Centre for
Process
Systems
Engineering

Global Optimization Issues in Parametric Programming and Control

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The Queen's Anniversary Prizes 2002

Outline

- Optimization under Uncertainty
- Parametric Programming
- Model Predictive Control
- Multi-parametric MILP
- Multi-parametric MIQP
- Multi-parametric Global Optimization
- Bilevel Programming
- Concluding Remarks

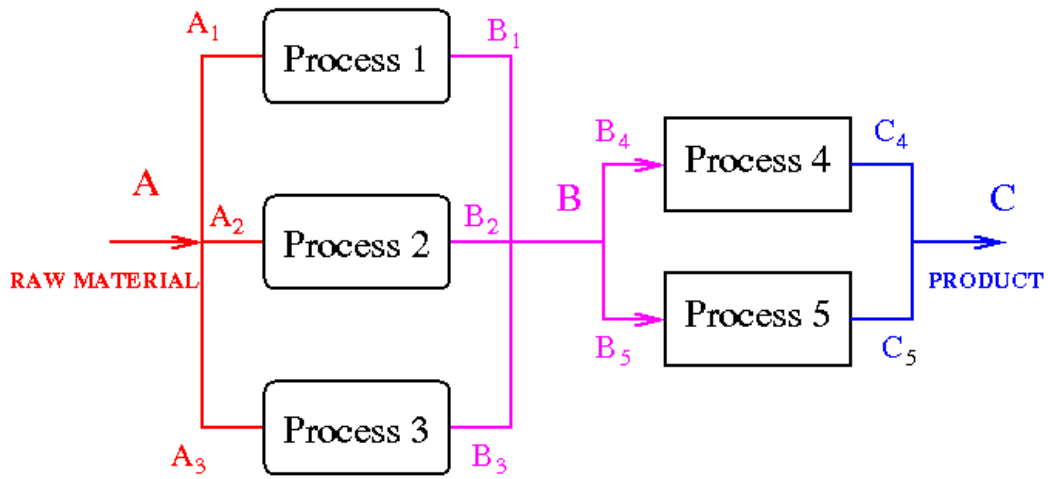
Uncertainty

So far as the laws of mathematics refer to reality, they are not certain. And so far as they are certain, they do not refer to reality.

Albert Einstein

- **Assumptions**
- **Simplifications**

Sources of Uncertainty



- Feed Availability
- Feed Composition
- Heat Transfer Coefficient
- Product Demand
- Temperature Variations
- Equipment Availability

Key Objectives

OBJECTIVE 1: Determine an "optimal" structure/ design/ operating policy in the presence of uncertainty

- "optimal"
  - profit / cost
  - operability objective
    - (flexibility, robustness)
- trade-offs

Stochastic Optimization

OBJECTIVE 2: Derive profile of ALL optimal solutions as a function of the uncertain parameters

NEW

Parametric Optimization

What is Parametric Optimization?

- Given:
  - a performance criterion to minimize/maximize
  - a vector of constraints
  - a vector of parameters
- Obtain:
  - the performance criterion and the optimization variables as a function of the parameters
  - the regions in the space of parameters where these functions remain valid

Parametric Optimization (POP)

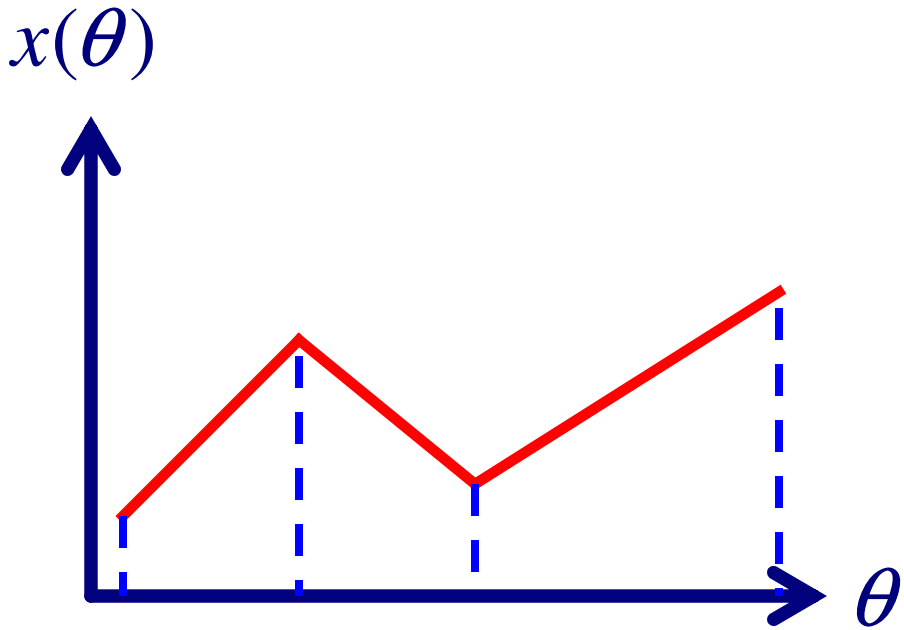
$$z(\theta) = \min_{x} f(x,\theta)$$

$$\text{s.t. } g(x,\theta) \le 0$$

$$x \in \Re^{n}$$

$$\theta \in \Re^{s}$$

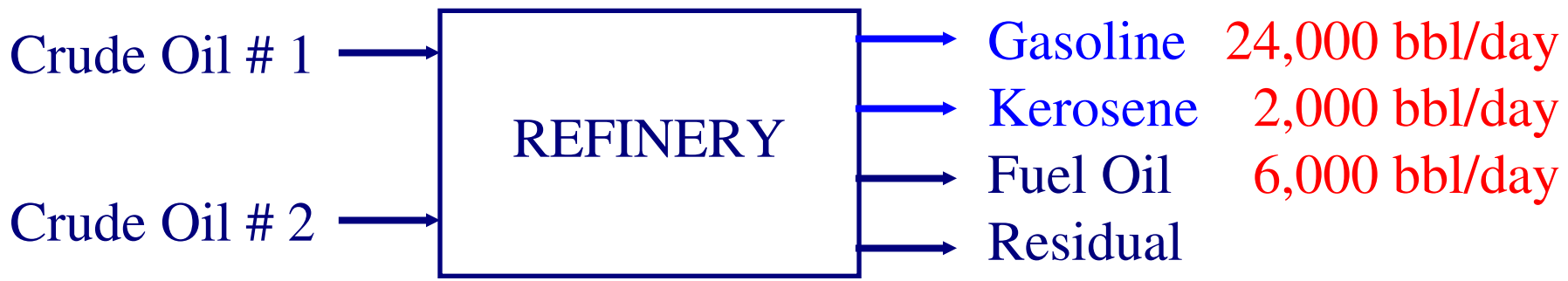
$$x(\theta)$$

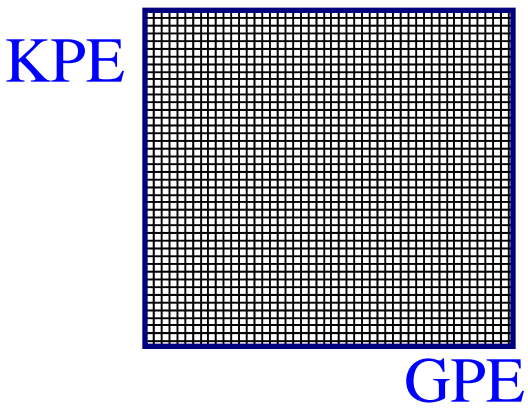


Obtain optimal solution as a function of parameters

An Example – Linear Model

(Edgar and Himmelblau, 1989)





