U(t) \ge f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in \mathcal{B}_i^U(X(t)) \cap D_x$, $\mathbf{z}_y \in Y(t) \cap D_y$
3. $\dot{y}_i^L(t) \le f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^L(Y(t)) \cap D_y$
4. $\dot{y}_i^U(t) \ge f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^U(Y(t)) \cap D_y$

Then $\mathbf{x}^L(t) \le \mathbf{x}(t, \mathbf{p}) \le \mathbf{x}^U(t)$ and $\mathbf{y}^L(t) \le \mathbf{y}(t, \mathbf{p}) \le \mathbf{y}^U(t)$, $\forall (t, \mathbf{p}) \in [t_0, t_f] \times P$.

Computing State Bounds

Let $\mathbf{x}^L, \mathbf{x}^U : [t_0, t_f] \to \mathbb{R}^{n_x}$ and $\mathbf{y}^L, \mathbf{y}^U : [t_0, t_f] \to \mathbb{R}^{n_y}$ be differentiable on (t_0, t_f) and satisfy

(IC): 1. $\mathbf{x}^L(t_0) \le \mathbf{x}(t_0, \mathbf{p}) \le \mathbf{x}^U(t_0)$.

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(RHS): For every $t \in (t_0, t_f]$ and each i, letting $X(t) \equiv [\mathbf{x}^L(t), \mathbf{x}^U(t)]$ and

$Y(t) \equiv \mathcal{N}(t, [\mathbf{x}^L(t), \mathbf{x}^U(t)], [\mathbf{y}^L(t), \mathbf{y}^U(t)])$:

1. $\dot{x}_i^L(t) \le f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in \mathcal{B}_i^L(X(t)) \cap D_x$, $\mathbf{z}_y \in Y(t) \cap D_y$
2. $\dot{x}_i^U(t) \ge f_{x,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in \mathcal{B}_i^U(X(t)) \cap D_x$, $\mathbf{z}_y \in Y(t) \cap D_y$
3. $\dot{y}_i^L(t) \le f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^L(Y(t)) \cap D_y$
4. $\dot{y}_i^U(t) \ge f_{y,i}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$ if $\mathbf{p} \in P$, $\mathbf{z}_x \in X(t) \cap D_x$, $\mathbf{z}_y \in \mathcal{B}_i^U(Y(t)) \cap D_y$

Then $\mathbf{x}^L(t) \le \mathbf{x}(t, \mathbf{p}) \le \mathbf{x}^U(t)$ and $\mathbf{y}^L(t) \le \mathbf{y}(t, \mathbf{p}) \le \mathbf{y}^U(t)$, $\forall (t, \mathbf{p}) \in [t_0, t_f] \times P$.

Computing State Bounds

- Integrate UODEs using interval arithmetic

$$\dot{x}_i^L(t) = \left[f_{x,i} \right]^L (t, P, \mathcal{B}_i^L(X(t)), Y(t)), \quad x_i^L(t_0) = \left[x_{0,i} \right]^L (P),$$

$$\dot{x}_i^U(t) = \left[f_{x,i} \right]^U (t, P, \mathcal{B}_i^U(X(t)), Y(t)), \quad x_i^U(t_0) = \left[x_{0,i} \right]^U (P),$$

$$\dot{y}_i^L(t) = \left[f_{y,i} \right]^L (t, P, X(t), \mathcal{B}_i^L(Y(t))), \quad y_i^L(t_0) = \left[y_{0,i} \right]^L (P),$$

$$\dot{y}_i^U(t) = \left[f_{y,i} \right]^U (t, P, X(t), \mathcal{B}_i^U(Y(t))), \quad y_i^U(t_0) = \left[y_{0,i} \right]^U (P),$$

$$X(t) \equiv [\mathbf{x}^L(t), \mathbf{x}^U(t)]$$

$$Y(t) \equiv \mathcal{N}(t, [\mathbf{x}^L(t), \mathbf{x}^U(t)], [\mathbf{y}^L(t), \mathbf{y}^U(t)])$$

