Applied Numerical Optimization

Prof. Alexander Mitsos, Ph.D.

Parametric optimization and uncertainty

Optimization Under Uncertainty

- Consider uncertain variables/parameters $\boldsymbol{y}$, e.g., :
  - $\boldsymbol{y}$ is a model parameter that can at best be estimated,
  - $\boldsymbol{y}$ results from a stochastic process, which is not yet resolved.

- $\boldsymbol{y}$ can affect objective function and constraints

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & f(\boldsymbol{x}, \boldsymbol{y}) \\ \text{s.t.} \quad & \boldsymbol{c}(\boldsymbol{x}, \boldsymbol{y}) \leq \boldsymbol{0} \end{aligned} \qquad \text{(PAR)}$$

  - $\boldsymbol{y}$ is not an optimization variable
  - if $\boldsymbol{y}$ is fixed then (PAR) is normal NLP in $\boldsymbol{x}$

- Alternative notions to handle uncertainty:
  - Parametric Optimization
  - Stochastic Programming
  - Robust Optimization

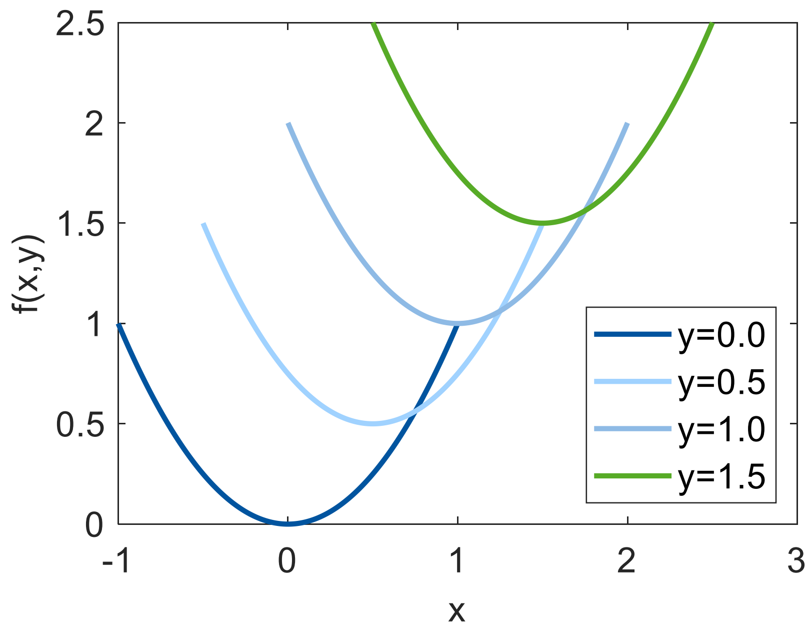
Parametric Optimization

- Parametric optimization is finding solution as function of parameter

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & f(\boldsymbol{x}, \boldsymbol{y}) \\ \text{s.t.} \quad & \boldsymbol{c}(\boldsymbol{x}, \boldsymbol{y}) \le \boldsymbol{0} \end{aligned} \qquad \text{(PAR)}$$

- The optimal solution point and optimal objective value depend on parameters: $\boldsymbol{x}^*(\boldsymbol{y})$ and $f^*(\boldsymbol{y}) = f(\boldsymbol{x}^*(\boldsymbol{y}), \boldsymbol{y})$

- Example:
  - $\min_x \; (x-y)^2 + y$
  - $x^*(y) = y$
  - $f^*(y) = f(x^*(y), y) = (y-y)^2 + y = y$



Parametric Optimization and Uncertainty

$$\begin{aligned} f^*(\boldsymbol{y}) = \min_{\boldsymbol{x}} \quad & f(\boldsymbol{x}, \boldsymbol{y}) \\ \text{s.t.} \quad & \boldsymbol{c}(\boldsymbol{x}, \boldsymbol{y}) \leq \boldsymbol{0} \end{aligned} \qquad \text{(PAR)}$$

- Suppose that $\boldsymbol{y}$ is uncertain parameter

- Parametric optimization is only useful under the following conditions:
  - The uncertainty is realized before the decision variables must be fixed
  - Once the uncertainty is realized, it is not practical to solve (PAR) for fixed $\boldsymbol{y}$

  These conditions hold for example in online control and resource allocation.

- Solution approaches typically identify parameter regions for which the solution stays qualitatively same.
  - So called critical region (CR), e.g., no active set change

Example: Parametric Quadratic Optimization

Consider convex quadratic parametric optimization problem

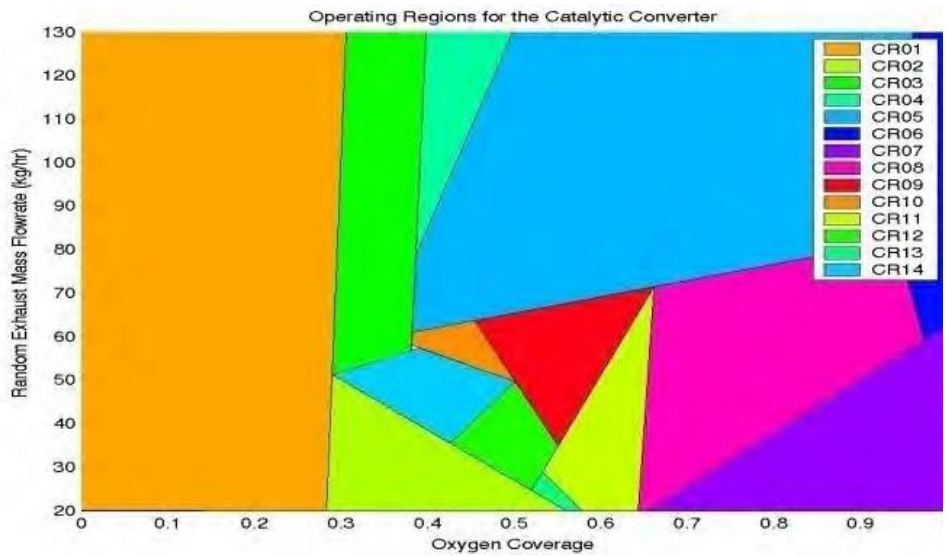
$$f^*(\boldsymbol{y}) = \min_{\boldsymbol{x} \in X} \frac{1}{2} \boldsymbol{x}^T \boldsymbol{G} \boldsymbol{x} + \boldsymbol{d}^T \boldsymbol{x} \quad \text{with} \quad \boldsymbol{y} \in Y$$
$$\text{s.t.} \quad \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{F}\boldsymbol{y}$$

- Solve for $\mathbf{y} = \bar{\boldsymbol{y}}$
- Recall that 1st order KKT are necessary and sufficient
  - Under mild assumptions
- Recall sensitivity analysis via KKT conditions
  - Yields $\boldsymbol{x}^*(\cdot)$ as an affine function of $\boldsymbol{y}$.
  - $\boldsymbol{x}^*(\cdot)$ seizes to be valid once one of the inequalities in the KKT conditions is violated.