<u>Objective</u>: Maximise Profit

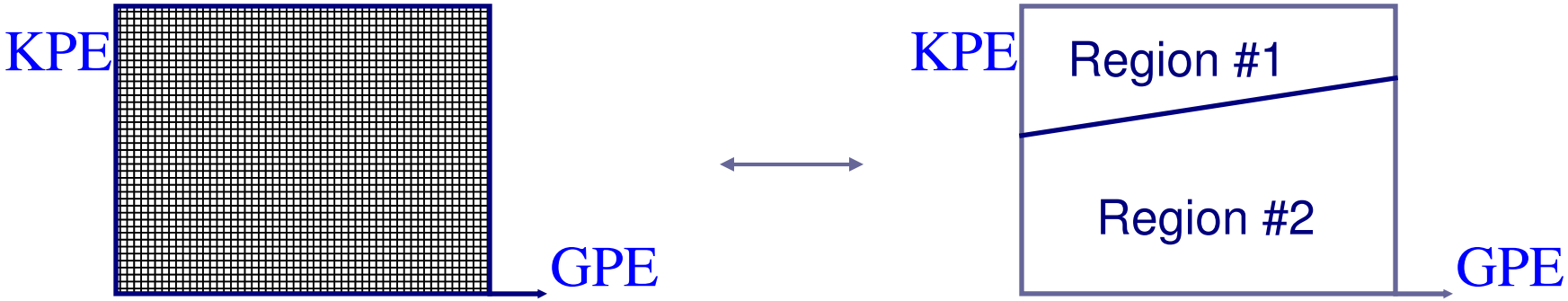
<u>Parameters:</u>

Gasoline Prod. Expansion (GPE)

Kerosene Prod. Expansion (KPE)

Solve optimization problems at many points?

Parametric Solution



Profit = 4.66 GPE + 87.5 KPE + 286759 Crude#1 = 1.72 GPE – 7.59 KPE + 26207 Crude#2 = -0.86 GPE + 13.79 KPE + 6897	if	-0.14 GPE + 4.21 KPE < 896.55 0 < GPE < 6000 0 < KPE (REGION #1)
Profit = 7.53 GPE + 30541 Crude#1 = 1.48 GPE + 24590 Crude#2 = -0.41GPE + 9836	if	-0.14 GPE + 4.21 KPE > 896.55 0 < GPE < 6000 KPE < 500 (REGION #2)

Only 2 optimization problems solved!

Parametric Optimization (POP)