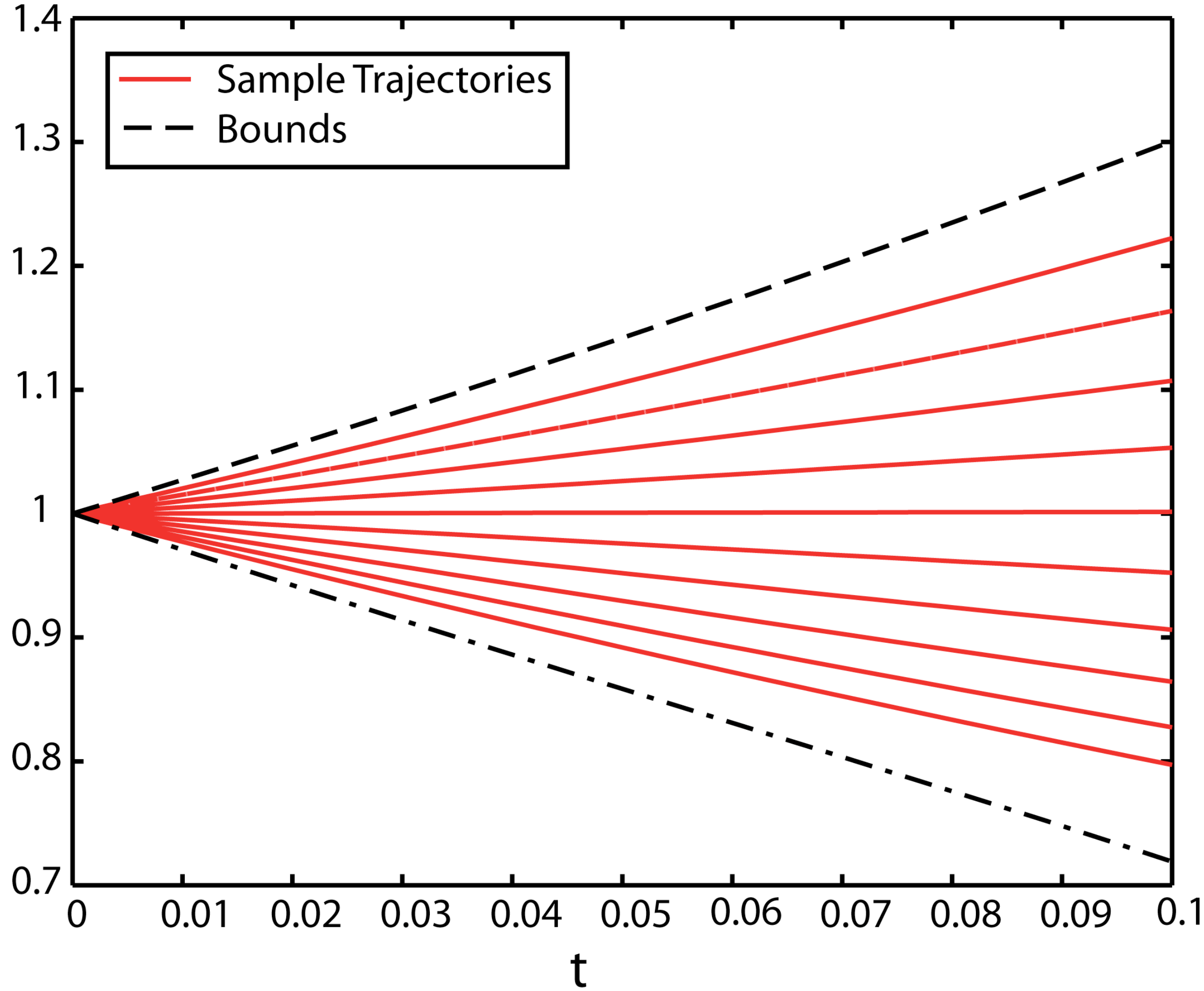
DAE Example

$$\dot{x}(t,p) = -px(t,p) + 0.01y(t,p), \quad x_0 = 1,$$

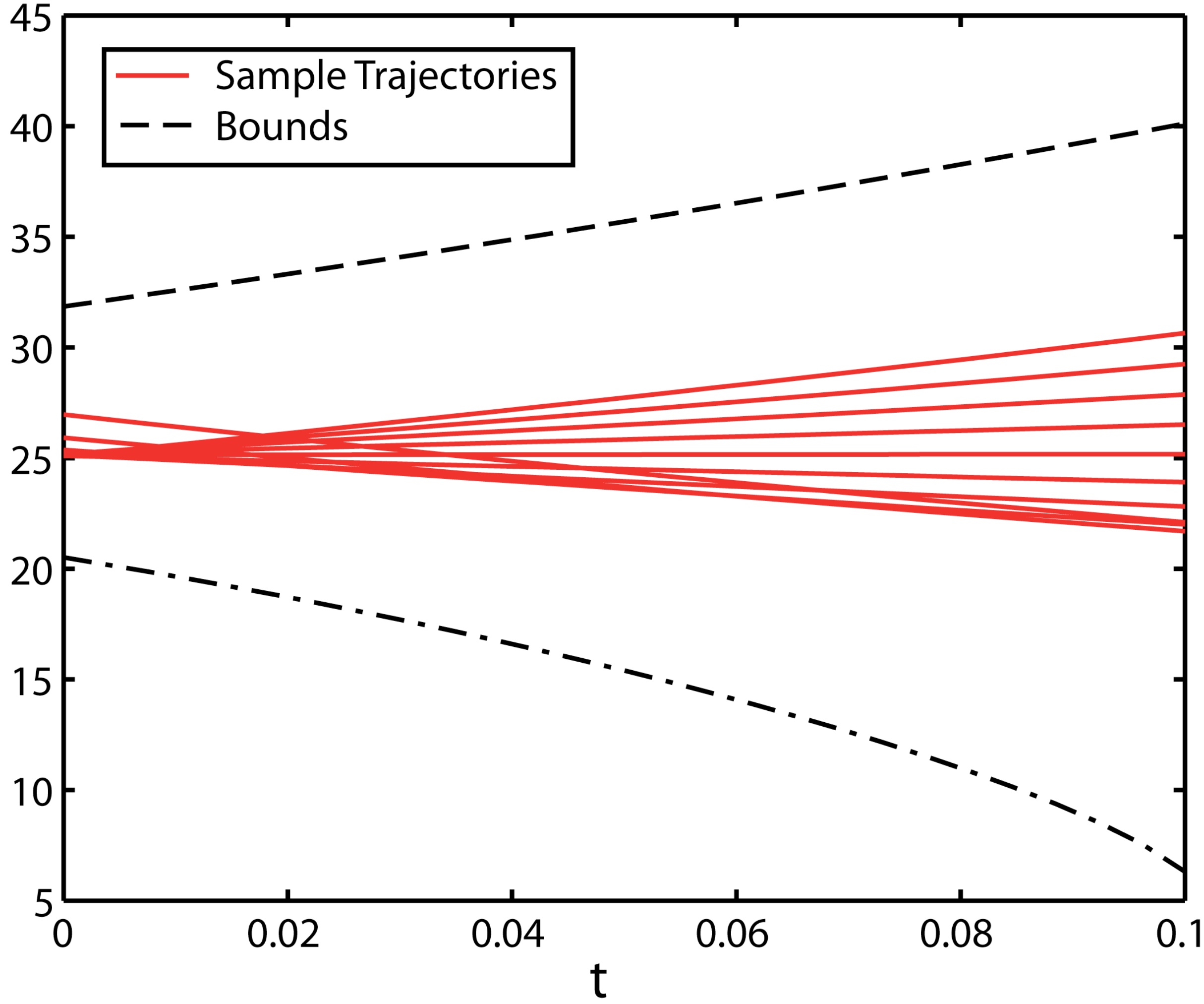
$$0 = y(t,p) - (y(t,p))^{-1/2}(p - p^3 / 6 + p^5 / 120) - 25x(t,p)$$

$$P = [0.5, 5.0], \quad I = [0, 0.1].$$

DAE Example: Bounds on $\mathbf{x}$



DAE Example: Bounds on y



State Bounds: Conclusions

- Can extend classical differential inequalities results to DAEs
- Computationally tractable procedure using interval Newton-type methods
- Computational cost is comparable to integration of the original dynamic model

Conclusions

- Sequential approach to dynamic optimization
  - Extended to global optimization through novel techniques for bounding & relaxing dynamics
- Extended theory for computing bounds and relaxations for ODE solutions to DAEs
- Relaxations can be propagated through arbitrary functions of the state variables
- Results in a rigorous global optimization algorithm for a wide range of problems with DAEs embedded