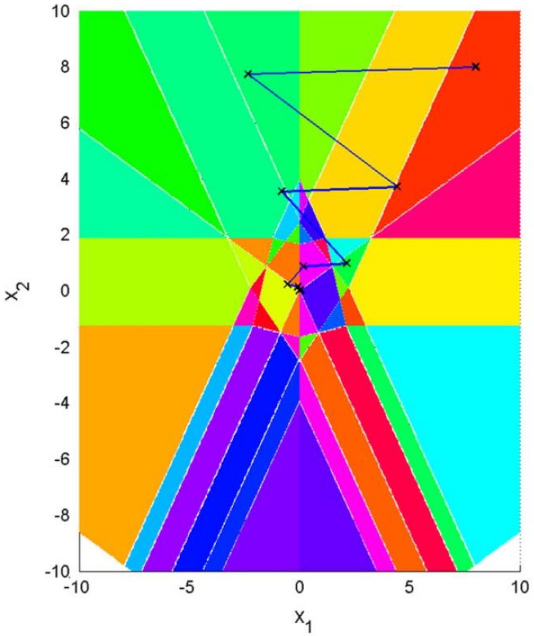
Example: Parametric Quadratic Optimization – Algorithm

1. Iterate $k = 1, 2, \ldots$
2. Solve (QPAR) with $\boldsymbol{y} \in Y$ as free variable
3. Fix $\bar{\boldsymbol{y}}$ to the solution and solve (QPAR) for $\boldsymbol{y} = \bar{\boldsymbol{y}}$
4. Derive parametric solution for current critical region $CR^{(k)}$
5. Derive constraints to define $CR^{(k)}$
6. If Y is covered with critical regions, STOP
7. Go to step 1 with $CR^{(k)}$ removed from the feasible set

$$
\begin{aligned}
f^*(\boldsymbol{y}) = \min_{\boldsymbol{x} \in X} \quad & \frac{1}{2}\boldsymbol{x}^T \boldsymbol{G}\boldsymbol{x} + \boldsymbol{d}^T\boldsymbol{x} \\
\text{s.t.} \quad & \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{F}\boldsymbol{y}
\end{aligned}
\qquad \text{(QPAR)}
$$



Picture from: Pistikopoulos, OSE 2012



Picture from: Oberdieck, Pistikopoulos, Automatica 2015

Check Yourself

- What is parametric optimization and how does it relate to uncertainty?

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Introduction to optimization under uncertainty

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Optimization Under Uncertainty

- Consider uncertain variables/parameters $\boldsymbol{y}$, e.g., :
  - $\boldsymbol{y}$ is a model parameter that can at best be estimated,
  - $\boldsymbol{y}$ results from a stochastic process, which is not yet resolved.

- $\boldsymbol{y}$ can affect objective function and constraints

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & f(\boldsymbol{x}, \boldsymbol{y}) \\ \text{s.t.} \quad & \boldsymbol{c}(\boldsymbol{x}, \boldsymbol{y}) \leq \mathbf{0} \end{aligned}$$

  - $\boldsymbol{y}$ is not an optimization variable
  - if $\boldsymbol{y}$ is fixed then we have normal NLP in $\boldsymbol{x}$

- Alternative notions to handle uncertainty:
  - Parametric Optimization
  - Stochastic Programming
  - Robust Optimization

Alternatives to Parametric Optimization

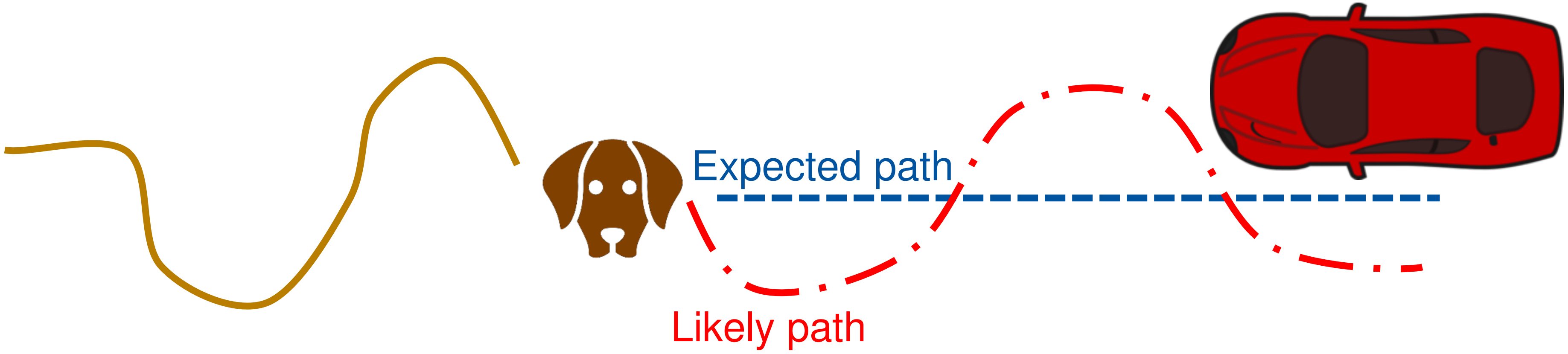
Different notions to account for uncertainty:

- Stochastic approaches consider probability measures over the set of possible uncertainty realizations
- Robust approaches consider worst-case uncertainty realization

	Stochastic	Robust
Assumption	Known probability for $\boldsymbol{y}$	$\mathbf{y}$ bounded, $\mathbf{y} \in Y$
Objective	e.g., $\min\limits_{\mathbf{x}} \mathbb{E}_Y(f(\mathbf{x}, \mathbf{y}))$	$\min\limits_{\mathbf{x}} \max\limits_{\mathbf{y} \in Y} f(\mathbf{x}, \mathbf{y})$
	Optimality in probabilistic sense	Optimality for the worst case
Constraint	e.g., $\mathbb{P}_Y(\mathbf{c}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0}) \geq \alpha,\ \alpha \in (0,1)$	$\mathbf{c}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0}, \forall \mathbf{y} \in Y$
	Chance for feasibility	Guaranteed feasibility

- Compared to neglecting uncertainties, both approaches result in more reliable and conservative solutions

Example: Optimization under Uncertainty (1)



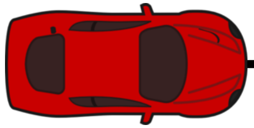
Inspired by Sam L. Savage, Stanford University

Nominal optimization:
- Consider expected path, drive straight. Likely result: 

Stochastic approach:
- Consider likely paths, drive to the side and slow down. Likely result: 

Robust approach:
- Consider all possible paths, stop the car. Guaranteed result: 

Example: Optimization under Uncertainty (2)



50% no traffic, 45min

40% moderate traffic, 60min

10% much traffic, 120min

Minimize time at airport (T@A), missed flight ⇒ 3h wait

- Nominal optimization:
  - Leave 58.5 min before flight: avg. T@A: 90min, 50% missed flights
- Stochastic approach:
  - Leave 60 min before flight: avg. T@A: 19.5min, 10% missed flights
- Robust approach:
  - Leave 120 min before flight: avg. T@A: 61.5min, 0% missed flights

Check Yourself

- What problems can arise if uncertainty is neglected in the solution of optimization problems?
- Name the basic notions of how uncertainty can be addressed. How do the approaches relate to each other?

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Two-stage stochastic optimization

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Two-Stage Stochastic Programming

Consider the following problem description:

- $\boldsymbol{y} \in Y$ is an uncertain parameter with some probability distribution.
- $\boldsymbol{x} \in X$ is a decision variable that must be fixed before the uncertainty is realized with constraints $\boldsymbol{c}^{\mathrm{U}}(\boldsymbol{x}) \leq \mathbf{0}$.
- $\boldsymbol{z} \in Z$ is a decision variable that can be fixed after the uncertainty is realized with constraints $\boldsymbol{c}^{\mathrm{L}}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}) \leq \mathbf{0}$.
- An objective function $f : X \times Y \times Z \to \mathbb{R}$ is to be minimized.
- f is separable such that $f(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}) = f^{\mathrm{U}}(\boldsymbol{x}) + f^{\mathrm{L}}(\boldsymbol{y}, \boldsymbol{z})$.