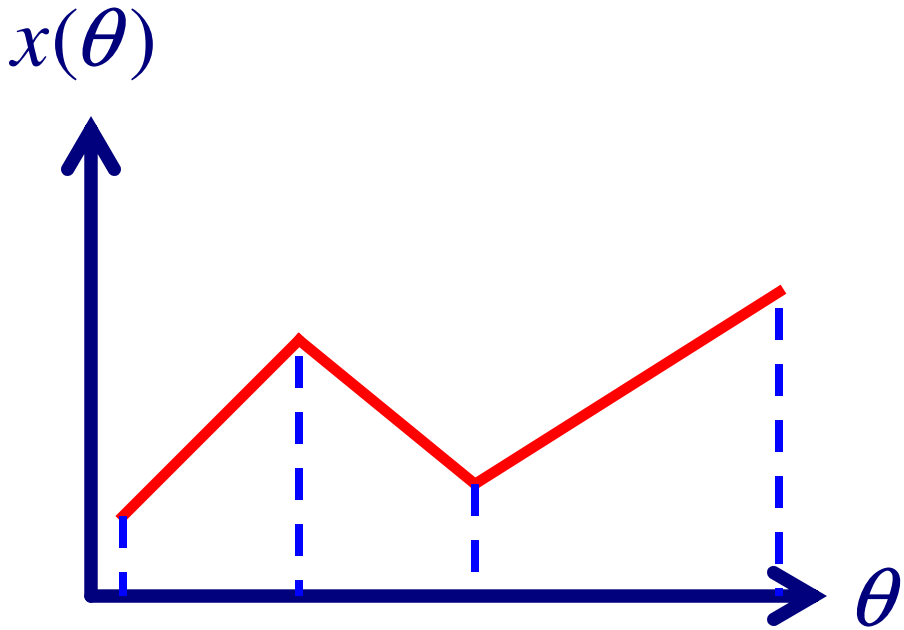
$$z(\theta) = \min_{x} f(x,\theta)$$

$$\text{s.t. } g(x,\theta) \le 0$$

$$x \in \Re^{n}$$

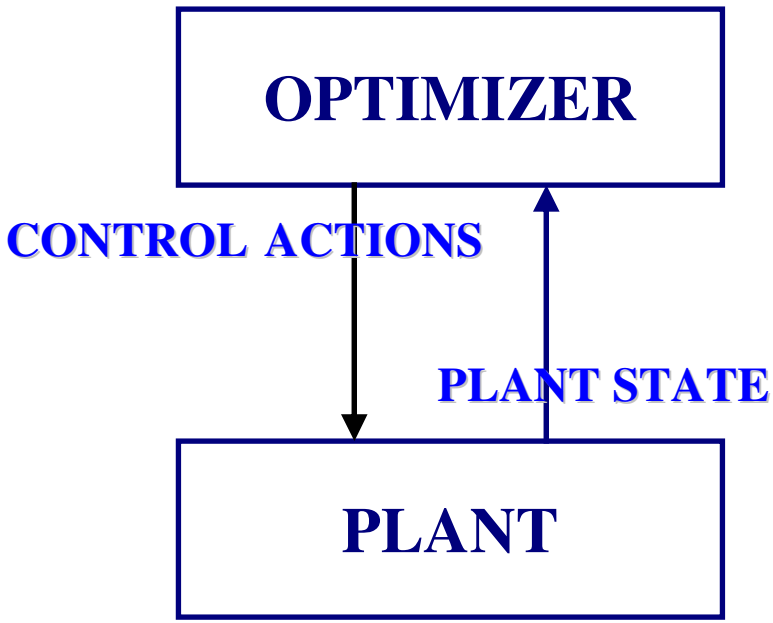
$$\theta \in \Re^{s}$$

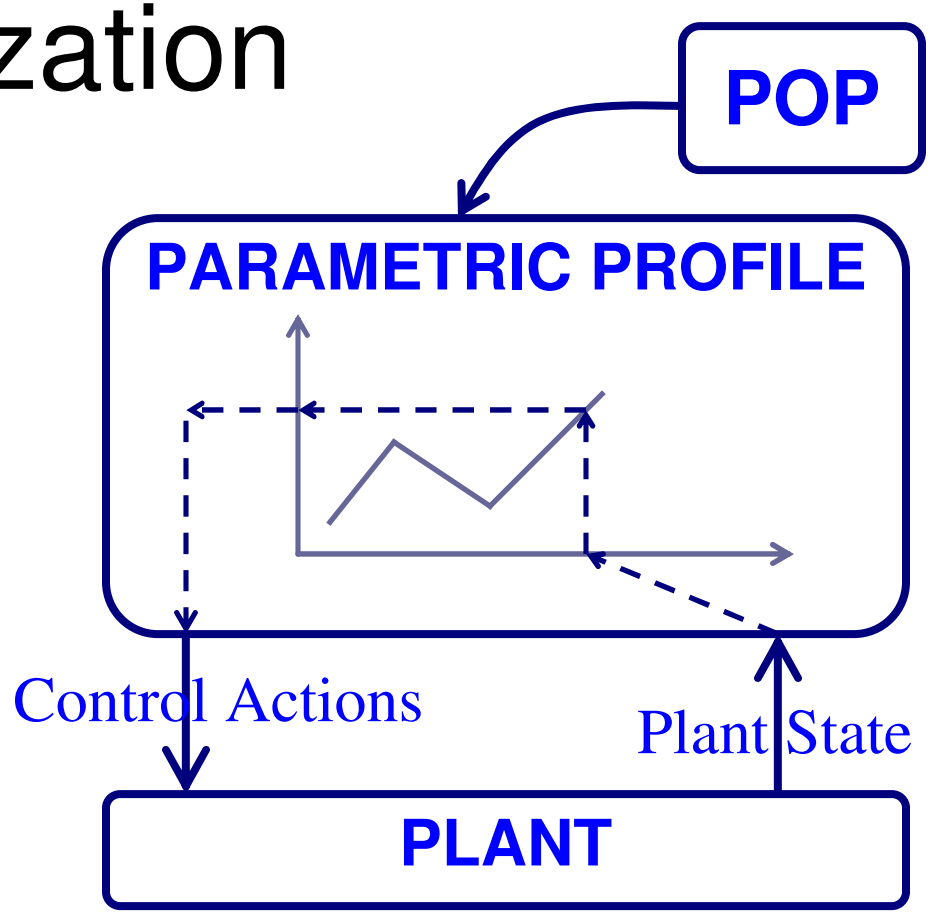
$$x(\theta)$$



Obtain optimal solution as a function of parameters

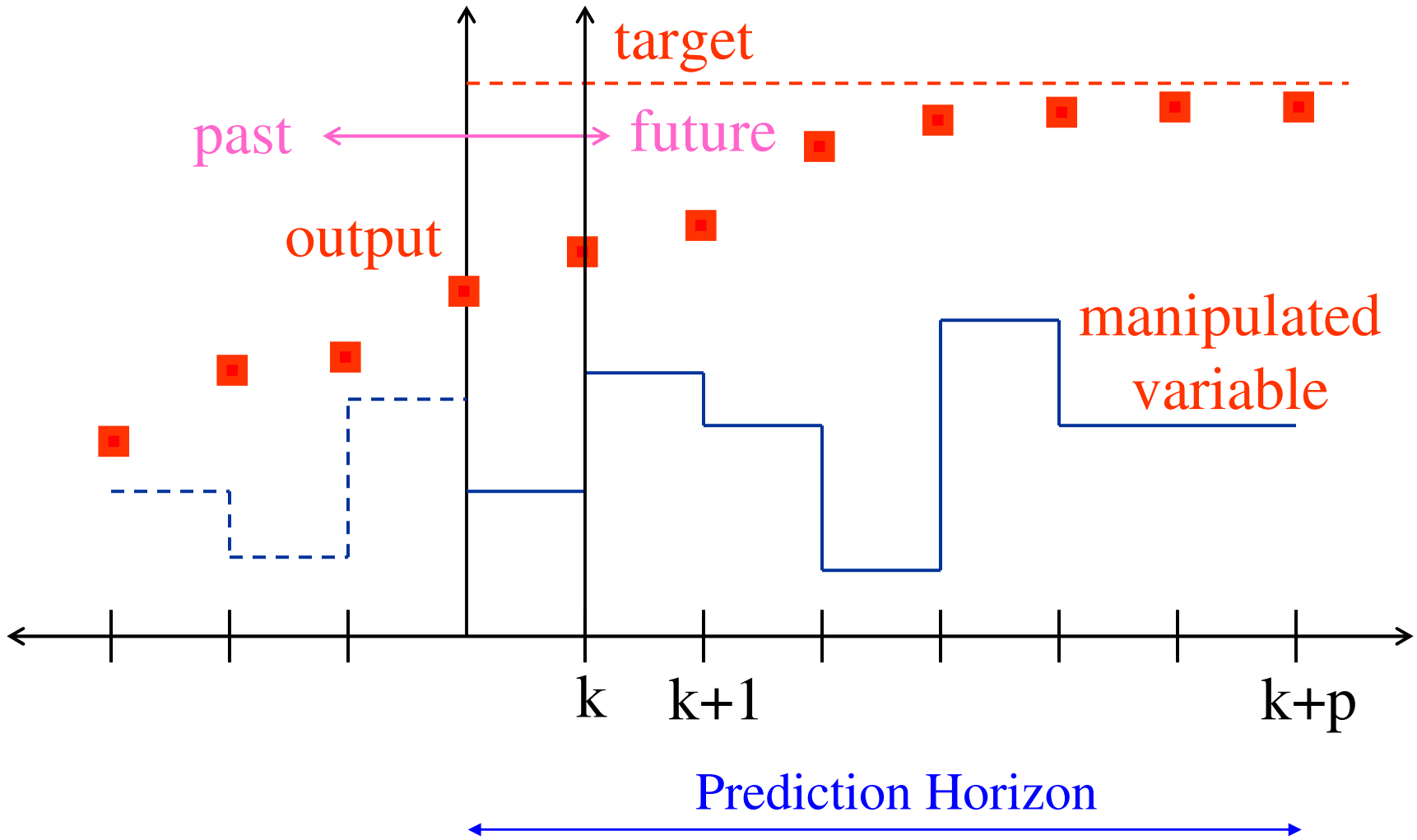
On-line Optimization





Function Evaluation!

Model Predictive Control (MPC)



Model Predictive Control

$$\min_{u(k),\ldots,u(k+Nu)} \sum_{k=0}^{N_y}[x'(k)Qx(k)] + \sum_{k=0}^{N_u}[u(k)'Ru(k)]$$

$$\text{s.t.} \quad x(k+1) = f(x(k), u(k))$$

$$x_{\min} \le x(k+1) \le x \le x_{\max}, k = 0,1,\ldots,N_c$$

$$u_{\min} \le u(k) \le u_{\max}, k = 0,1,\ldots,N_c$$

- Solve an optimization problem at each time interval k

Model Predictive Control (MPC)

min A quadratic and convex function of discretised state and control variables

s.t. 1. Constraints linear in discretised state and control variables

2. Lower and upper bounds on state and control variables

Solve a QP at each time interval

Parametric Programming Approach

- State variables à Parameters
- Control variables à Optimization variables

- MPC à Parametric Optimization problem

- Control variables = F(State variables)

Multi-parametric Quadratic Programs

$$z(\theta) = \min_x \frac{1}{2} x^T Q x$$

$$\text{s.t. } Ax \le b + F\theta$$

$$x \in \Re^n$$

$$\theta \in \Theta \subseteq \Re^m$$

- Theorem 1:
  x and λ are linear function of θ
- Theorem 2:
  $z(\theta)$ is continuous, convex and quadratic

x continuous variables ; θ parameters ; λ Lagrange multipliers

Q positive definite constant matrix ; b, A, F constant vector/matrices

RHS Uncertainty

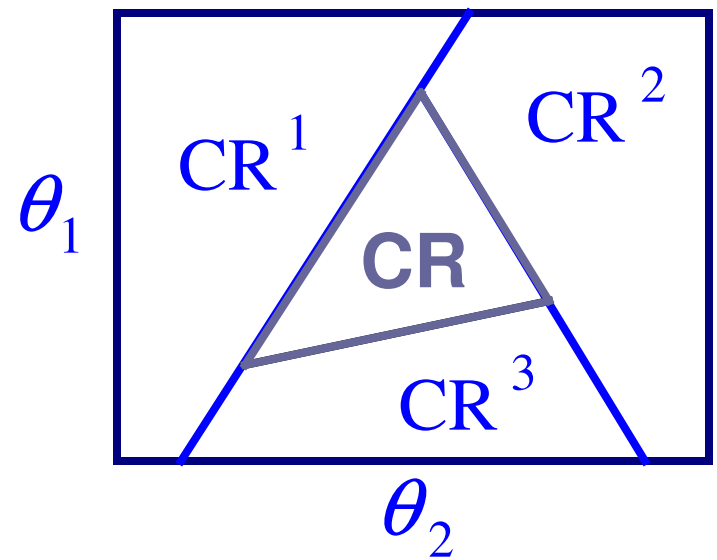
Critical Region (CR)

- CR: the region where a solution remains optimal
  - Feasibility Condition:

$$Ax(\theta) \le b + F\theta$$

  - Optimality Condition:

$$\lambda(\theta) \ge 0$$



- CR:
  - A polyhedron
  - Obtain:

$$\mathrm{CR}^{\mathrm{rest}} = \Theta - \mathrm{CR} = \mathrm{CR}^1 \cup \mathrm{CR}^2 \cup \mathrm{CR}^3$$

Example

$$J(x_t) = \min_{u_t, u_{t+1}} \frac{1}{2} x_{t+2}{}^T P x_{t+2} + \frac{1}{2} \sum_{k=0}^{1} [x_{t+k}{}^T Q x_{t+k} + u_{t+k}{}^T R u_{t+k}]$$

s.t.