Future Work

- Extension to fully implicit DAEs
- High-index problems
- DAE reachability analysis

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Supplementary Material

Alternative Approaches

$$\min_{\mathbf{p}\in P} \; J(\mathbf{p}) \equiv \phi(\mathbf{p},\mathbf{x}(t_f,\mathbf{p}),\mathbf{y}(t_f,\mathbf{p})) + \int_{t_0}^{t_f} \ell(s,\mathbf{p},\mathbf{x}(s,\mathbf{p}),\mathbf{y}(s,\mathbf{p}))ds$$

$$\text{s.t.} \;\; \mathbf{G}(\mathbf{p}) \equiv \psi(\mathbf{p},\mathbf{x}(t_f,\mathbf{p}),\mathbf{y}(t_f,\mathbf{p})) + \int_{t_0}^{t_f} \xi(s,\mathbf{p},\mathbf{x}(s,\mathbf{p}),\mathbf{y}(s,\mathbf{p}))ds \leq \mathbf{0}$$

$$\begin{aligned} \dot{\mathbf{x}}(t,\mathbf{p}) &= \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad & \mathbf{x}(t_0,\mathbf{p}) &= \mathbf{x}_0(\mathbf{p}), \\ \mathbf{0} &= \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p})), \quad & \mathbf{y}(t_0,\hat{\mathbf{p}}) &= \mathbf{y}_0(\hat{\mathbf{p}}). \end{aligned}$$

- Simultaneous/ full discretization approach
  - Introduces too many variables for global algorithms
- No other relaxation methods have been proposed

Computing State Bounds

- Interval Arithmetic
  - Compute cheap bounds on the range of functions over intervals

$$[a^L, a^U] + [b^L, b^U] = [a^L + b^L, a^U + b^U]$$

$$[a^L, a^U] \times [b^L, b^U] = [\min(a^L b^L, a^L b^U, a^U b^L, a^U b^U), \max(a^L b^L, a^L b^U, a^U b^L, a^U b^U)]$$

  - As long as the feasible set is an interval . . .

$$\dot{x}_i^L(t) = \left[\, f \,\right]_i^L < \min f_i(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$$
$$s.t. \quad \mathbf{z}_x \in \mathcal{B}_i^L[\mathbf{x}^L(t), \mathbf{x}^U(t)],$$
$$\mathbf{z}_y \in [\mathbf{y}^L(t), \mathbf{y}^U(t)]$$
$$\mathbf{p} \in P$$

Computing State Bounds

- Implement algebraic constraints in differential inequalities. . .

$$\dot{x}_i^L(t) = \left[f \right]_i^L < \min f_i(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y)$$

$$\begin{aligned} s.t.\quad & \mathbf{z}_x \in \mathcal{B}_i^L[\mathbf{x}^L(t), \mathbf{x}^U(t)], \\ & \mathbf{z}_y \in [\mathbf{y}^L(t), \mathbf{y}^U(t)] \\ & \mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0} \\ & \mathbf{p} \in P \end{aligned}$$

Feasible set is no longer an interval

Interval Newton Methods

$$\mathbf{0} = \mathbf{g}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p}))$$

Fix $(t, \mathbf{p}) \in [t_0, t_f] \times P$ and $i \in \{1, \ldots, n_x\}$ and suppose $\mathbf{x}(t, \mathbf{p}) \in [\mathbf{x}^L, \mathbf{x}^U]$ and $\mathbf{y}(t, \mathbf{p}) \in [\mathbf{y}^L, \mathbf{y}^U]$. For any $\tilde{\mathbf{y}} \in [\mathbf{y}^L, \mathbf{y}^U]$, $\exists \xi \in [\mathbf{y}^L, \mathbf{y}^U]$:

$$-g_i(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \tilde{\mathbf{y}}) = \frac{\partial g_i}{\partial \mathbf{y}}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \xi)\Big(\mathbf{y}(t, \mathbf{p}) - \tilde{\mathbf{y}}\Big)$$