- The corresponding two-stage stochastic program can be written as

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & f^{\mathrm{U}}(\boldsymbol{x}) + \mathbb{E}_Y(F(\boldsymbol{x}, \boldsymbol{y})) \\ \text{s.t.} \quad & \boldsymbol{c}^{\mathrm{U}}(\boldsymbol{x}) \leq \mathbf{0} \end{aligned} \qquad \text{(ST1)}$$

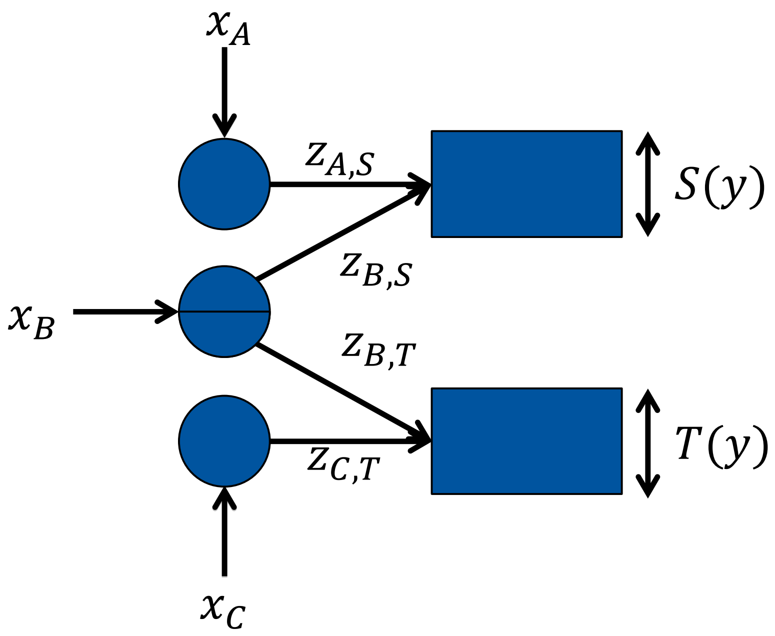
$$\begin{aligned} F(\boldsymbol{x}, \boldsymbol{y}) = \min_{\boldsymbol{z}} \quad & f^{\mathrm{L}}(\boldsymbol{y}, \boldsymbol{z}) \\ \text{s.t.} \quad & \boldsymbol{c}^{\mathrm{L}}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}) \leq \mathbf{0} \end{aligned} \qquad \text{(ST2)}$$

- (ST1) determines the fist-stage decision process before the uncertainty is realized.
- (ST2) describes the second-stage decision process for a specific uncertainty scenario.

Two-Stage Stochastic Programming Example: Plant design

Determine sizing (x_A, x_B, x_C) of different production tracks to maximize profit under uncertain demand $(S(y), T(y))$.

1. Decide on investment into tracks A, B, C: (x_A, x_B, x_C).
2. Realize uncertainty y and obtain demand: $S(y)$ and $T(y)$.
3. Decide on production of products S and T from tracks A, B, C: $(z_{A,S}, z_{B,S}, z_{B,T}, z_{C,T})$.



$$\min_{\boldsymbol{x}} \; d_A x_A + d_B x_B + d_C x_C + \mathbb{E}_Y(F(x,y))$$
$$\text{s.t.} \; x_A + x_B + x_C \le x_{max}$$
$$x_A, x_B, x_C \ge 0$$

$$F(x,y) = \min_{z} -d_S\left(z_{A,S} + z_{B,S}\right) - d_T\left(z_{B,T} + z_{C,T}\right)$$
$$\text{s.t.} \; z_{A,S} \le x_A \qquad z_{A,S} + z_{B,S} \le S(y)$$
$$z_{B,S} + z_{B,T} \le x_B \qquad z_{B,T} + z_{C,T} \le T(y)$$
$$z_{C,T} \le x_C$$

A Single-Stage Reformulation

$$\begin{aligned} &\min_{\boldsymbol{x}} f^{\mathrm{U}}(\boldsymbol{x}) + \mathbb{E}_Y(F(\boldsymbol{x},\boldsymbol{y})) \\ &\text{s.t.}\ \ \boldsymbol{c}^{\mathrm{U}}(\boldsymbol{x}) \le \boldsymbol{0} \end{aligned} \qquad \text{(ST1)}$$

$$\begin{aligned} F(\boldsymbol{x},\boldsymbol{y}) = &\min_{\boldsymbol{z}}\ f^{\mathrm{L}}(\boldsymbol{y},\boldsymbol{z}) \\ &\text{s.t.}\ \boldsymbol{c}^{\mathrm{L}}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{z}) \le \boldsymbol{0} \end{aligned} \qquad \text{(ST2)}$$

- If $\boldsymbol{y}$ has a continuous or large discrete distribution, $\mathbb{E}_Y(F(\boldsymbol{x},\boldsymbol{y}))$ is difficult if not impossible to evaluate exactly.
- The distribution can be approximated by finitely many scenarios $s \in \mathcal{S}$ with $\mathbf{y} = \boldsymbol{y}_s > \mathbf{0}$ and probability of occurrence P_s such that $\sum_{s\in\mathcal{S}} P_s = 1$
- Then, the two-stage stochastic program can be approximated by the single-stage program

$$\begin{aligned} &\min_{\boldsymbol{x},\boldsymbol{z}_s} f^{\mathrm{U}}(\boldsymbol{x}) + \sum_{s\in\mathcal{S}} P_s \cdot f^{\mathrm{L}}(\boldsymbol{y}_s,\boldsymbol{z}_s) \\ &\text{s.t.}\ \boldsymbol{c}^{\mathrm{U}}(\boldsymbol{x}) \le \boldsymbol{0} \\ &\qquad \boldsymbol{c}^{\mathrm{L}}(\boldsymbol{x},\boldsymbol{y}_s,\boldsymbol{z}_s) \le \boldsymbol{0}, \forall s \in \mathcal{S} \end{aligned}$$

- The resulting problem is potentially very large and challenging to solve.
- More efficient approaches have been proposed in literature.

Check Yourself

- What is the essential feature of a two-stage stochastic program?
- When can a two-stage stochastic program be reformulated exactly into a single-stage program?

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Introduction to Semi Infinite Programs

Semi-Infinite Optimization Problems

What does the following mean?

$$\min_{\boldsymbol{x} \in X} \; f(\boldsymbol{x}) \qquad \text{(SIP)}$$
$$\text{s.t. } \; c(\boldsymbol{x}, y) \leq 0, \forall y \in Y$$

- A point $\boldsymbol{x} \in X$ is feasible if and only if $c(\boldsymbol{x}, y) \leq 0$ holds for all possible values of $y \in Y$.
- If $|Y| = \infty$, we speak of a semi-infinite optimization problem (SIP)
- For simplicity of notation we take a single SIP constraint, and a single uncertain variable $y \in Y \subset R$
- SIP has finitely many variables and infinitely many constraints
- SIPs date back to at least 1960s
- SIPs are useful for worst-case optimization="robust optimization"
- Many generalizations exist, including to $Y(\boldsymbol{x})$, existence constraints
- It is important special case of hierarchical problems (bilevel, trilevel)

Semi-Infinite Optimization Problems: A Useful Reformulation

$$\min_{\boldsymbol{x}\in X} \; f(\boldsymbol{x}) \qquad \text{(SIP)}$$
$$\text{s.t.} \;\; c(\boldsymbol{x}, y) \leq 0, \forall y \in Y$$