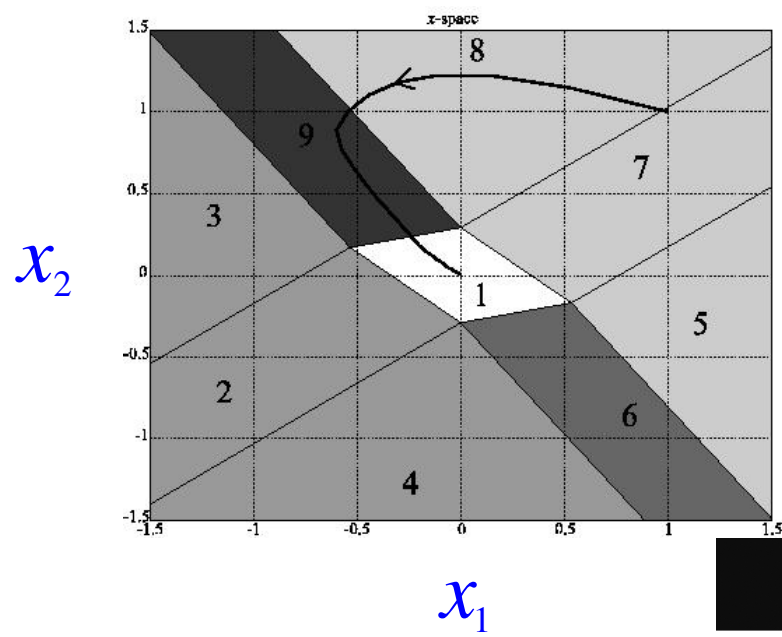
$$x_{t+1} = \begin{bmatrix} 0.7326 & -0.0861 \\ 0.1722 & 0.9909 \end{bmatrix} x_t + \begin{bmatrix} 0.0609 \\ 0.0064 \end{bmatrix} u_t$$

$$y_t = \begin{bmatrix} 0 & 1.4142 \end{bmatrix} x_t$$

$$-2 \le u_{t+k} \le 2, k = 0,1$$

Explicit Solution

$$u = \begin{cases} \begin{bmatrix} -5.9220 & -6.8883 \end{bmatrix} x & \text{if} \quad \begin{bmatrix} -5.9220 & -6.8883 \\ 5.9220 & 6.8883 \\ -1.5379 & 6.8291 \\ 1.5379 & -6.8291 \end{bmatrix} x \le \begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \end{bmatrix} & \mathbf{1} \\ 2 & \text{if} \quad \begin{bmatrix} -3.4155 & 4.6452 \\ 0.1044 & 0.1215 \\ 0.1259 & 0.0922 \end{bmatrix} x \le \begin{bmatrix} 2.6341 \\ -0.0353 \\ -0.0267 \end{bmatrix} & \mathbf{2,4} \\ \vdots & \end{cases}$$



Explicit Solution

$$
u = \begin{cases}
\begin{bmatrix} -5.9220 & -6.8883 \end{bmatrix} x & \text{if} \quad \begin{bmatrix} -5.9220 & -6.8883 \\ 5.9220 & 6.8883 \\ -1.5379 & 6.8291 \\ 1.5379 & -6.8291 \end{bmatrix} x \le \begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \end{bmatrix} & \mathbf{1} \\
2 & \text{if} \quad \begin{bmatrix} -3.4155 & 4.6452 \\ 0.1044 & 0.1215 \\ 0.1259 & 0.0922 \end{bmatrix} x \le \begin{bmatrix} 2.6341 \\ -0.0353 \\ -0.0267 \end{bmatrix} & \mathbf{2,4} \\
2 & \text{if} \quad \begin{bmatrix} 0.0679 & -0.0924 \\ 0.1259 & 0.0922 \end{bmatrix} x \le \begin{bmatrix} -0.0524 \\ -0.0519 \end{bmatrix} & \mathbf{3} \\
-2 & \text{if} \quad \begin{bmatrix} -0.1259 & -0.0922 \\ -0.0679 & 0.0924 \end{bmatrix} x \le \begin{bmatrix} -0.0519 \\ -0.0524 \end{bmatrix} & \mathbf{5} \\
\begin{bmatrix} -6.4159 & -4.6953 \end{bmatrix} x + 0.6423 & \text{if} \quad \begin{bmatrix} -6.4159 & -4.6953 \\ -0.0275 & 0.1220 \\ 6.4159 & 4.6953 \end{bmatrix} x \le \begin{bmatrix} 1.3577 \\ -0.0357 \\ 2.6423 \end{bmatrix} & \mathbf{6} \\
-2 & \text{if} \quad \begin{bmatrix} 3.4155 & -4.6452 \\ -0.1044 & -0.1215 \\ -0.1259 & -0.0922 \end{bmatrix} x \le \begin{bmatrix} 2.6341 \\ -0.0353 \\ -0.0267 \end{bmatrix} & \mathbf{7,8} \\
\begin{bmatrix} -6.4159 & -4.6953 \end{bmatrix} x - 0.6423 & \text{if} \quad \begin{bmatrix} 6.4159 & 4.6953 \\ 0.0275 & -0.1220 \\ -6.4159 & -4.6953 \end{bmatrix} x \le \begin{bmatrix} 1.3577 \\ -0.0357 \\ 2.6423 \end{bmatrix} & \mathbf{9}
\end{cases}
$$

Worst-Case Computational Complexity

Number of Regions: $$N_r = \sum_{k=0}^{\eta} k! c^k$$

where: $$\eta = \sum_{i=0}^{m} \frac{c!}{(c-i)!i!}$$

where m is the number of optimization variables and c is the number of inequalities

Computational Experience

Computational Time (s):

c	m/n	2	3	4	5
4	2	3.02	4.12	5.05	5.33
6	3	10.44	26.75	31.7	70.19
8	4	25.27	60.20	53.93	58.61

Number of Regions:

c	m/n	2	3	4	5
4	2	7	7	7	7
6	3	17	47	29	43
8	4	29	99	121	127

Applications

- Control of Type 1 diabetes
- Control of Pilot Plant Reactor
- Control of Industrial Air Separation Units
- Control of Automotive Systems