Interval Newton Methods

$$\mathbf{0} = \mathbf{g}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p}))$$

$$\frac{\partial g_i}{\partial y_i}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \xi)\Big(y_i(t, \mathbf{p}) - \tilde{y}_i\Big)$$

$$= -g_i(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \tilde{\mathbf{y}}) - \sum_{j \neq i} \frac{\partial g_i}{\partial y_j}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \xi)\Big(y_j(t, \mathbf{p}) - \tilde{y}_j\Big)$$

Interval Newton Methods

$$\mathbf{0} = \mathbf{g}(t, \mathbf{p}, \mathbf{x}(t,\mathbf{p}), \mathbf{y}(t,\mathbf{p}))$$

$$\frac{\partial g_i}{\partial y_i}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\xi)\Big(y_i(t,\mathbf{p}) - \tilde{y}_i\Big) = -g_i(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\tilde{\mathbf{y}}) - \sum_{j\neq i}\frac{\partial g_i}{\partial y_j}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\xi)\Big(y_j(t,\mathbf{p}) - \tilde{y}_j\Big)$$

- Supposing $\frac{\partial g_i}{\partial y_i}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\xi) \neq 0,$

$$y_i(t,\mathbf{p}) = \tilde{y}_i - \left(\frac{\partial g_i}{\partial y_i}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\xi)\right)^{-1}\left(g_i(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\tilde{\mathbf{y}}) + \sum_{j\neq i}\frac{\partial g_i}{\partial y_j}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\xi)\Big(y_j(t,\mathbf{p}) - \tilde{y}_j\Big)\right)$$

Interval Newton Methods

$$\mathbf{0} = \mathbf{g}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p}))$$

$$y_i(t, \mathbf{p}) = \tilde{y}_i - \left(\frac{\partial g_i}{\partial y_i}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \xi) \right)^{-1} \left(g_i(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \tilde{\mathbf{y}}) + \sum_{j \neq i} \frac{\partial g_i}{\partial y_j}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \xi) \left(y_j(t, \mathbf{p}) - \tilde{y}_j \right) \right)$$

Interval Newton Methods

$$\mathbf{0} = \mathbf{g}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p}))$$

$$y_i(t, \mathbf{p}) = \tilde{y}_i - \left(\frac{\partial g_i}{\partial y_i}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \xi) \right)^{-1} \left(g_i(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \tilde{\mathbf{y}}) + \sum_{j \neq i} \frac{\partial g_i}{\partial y_j}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \xi) \left(y_j(t, \mathbf{p}) - \tilde{y}_j \right) \right)$$

- Compute refined bounds for $y_i(t,\mathbf{p})$

$$y_i(t, \mathbf{p}) \in \tilde{y}_i - \left(\frac{\partial g_i}{\partial y_i}(t, P, X(t), Y(t)) \right)^{-1} \left(g_i(t, P, X(t), \tilde{\mathbf{y}}) + \sum_{j \neq i} \frac{\partial g_i}{\partial y_j}(t, P, X(t), Y(t)) \left(Y_j(t) - \tilde{y}_j \right) \right)$$

Interval Newton Methods

$$\mathbf{0} = \mathbf{g}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p}))$$

- Interval Gauss-Seidel:

$$\tilde{Y}_1(t) = \tilde{y}_1 - \left(\frac{\partial g_1}{\partial y_1}(t, P, X(t), Y(t))\right)^{-1} \left(g_1(t, P, X(t), \tilde{\mathbf{y}}) + \sum_{j \neq i} \frac{\partial g_1}{\partial y_j}(t, P, X(t), Y(t)) \big(Y_j(t) - \tilde{y}_j\big)\right)$$

$$\tilde{Y}_i(t) = \tilde{y}_i - \left(\frac{\partial g_i}{\partial y_i}(t, P, X(t), Y(t))\right)^{-1} \Big(g_i(t, P, X(t), \tilde{\mathbf{y}}) + \sum_{j < i} \frac{\partial g_i}{\partial y_j}(t, P, X(t), Y(t)) \big(\tilde{Y}_j(t) - \tilde{y}_j\big) + \\ + \sum_{j > i} \frac{\partial g_i}{\partial y_j}(t, P, X(t), Y(t)) \big(Y_j(t) - \tilde{y}_j\big)\Big)$$