- If $\max_{y\in Y} c(\boldsymbol{x}, y)$ exists, we can rewrite (SIP) as

$$\min_{\boldsymbol{x}\in X} \; f(\boldsymbol{x})$$
$$\text{s.t.} \;\; 0 \geq \max_{y\in Y} c(\boldsymbol{x}, y)$$

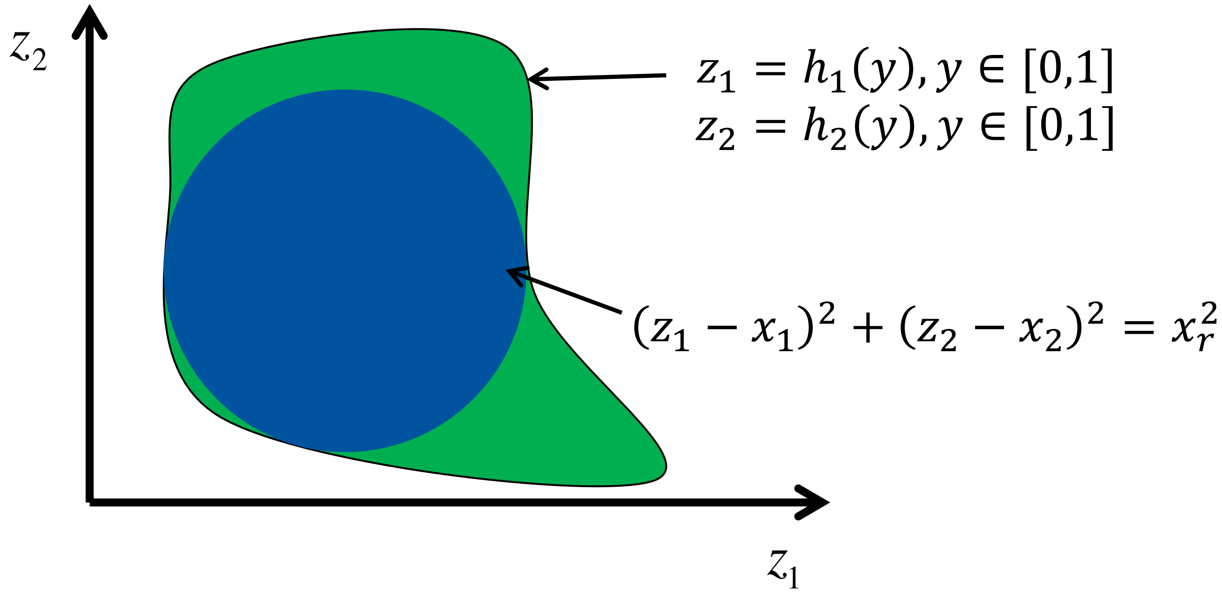
- We call $\max_{y\in Y} c(\boldsymbol{x}, y)$ the lower-level problem (LLP)
- A point $\boldsymbol{x} \in X$ is feasible if and only if the global solution to LLP is ≤ 0

Design Centering as Semi-Infinite Program

- Fit the largest Shape A that fits into Shape B

- Example: circle
  - Variables: center coordinates & radius $\boldsymbol{x} = (x_1, x_2, x_r)$
  - Objective: maximal radius $\Rightarrow \max_{\boldsymbol{x}} x_r$
  - Constraint: Shape A shall fit into Shape B

$$\Rightarrow (h_1(y) - x_1)^2 + (h_2(y) - x_2)^2 \geq x_r^2,\ \forall y \in [0,1]$$



- Real-life applications:
  - Diamond cutting: Stein, Optimization with Multivalued Mappings: Theory, Applications and Algorithms, 2006
  - Model reduction: Oluwole et. al, Combustion and Flame, 2006

Example: Path Constraints in Dynamic Optimization

- Dynamic optimization: infinite # variables
  - Handled by control-vector parametrization
- States uniquely determined as function of time by model
- Path constraints hold for $\forall\, t \rightarrow$ semi-infinite problem
- Standard algorithms & solvers enforce the path constraints for a finite # times:
  - $[0, t_f]$ is discretized to $\{t_1, t_2, \dots, t_N\} \subset [0, t_f]$
  - Relaxation that may result in violations
- Motivates the use of SIP techniques[1,2]

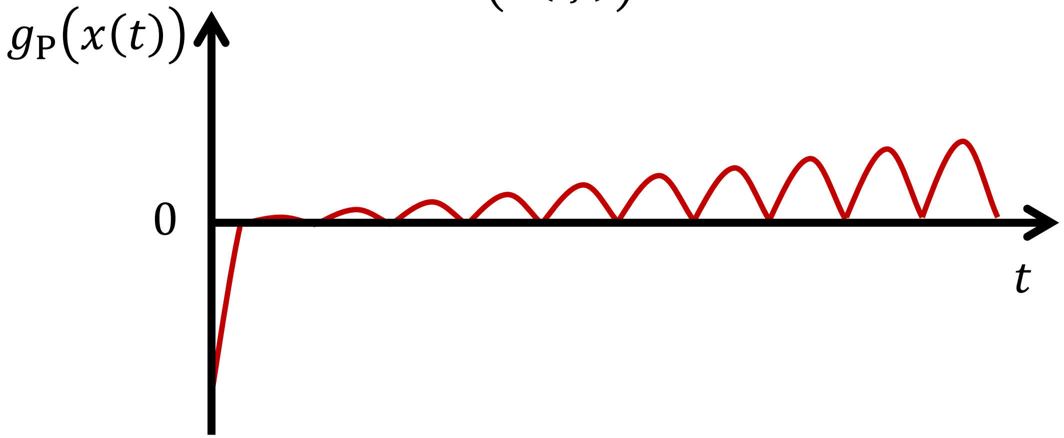
$$\min_{\boldsymbol{x}(\cdot),\boldsymbol{u}(\cdot)} \Phi\left(\boldsymbol{x}(t_f)\right)$$

$$\text{s.t.} \quad \dot{\boldsymbol{x}}(t) = \boldsymbol{f}\left(\boldsymbol{x}(t), \boldsymbol{u}(t)\right), t \in [t_0, t_f]$$

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

$$\boldsymbol{g}_{\mathrm{P}}\left(\boldsymbol{x}(t), \boldsymbol{u}(t)\right) \leq \boldsymbol{0}\ \forall t \in [t_0, t_f]$$

$$\boldsymbol{g}_{\mathrm{T}}\left(\boldsymbol{x}(t_f)\right) \leq \boldsymbol{0}$$



[1] Polak, SIAM Review, 1987
[2] Fu et. int Mitsos, Automatica, 2015

Example: Optimal Operation Under Parametric Uncertainty

$$\min_{\boldsymbol{x}(\cdot),\boldsymbol{u}(\cdot)} \Phi\left(\boldsymbol{x}(t_f)\right)$$

s.t. $\dot{\boldsymbol{x}}(t) = \boldsymbol{f}(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{y}), t \in [t_0, t_f]$

$\boldsymbol{x}(t_0) = \boldsymbol{x}_0(\boldsymbol{y})$

$\boldsymbol{g}_{\mathrm{P}}(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{y}) \leq \mathbf{0}\ \forall t \in [t_0, t_f]$

$$\min_{\boldsymbol{u}(\cdot)} \Phi\left(\boldsymbol{x}(t_f)\right)$$

s.t. $\boldsymbol{g}_{\mathrm{P}}(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{y}) \leq \mathbf{0}\ \forall t \in [t_0, t_f]$

Where $\boldsymbol{x}(\cdot)$ is the solution of

$\dot{\boldsymbol{x}}(t) = \boldsymbol{f}(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{y}), t \in [t_0, t_f]$