Hybrid Control

Multi-Parametric Mixed Integer Linear Programs

$$z(\theta) = \min_{x,y} c^T x + d^T y$$

$$\text{s.t. } Ax + Ey \leq b + F\theta$$

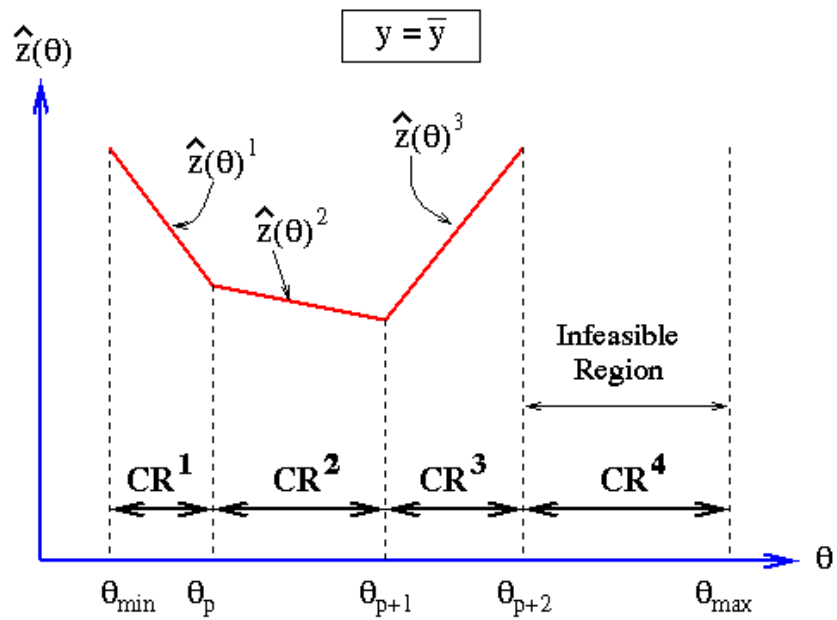
$$x \in \Re^n$$

$$y \in \{0,1\}^m$$

$$\theta \in \Theta \subseteq \Re^s$$

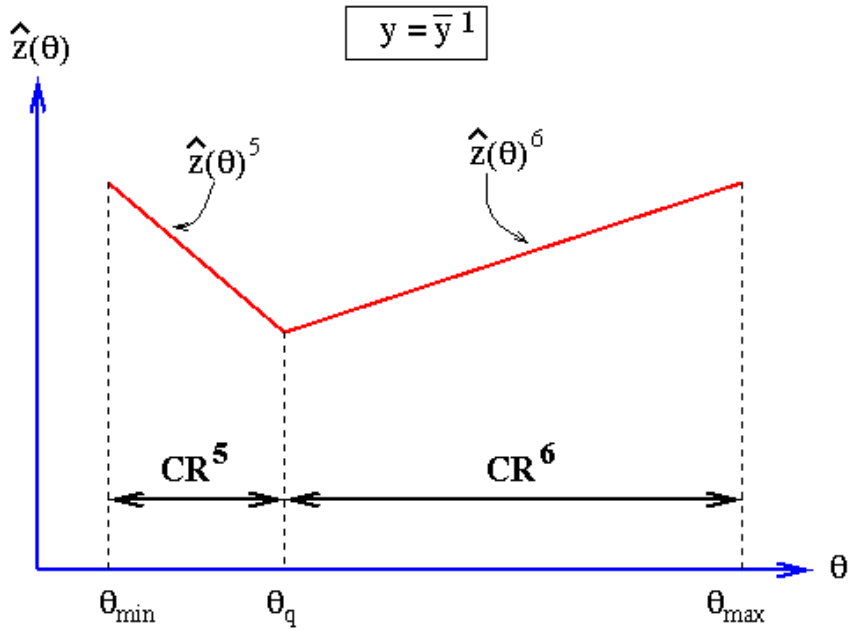
mp-MILP Algorithm - Step 1

- fix integer variables
- solve the multi-parametric LP => parametric upper bound
- infeasible region for multi-parametric case given by a set of convex regions



Next Integer Solution

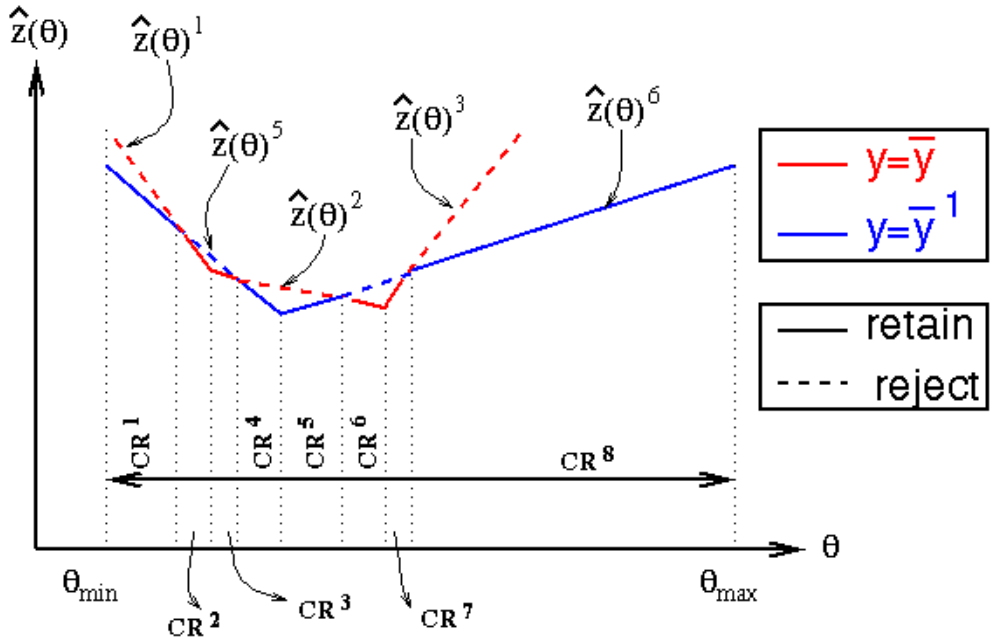
- obtain another integer solution by:
  - treating parameters as variables
  - introducing integer and parametric cuts



- solve multiparametric LP for next integer solution

Compare Parametric Solutions

- keep lower of the two parametric solutions

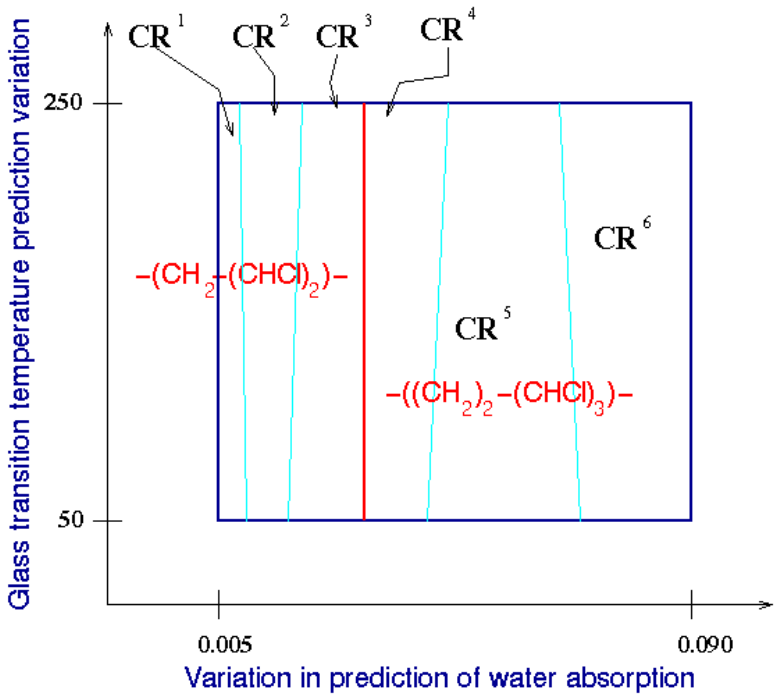


- for the multiparametric case, comparison is more difficult as it involves hyperplanes

Material Design under Uncertainty

- Objective: minimize the maximum deviation from the target property
- Constraints: property upper and lower bounds, property prediction correlations
- Integer Variables: number of each constituent molecular group
- Uncertainty: property prediction parameters

Polymer Design under Uncertainty



Parametric Solution

Parametric Solution	Critical Region
$s^1 = 0.02596 - 1.802\theta_1$	$76600\theta_1 + \theta_2 \leq 916.806$ $0.005 \leq \theta_1, 50 \leq \theta_2 \leq 250$
$s^2 = 0.0044 + 2.352 \times 10^{-5}\theta_2$	$-76600\theta_1 - \theta_2 \leq -916.806$ $76600\theta_1 - \theta_2 \leq 1290.806$ $50 \leq \theta_2 \leq 250$
$s^3 = -0.02596 + 1.802\theta_1$	$-76600\theta_1 + \theta_2 \leq -1290.806$ $\theta_1 \leq 0.03075, 50 \leq \theta_2 \leq 250$
$s^4 = 0.06491 - 1.15274\theta_1$	$76600\theta_1 - \theta_2 \leq 3262.846$ $0.03075 \leq \theta_1, 50 \leq \theta_2 \leq 250$
$s^5 = 0.0158 - 1.505 \times 10^{-5}\theta_2$	$76600\theta_1 + \theta_2 \leq 5363.846$ $-76600\theta_1 + \theta_2 \leq -3262.846$ $50 \leq \theta_2 \leq 250$
$s^6 = -0.06491 + 1.15274\theta_1$	$-76600\theta_1 - \theta_2 \leq -5363.846$ $\theta_1 \leq 0.09, 50 \leq \theta_2 \leq 250$

Multi-Parametric Mixed Integer Quadratic Programs

$$z(\theta) = \min_{x,y} c^T x + \tfrac{1}{2} x^T Q x + d^T y$$

$$\text{s.t. } Ax + Ey \le b + F\theta$$

$$x \in \Re^n$$

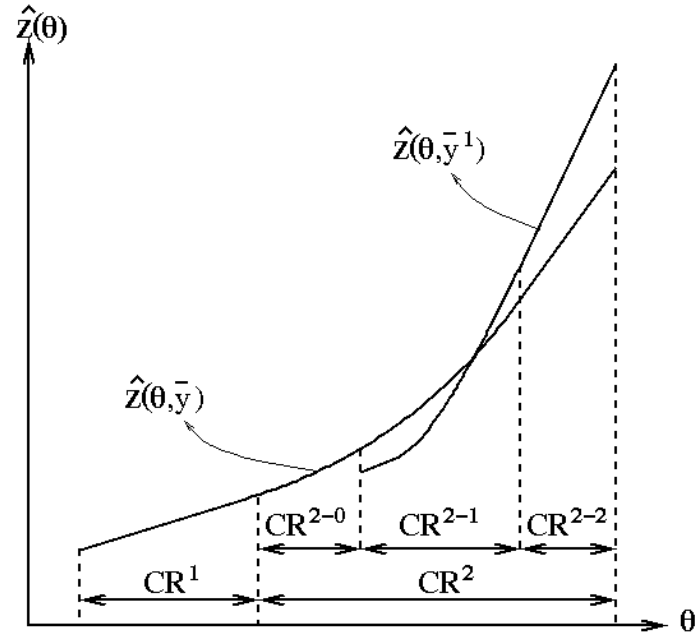
$$y \in \{0,1\}^m$$

$$\theta \in \Theta \subseteq \Re^s$$

An Enclosure of the Solution

- Fix integer variables
  - solve mp-QP
  - parametric upper bound
  - critical regions
- Introduce cuts:
  - previous integer solution
  - parametric upper bound

  (Nonconvex formulation)



- Remove redundant parametric solns
- Retain ALL non-redundant parametric solns

Multi-Parametric Global Optimization

$$z(\theta) = \min_{x} f(x)$$

$$\text{s.t. } g(x) \le b + F\theta$$

$$x^L \le x \le x^U$$

$$\theta^L \le \theta \le \theta^U$$

$$x \in X \subseteq \Re^n$$

$$\theta \in \Theta \subseteq \Re^s$$

- Formulate Convex Multi-Parametric Overestimating and Underestimating Subproblems
- Branch and Bound on the space of optimization variables and parameters to:
  - Obtain tighter subproblems
  - Compare parametric solutions
  - Fathom spaces of variables and parameters

Key Problems:

- Research in Global Optimization
  - Not much work on Overestimators
  - A local solution provides an upper bound
- Upper Bound: Solution of Multi-Parametric Non-convex Programs by using Multi-Parametric Convex Programming Techniques does not provide a parametric upper bound

An Example

$$z(\theta) = \min_x \cos(x)$$

$$\text{s.t.} \quad x \le \theta$$

$$x \ge \theta$$

$$\pi \le \theta \le 5\pi$$

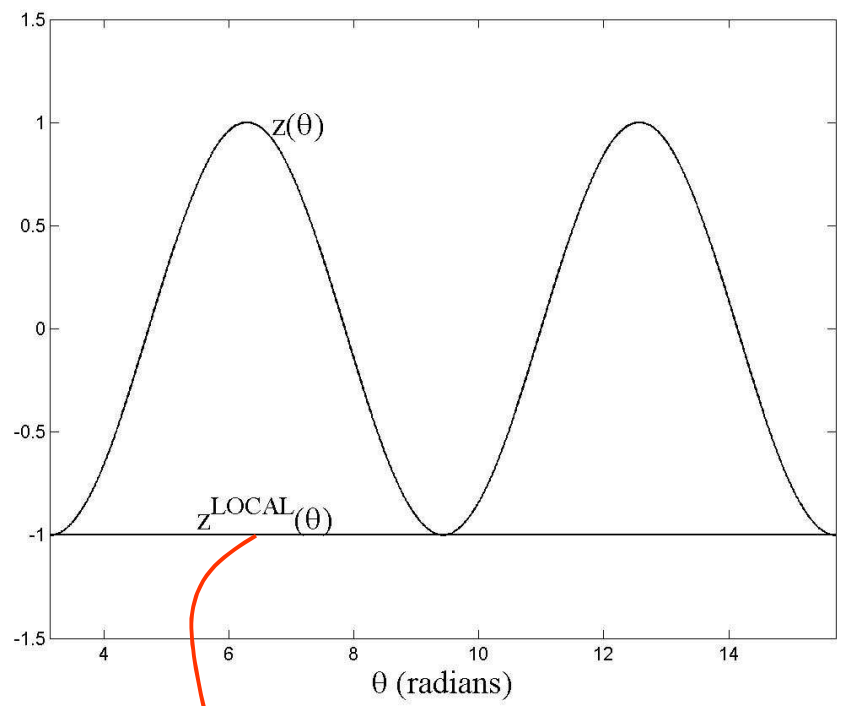
Outer-Approximation at θ = π

$$z^{\text{LOCAL}}(\theta) = \min_x \; -1$$

$$\text{s.t.} \quad x \le \theta$$

$$x \ge \theta$$

$$\pi \le \theta \le 5\pi$$



Not an upper bound!