$\boldsymbol{x}(t_0) = \boldsymbol{x}_0(\boldsymbol{y})$

- Recall sequential interpretation
- Worst-case formulation by introducing parametric solution of states

$$\min_{\boldsymbol{u}(\cdot)} \Phi\left(\boldsymbol{x}(t_f)\right)$$

$\boldsymbol{g}_{\mathrm{P}}\left(\boldsymbol{x}_{\boldsymbol{y}}(t), \boldsymbol{u}(t), \boldsymbol{y}\right) \leq \mathbf{0}\ \forall \boldsymbol{y}, \forall t \in [t_0, t_f]$

Where $\boldsymbol{x}(\cdot)$ is the solution of nominal $\boldsymbol{y} = \bar{\boldsymbol{y}}$

$\dot{\boldsymbol{x}}(t) = \boldsymbol{f}(\boldsymbol{x}(t), \boldsymbol{u}(t), \bar{\boldsymbol{y}}), t \in [t_0, t_f]$

$\boldsymbol{x}(t_0) = \boldsymbol{x}_0(\bar{\boldsymbol{y}})$

and $\boldsymbol{x}_{\boldsymbol{y}}(\cdot)$ is the solution for given $\boldsymbol{y}$

$\dot{\boldsymbol{x}}(t) = \boldsymbol{f}(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{y}), t \in [t_0, t_f]$

$\boldsymbol{x}(t_0) = \boldsymbol{x}_0(\boldsymbol{y})$

[1] Puschke et. int Mitsos, Comp&Chem Eng, 2018

Check Yourself

- For which kind of constraint functions is an SIP particularly difficult to solve? Why is this the case?
- What are applications of SIP?

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Basic solution methods for Semi Infinite Programs

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Semi-Infinite Optimization Problems: A Useful Reformulation

$$\begin{aligned} \min_{\boldsymbol{x}\in X}\ & f(\boldsymbol{x}) \\ \text{s.t.}\ & c(\boldsymbol{x},y) \le 0, \forall y \in Y \end{aligned} \qquad \text{(SIP)}$$

- If $\max_{y\in Y} c(\boldsymbol{x},y)$ exists, we can rewrite (SIP) as

$$\begin{aligned} \min_{\boldsymbol{x}\in X}\ & f(\boldsymbol{x}) \\ \text{s.t.}\ & 0 \ge \max_{y\in Y} c(\boldsymbol{x},y) \end{aligned}$$

- We call $\max_{y\in Y} c(\boldsymbol{x},y)$ the lower-level problem (LLP)
- A point $\boldsymbol{x} \in X$ is feasible if and only if the global solution to LLP is ≤ 0

Intuitive Solution Approach as Nested Problem?

- Treat semi-infinite constraint as black box function

$$c^*(\boldsymbol{x}) = \max_{y \in Y} c(\boldsymbol{x}, y)$$

- Use local solver to solve

$$\min_{\boldsymbol{x} \in X} \; f(\boldsymbol{x})$$
$$\text{s.t. } c^*(\boldsymbol{x}) \leq 0$$

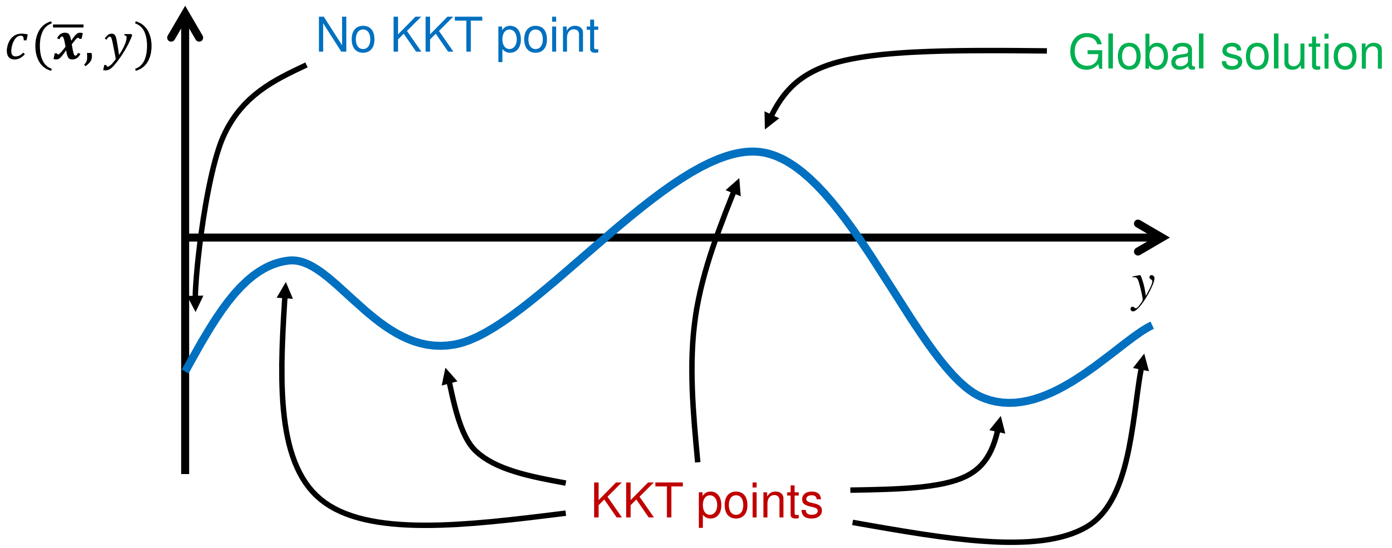
- For any particular $\boldsymbol{x} \in X$ obtain $c^*(\boldsymbol{x})$ by solving (LLP) globally

- Problems
  - Gradient-based methods are not applicable: $c^*(\cdot)$ is not differentiable
  - Gradient-free local solvers evaluate many points $\boldsymbol{x} \in X$ requiring many global solutions of (LLP)
  - Parametric solution of $c^*(\cdot)$ is extremely expensive

- Nonsmooth local solvers of interest

Intuitive Solution Approach using Optimality Conditions of LLP?

- Replace the lower-level problem with its KKT conditions
- The resulting problem is finite and can be solved by NLP methods
  - Recall that the KKT conditions have nonsmoothness
- In general wrong since KKT conditions are **not sufficient for the global** maximization of LLP



- Relaxation of the SIP: resulting point is not necessarily feasible in the SIP

Solution Methods of SIP: Local Reduction and Discretization

1. Local reduction

- For a point $\bar{\boldsymbol{x}} \in X$, find all KKT points of the LLP
- Track all KKT points
- The resulting problem is finite and can be solved by NLP methods

2. Discretization

- Replace Y with a finite discretization $Y^D \subset Y$
- The resulting problem is a finite approximation of the SIP and can be solved by NLP methods
- The resulting problem is a relaxation
- The discretization Y^D is populated to better approximate the SIP
- The relaxation can be tightened by using also KKT conditions of LLP

Check Yourself

- For which kind of constraint functions is an SIP particularly difficult to solve? Why is this the case?
- Why not solve the nested problem directly?
- Name the basic approaches to the solution of SIPs.
- How does the discretized version of an SIP relate to the original problem?