Four Overestimators

OVERESTIMATOR-1

- Substitute the solution of the underestimating subproblem into the original problem
- Minimum computational effort
- If the parametric profile is linear it can be compared to the solution of the underestimating subproblem to check for convergence

OVERESTIMATOR-2: Bilinear

Problem:

$$z(\theta) = \min_{x} f(x) + x_1 x_2$$

$$\text{s.t. } g(x) \le b + F\theta$$

Underestimating Problem:

$$\check{z}(\theta) = \min_{x,w} f(x) + w$$

$$\text{s.t. } g(x) \le b + F\theta$$

$$w \ge x_1^L x_2 + x_2^L x_1 - x_1^L x_2^L$$

$$w \ge x_1^U x_2 + x_2^U x_1 - x_1^U x_2^U$$

McCormick Underestimator

Lemma 1 (Floudas and co-workers): the maximum separation distance between the bilinear term and its convex underestimator is given by δ where:

$$\delta = \frac{(x_1^U - x_1^L)(x_2^U - x_2^L)}{4}$$

OVERESTIMATOR-2

Overestimating Subproblem:

$$\hat{z}(\theta) = \min_{x,w} f(x) + w + \delta$$

$$\text{s.t. } g(x) \le b + F\theta$$

$$w \ge x_1^L x_2 + x_2^L x_1 - x_1^L x_2^L$$

$$w \ge x_1^U x_2 + x_2^U x_1 - x_1^U x_2^U$$

- δ is a function of space of x under consideration => finite convergence within ε

- LEMMA 2 (Dua, Papalexandri, Pistikopoulos): The difference between the solution of the overestimating and the underestimating subproblem is given by δ. Only one subproblem: overestimating or underestimating, needs to be solved

OVERESTIMATOR-3

- Replace the non-convex term by its overestimating expressions: quite general
- Requires solving an optimization problem

McCormick Overestimator:

$$w \geq x_1^L x_2 + x_2^U x_1 - x_1^L x_2^U$$

$$w \geq x_1^U x_2 + x_2^L x_1 - x_1^U x_2^L$$

- Lemma 3 (Dua, Papalexandri, Pistikopoulos, 2003): For the case when only bilinear non-convexities are present, the Overestimator-2 is tighter than the Overestimator-3 in 87.5% of the area of the rectangle: $(x_1^U - x_1^L)(x_2^U - x_2^L)$

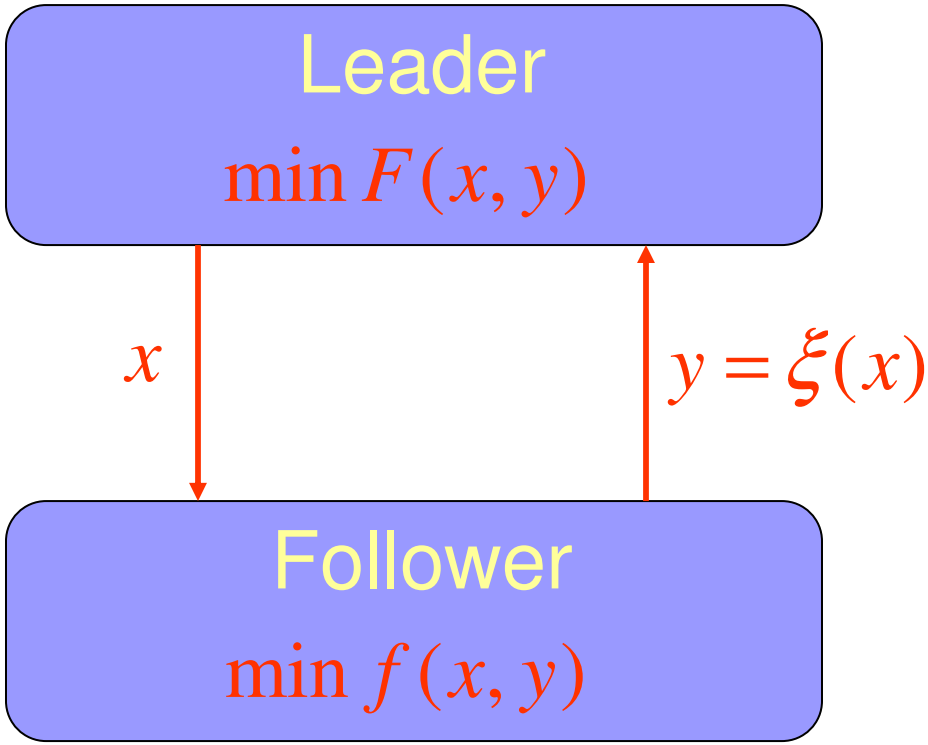
Overestimator-4

- When only bilinear terms are present in the objective function
- Replace the bilinear terms by McCormick overestimating expressions and reverse the sign of inequalities in the expressions
- Replace ‘min’ by ‘max’ in the objective function: solve an optimization problem
- Overestimator-4 is tighter than Overestimator-3

Parametric Overestimators Selection Criterion: Problem Specific

- Ease of obtaining: computational effort
  - O1,O2 < O3, O4
- Tightness: special cases
  - Case-1: O2<O3
  - Case-2: O4 < O3
- Functional Description: Linear or Nonlinear – for comparison purposes
  - O1 is sometimes non-linear

What is Bilevel Programming?



Mathematical Formulation

$$\min \quad F(x, y)$$
$$s.t. \quad G(x, y) \leq 0$$

Outer Problem

$$\min \quad f(x, y)$$
$$s.t. \quad g(x, y) \leq 0$$
$$x \in X, \; y \in Y$$

Inner Problem

- Linear Formulation is NP hard and Nonconvex
- Extensive Literature on Applications and Solution Techniques

Illustration: Bilevel Linear Programming Problem

$$\min_{x} \; F(x, y) = c_1^T x + d_1^T y$$

$$s.t. \quad A_1 x + B_1 y \le b_1$$

$$\min_{y} \; f(x, y) = c_2^T x + d_2^T y$$

$$s.t. \quad A_2 x + B_2 y \le b_2$$

Bilevel Programming via Parametric Programming

Step 1. Solve the inner problem as a parametric programming problem

(Reactions of the inner problem are computed as a function of the outer problem variables)

Step 2. Formulate the outer problem as a number of single optimisation problems

Step 3. Solve the single optimisation problems

(Global optimisation solutions are obtained)

Reformulation and Solution as a Parametric Program

$$\min_{y} \; f(x,y) = c_2^T x + d_2^T y$$
$$s.t. \quad A_2 x + B_2 y \le b_2$$

Inner Problem
(LP or QP)

Transform →

$$\min_{y} \; f(x,y) = d_2^T y + c_2^T x$$
$$s.t. \quad B_2 y \le b_2 - A_2 x$$

mp-LP/QP

↓

$$\xi_1(x) = m_1 + n_1 x \quad \text{if } H_1 x \le h_1$$
$$\xi_2(x) = m_2 + n_2 x \quad \text{if } H_2 x \le h_2$$
$$\vdots \qquad \vdots \qquad \vdots$$
$$\xi_k(x) = m_k + n_k x \quad \text{if } H_k x \le h_k$$

Critical region

Formulation and Solution of Single Optimization Problems

$$\min_x F(x,y) = c_1^T x + d_1^T y$$

$$s.t. \quad \begin{cases} A_1 x + B_1 y \le b_1 \\ \text{Inner Problem} \end{cases}$$

$$\begin{aligned} \min_x \quad & c_1^T x + d_1^T \xi_1(x) \\ s.t. \quad & A_1 x + B_1 \xi_1(x) \le b_1 \\ & H_1 x \le h_1 \end{aligned}$$

$$\begin{aligned} \min_x \quad & c_2^T x + d_2^T \xi_2(x) \\ s.t. \quad & A_2 x + B_2 \xi_2(x) \le b_2 \\ & H_2 x \le h_2 \end{aligned}$$

$$\vdots$$

$$\begin{aligned} \min_x \quad & c_k^T x + d_k^T \xi_k(x) \\ s.t. \quad & A_k x + B_k \xi_k(x) \le b_k \\ & H_k x \le h_k \end{aligned}$$

Numerical Example: Linear – Linear Case

Bard (1983), Visweswaran et al. (1996)

$$\min_{x} \quad F(x, y) = x + y$$

$$s.t. \quad -x \leq 0$$

$$\min_{y} \quad f(x, y) = -5x - y$$

$$s.t. \quad -x - 0.5y \leq -2$$

$$-0.25x + y \leq 2$$

$$x + 0.5y \leq 8$$

$$x - 2y \leq 2$$

$$-y \leq 0$$

Numerical Example: Linear – Linear Case

Transformation of the inner problem as an mp-LP problem

$$\min_{y} -y-5x$$

$$s.t. \quad \begin{bmatrix} -0.5 \\ 1 \\ 0.5 \\ -2 \\ -1 \end{bmatrix} y \le \begin{bmatrix} -2 \\ 2 \\ 8 \\ 2 \\ 0 \end{bmatrix} + \begin{bmatrix} 1 \\ 0.25 \\ -1 \\ -1 \\ 0 \end{bmatrix} x \quad \Rightarrow \quad y = \begin{cases} 0.25x+2 & \text{if } 0.8889 \le x \le 6.22 \quad (1) \\ -2x+16 & \text{if } \quad 6.22 \le x \le 6.8 \quad (2) \end{cases}$$

Computation of Global Optimum

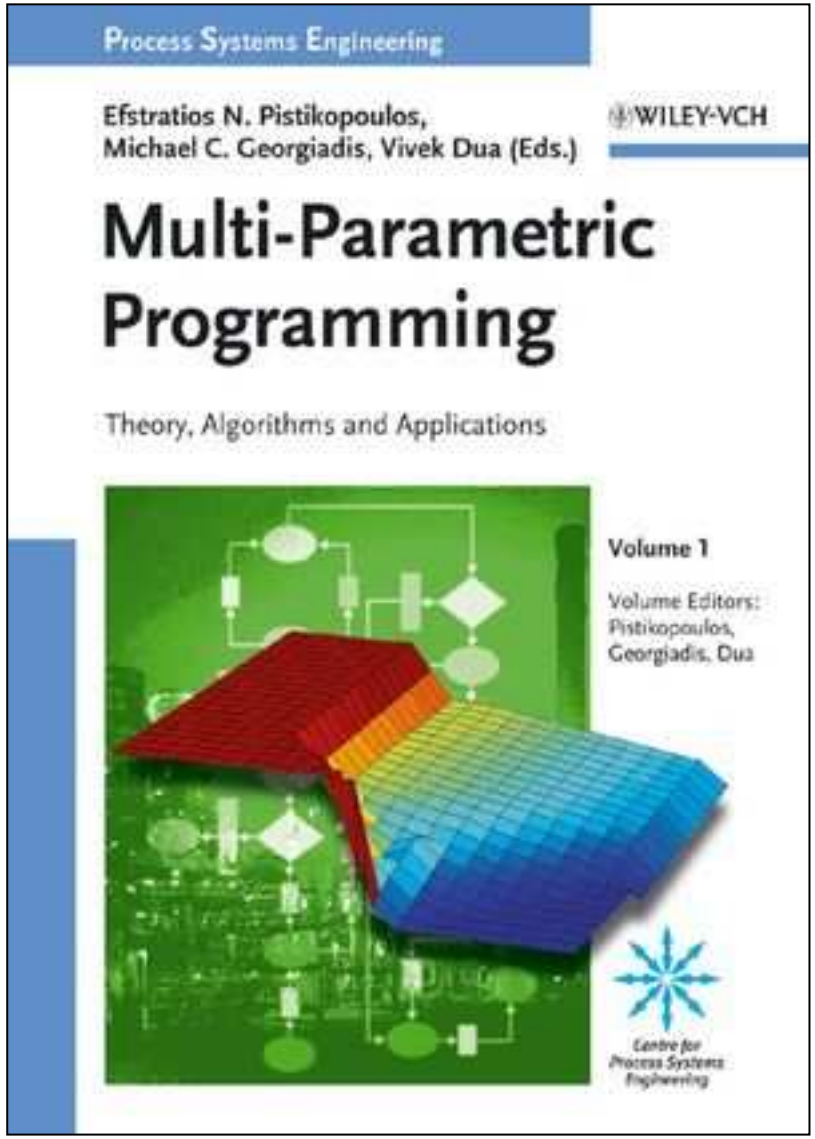
$$(1) \quad \min_{x} 1.25x + 2 \qquad s.t. \quad 0.8889 \le x \le 6.22$$

$$(2) \quad \min_{x} -x + 16 \qquad s.t. \quad 6.22 \le x \le 6.8$$

	CR (1)	CR (2)
F	3.111 (Global optimum)	9.20
x	0.8889	6.80
y	2.2222	2.40

Concluding Remarks

- Parametric Programming
  - Theory and algorithms for a wide range of mathematical programs
- Applications:
  - Optimization under Uncertainty
  - On-line Control and Optimization of Chemical, Biomedical, Automotive Systems
  - Bilevel programming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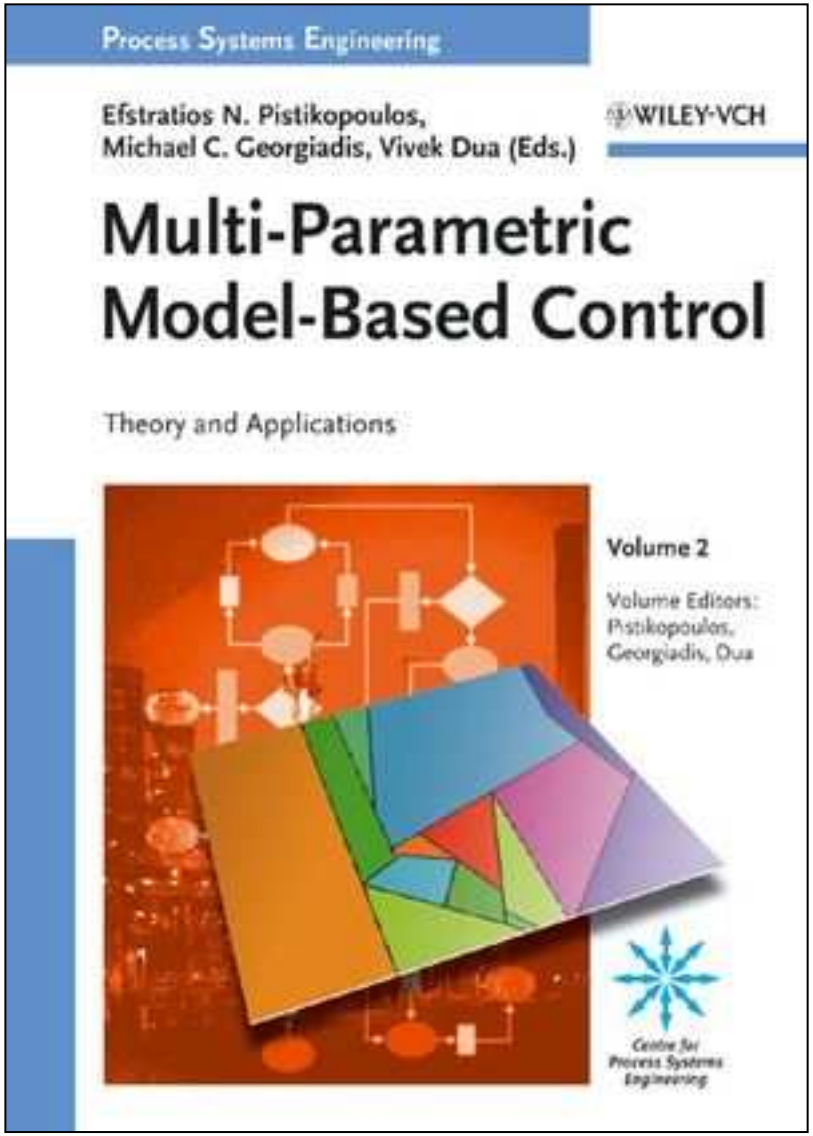
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