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Deterministic global solution of Semi Infinite Programs

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Semi-Infinite Optimization Problems: A Useful Reformulation

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- If $\max_{y\in Y} c(\boldsymbol{x},y)$ exists, we can rewrite (SIP) as

$$\min_{\boldsymbol{x}\in X} f(\boldsymbol{x}) \quad \text{s.t.} \quad 0 \geq \max_{y\in Y} c(\boldsymbol{x},y)$$

- We call $\max_{y\in Y} c(\boldsymbol{x},y)$ the lower-level problem (LLP)

- Goal: solve the SIP globally using discretization-based lower & upper bounding procedures
  - up to optimality gap $f^{UBD} - f^{LBD} \leq \varepsilon^f$
  - Assuming an SIP Slater point, continuous functions and compact X, Y

Mitsos, Optimization, 2011

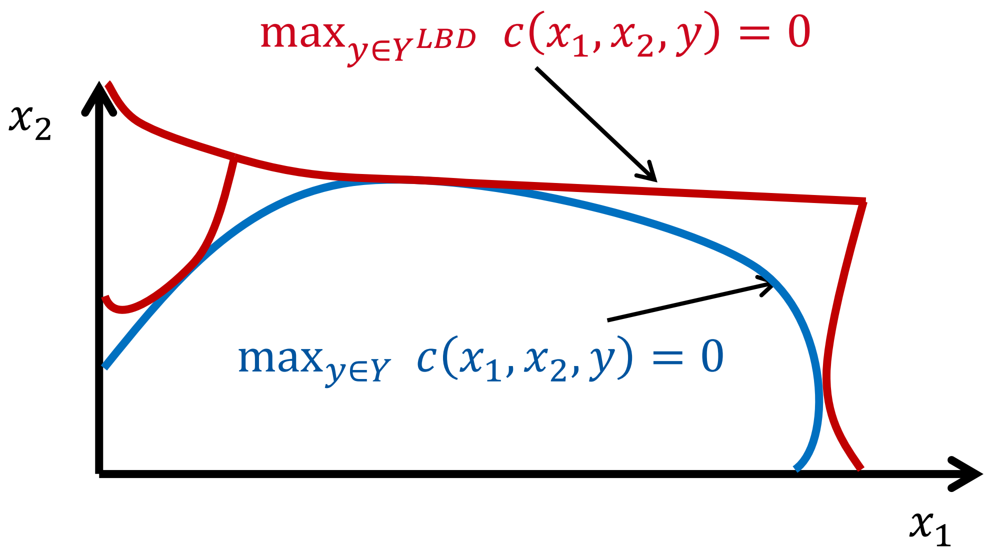
Discretization Approach from Blankenship & Falk

- Approximate Y with $Y^{LBD} \subset Y$, $|Y^{LBD}| < \infty$ to lower bounding problem (LBD)
  - The LLP is restricted and thus the SIP relaxed
  - Outer approximation

$$\begin{aligned} \min_{\boldsymbol{x} \in X} \quad & f(\boldsymbol{x}) \\ \text{s.t.} \quad & c(\boldsymbol{x}, y) \leq 0, \ \forall y \in Y^{LBD} \end{aligned} \qquad \text{(LBD)}$$

- Solve (LBD) and obtain $\bar{\boldsymbol{x}}$

- Solve (LLP) **globally** for $\boldsymbol{x} = \bar{\boldsymbol{x}}$ to alternatively obtain
  - $c^*(\bar{\boldsymbol{x}}) \leq 0$, $\bar{\boldsymbol{x}}$ is SIP feasible
  - $\bar{y}$: $c(\bar{\boldsymbol{x}}, \bar{y}) > 0$



Blankenship and Falk, J. Optim. Theory Appl.,1976

Lower Bounding Procedure

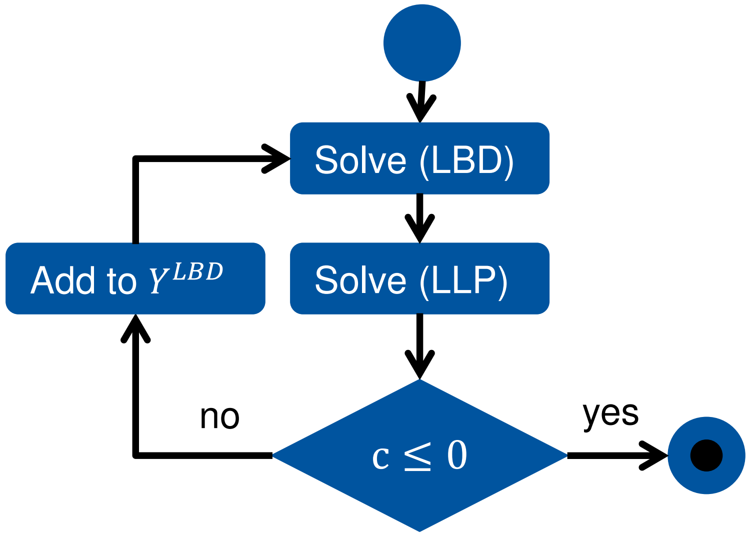
- (LBD) is a relaxation of (SIP) for any $Y^{LBD} \subset Y$
- The global solution of (LBD) gives a lower bound on the globally optimal objective value of (SIP)

- Algorithm:

1. Initialize $Y^{LBD} \subset Y, f^{LBD} \leftarrow -\infty$

2. Solve (LBD) globally to obtain $\bar{x}$
   - Set $f^{LBD} \leftarrow f(\bar{\boldsymbol{x}})$

3. Solve (LLP) globally for $\bar{\boldsymbol{x}}$ to obtain $\bar{y}$
   - If $c(\bar{\boldsymbol{x}}, \bar{y}) \leq 0$ then set $\boldsymbol{x}^* \leftarrow \bar{\boldsymbol{x}}$ and terminate ($\boldsymbol{x}^*$ is feasible)
   - Else set $Y^{LBD} \leftarrow \{\bar{y}\} \cup Y^{LBD}$ and go to step 2



- The algorithm converges to the global solution to (SIP) in the limit
- Finite generation of a feasible point is not guaranteed

Discretization with Guaranteed Feasibility

- Recall (LBD)

$$\begin{aligned} \min_{\boldsymbol{x}\in X} \quad & f(\boldsymbol{x}) \\ \text{s.t.} \quad & c(\boldsymbol{x},y) \leq 0, \forall y \in Y^{LBD} \end{aligned} \qquad \text{(LBD)}$$

- Restrict ($\varepsilon > 0$) the right-hand-side of the constraint to obtain the upper bounding problem (UBD)[1]

$$\begin{aligned} \min_{\boldsymbol{x}\in X} \quad & f(\boldsymbol{x}) \\ \text{s.t.} \quad & c(\boldsymbol{x},y) \leq -\varepsilon, \forall y \in Y^{UBD} \end{aligned} \qquad \text{(UBD)}$$

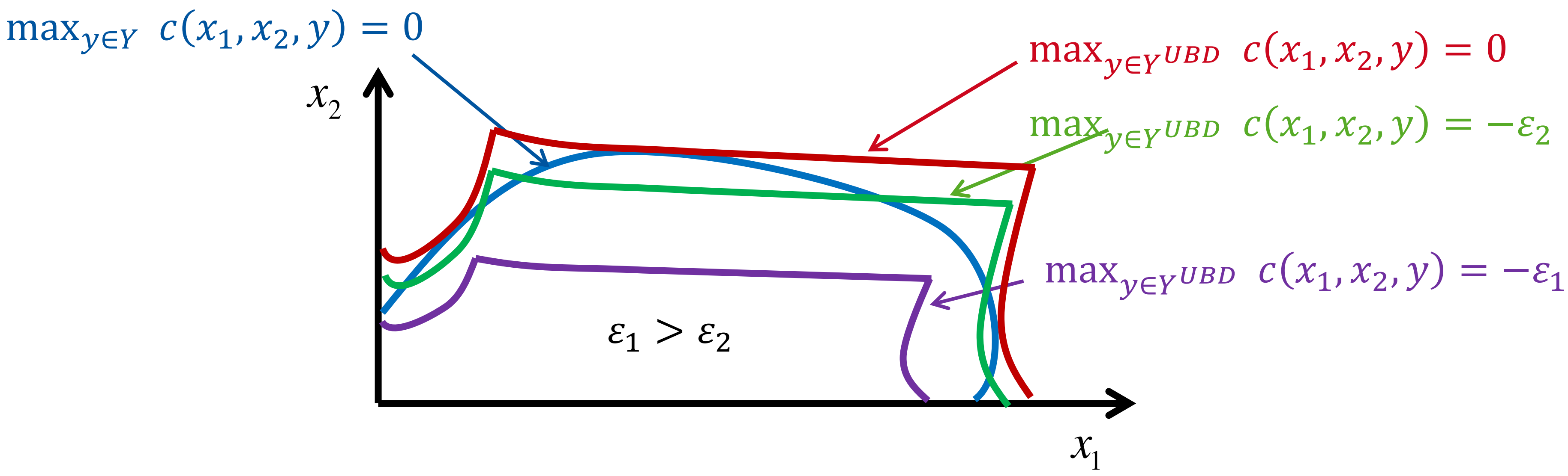
- (UBD) is neither a relaxation nor a restriction of (SIP)

[1] Mitsos, Optimization, 2011

Upper Bounding Problem

- (UBD) is neither a relaxation nor a restriction of (SIP)

$$\min_{\boldsymbol{x}\in X} \quad f(\boldsymbol{x}) \qquad \text{(UBD)}$$
$$\text{s.t.} \quad c(\boldsymbol{x}, y) \le -\varepsilon, \forall y \in Y^{UBD}$$



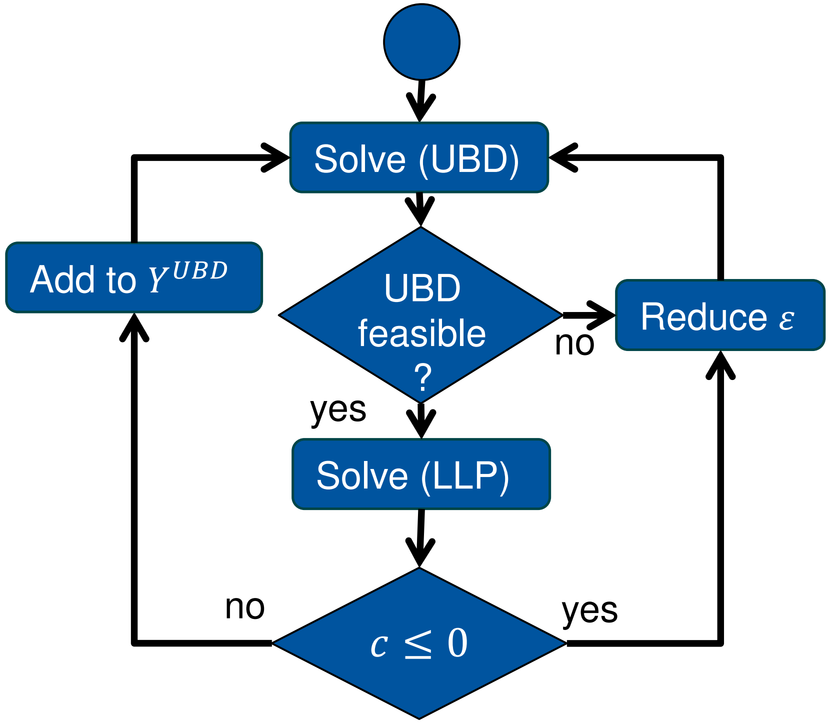
- By populating Y^{UBD}, the relaxation is made tighter → better approximate (SIP)
- By reducing $\varepsilon > 0$, the restriction is less severe → better approximate (SIP)

[1] Mitsos, Optimization, 2011

Simplified Upper Bounding Procedure

- Algorithm:

1. Initialize $Y^{UBD} \subset Y, f^{UBD} \leftarrow \infty, \varepsilon > 0, r > 1$
2. Solve (UBD) globally to obtain $\bar{\boldsymbol{x}}$
3. Solve (LLP) globally for $\bar{\boldsymbol{x}}$ to obtain $\bar{y}$
   - If $c(\bar{\boldsymbol{x}}, \bar{y}) \leq \mathbf{0}$ then set $\boldsymbol{x}^* \leftarrow \bar{\boldsymbol{x}}$ and $\varepsilon \leftarrow \varepsilon / r$
   - Else set $Y^D \leftarrow \{\bar{y}\} \cup Y^{UBD}$
   - Go to step 2



- Finite convergence to global optimum if SIP-Slater point exists
  – If for $\varepsilon^f > 0$, $\exists \boldsymbol{x}^S \in X$: $c(\boldsymbol{x}^S, y) < 0$, $\forall y \in Y$, $f(\boldsymbol{x}^S) \leq f^* + \varepsilon^f$ the procedure finitely produces an ε^f-optimal, feasible point

Check Yourself

- How does the discretized version of an SIP relate to the original problem?
- Describe a global solution method for SIP

Applied Numerical Optimization

Prof. Alexander Mitsos, Ph.D.

Parameter estimation in thermodynamics as bilevel/SIP

Aachener Verfahrenstechnik

RWTH AACHEN UNIVERSITY

Parameter Estimation for Thermodynamic Property Models

- Accurate prediction of phase separation behavior is needed, e.g., in separation design.
- Excess-Gibbs free energy models are used for liquid phases $G(T, P, \boldsymbol{x}, \boldsymbol{q})$
  - NRTL, UNIQUAC, Wilson, … :
- EOS models are used for vapor phases
  - No adjustment of parameters for binary interaction
- Binary interaction parameters $\boldsymbol{q}$ estimated via equilibrium experiments
- Parameters must be fit for model equations in equilibrium state.
  - Necessary equilibrium criterion: Isopotential (equality of chemical potential between phases)
  - Necessary and sufficient equilibrium criterion: $\min_{\boldsymbol{x}} G(T, P, \boldsymbol{x}, \boldsymbol{q})$
    - Specialized criteria exist: Gibbs tangent plane (Michelsen 1980) supporting hyperplane (Mitsos & Barton AIChEJ 2007)

Parameter Estimation: Classical approach

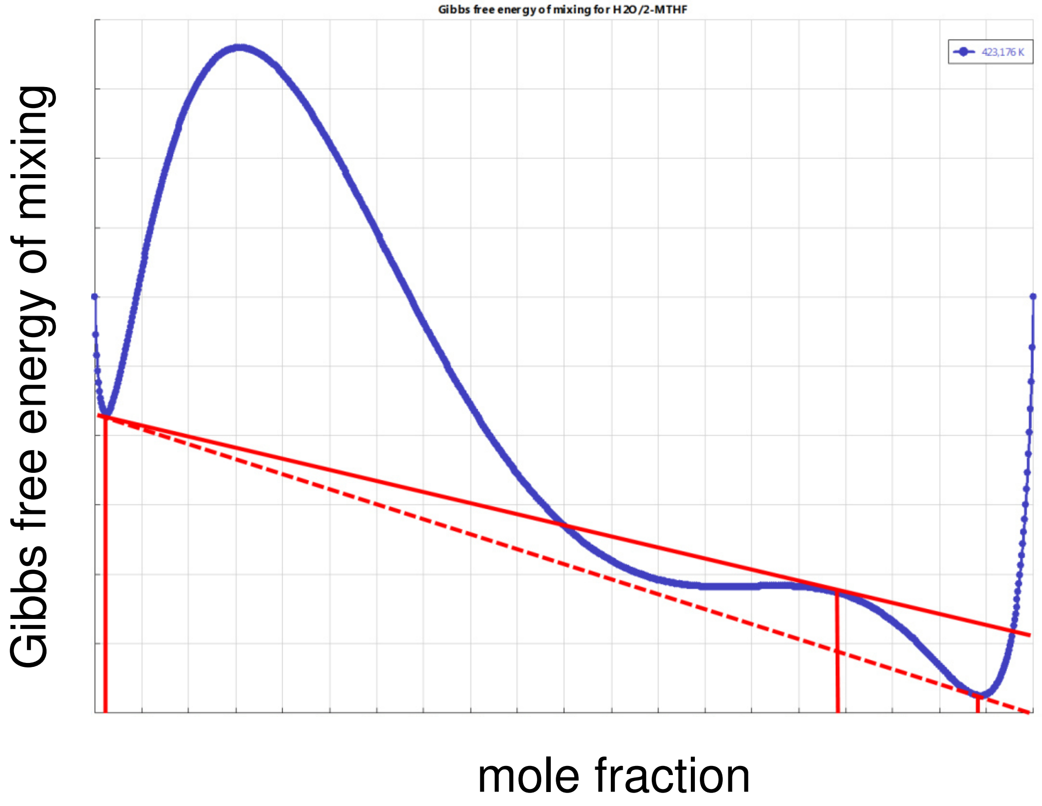
- Measure phase compositions $x^{m,i,k}$ at different temperatures T^i and constant pressure P.

- Minimize prediction-measurement discrepancy

- Enforce isopotential for thermodynamic equilibrium

- $$\min_{\boldsymbol{q}} LS(x^{p,i,k} - x^{m,i,k})$$
  $$\mu_1^1(T^i, P, x^{p,i,1}, \boldsymbol{q}) = \mu_1^k(T^i, P, x^{p,i,k}, \boldsymbol{q}) \ \forall\, i, k$$
  $$\mu_2^1(T^i, P, x^{p,i,1}, \boldsymbol{q}) = \mu_2^k(T^i, P, x^{p,i,k}, \boldsymbol{q}) \ \forall\, i, k$$

- Problem: isopotential is only **necessary**, not sufficient.



Glass, et int., Mitsos, *Fluid Phase Equilibria* 433 (2017): 212-225.

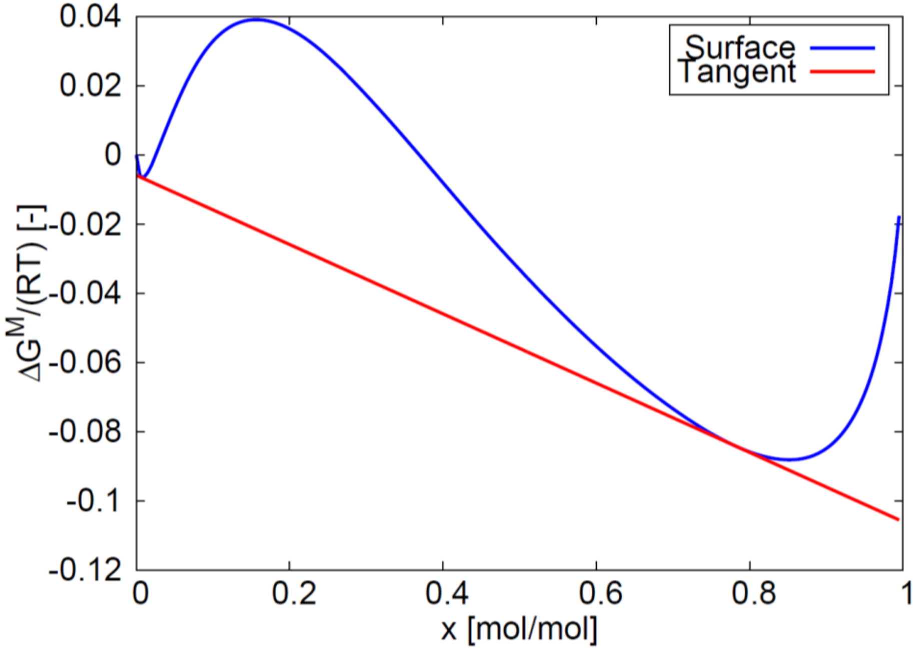
Parameter Estimation: Bilevel Formulation

- Developed by Mitsos, Bollas & Barton CES 2009
  - Extended by Glass & Mitsos
  - Implemented in BOARPET

- Introduce tangent plane criterion

$$\Delta g\left(T^i, P^i, x^{p,i,1}, \boldsymbol{q}\right) + \left.\frac{\delta \Delta g}{\delta x}\right|_{T^i, P^i, x^{p,i,1}, \boldsymbol{q}} \left(x - x^{p,i,1}\right) \leq \Delta g\left(T^i, P^i, x, \boldsymbol{q}\right) \quad \forall x \in [0,1]$$

- Additional constraints:
  - correct number of phase splits
  - correct number of phases for each split



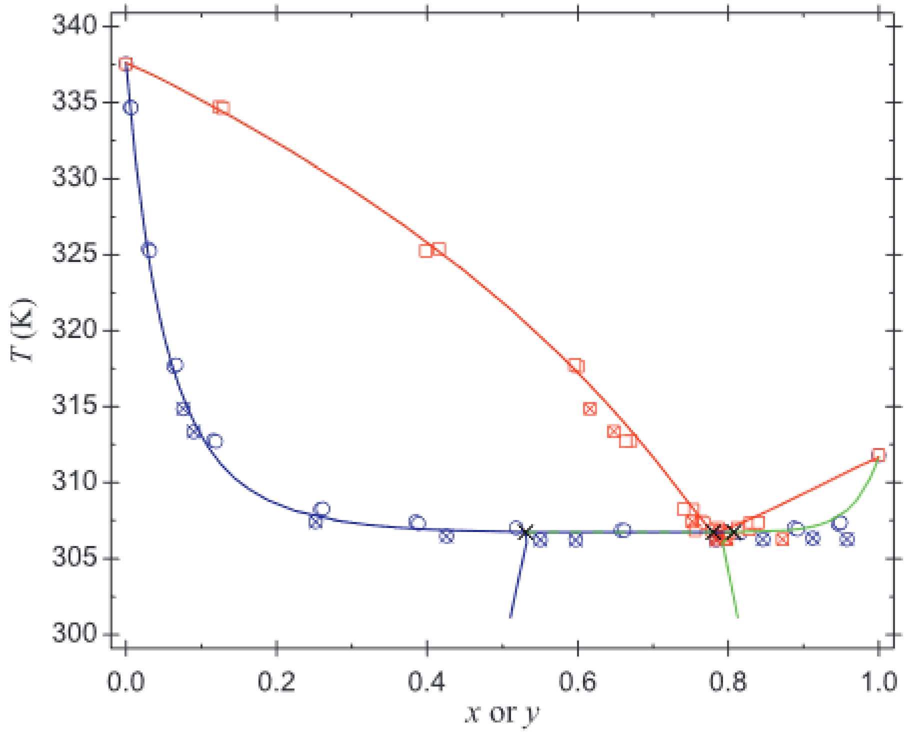
Glass, et int., Mitsos, *Fluid Phase Equilibria* 433 (2017): 212-225.

https://www.avt.rwth-aachen.de/cms/AVT/Forschung/Software/~kvkz/BOARPET/

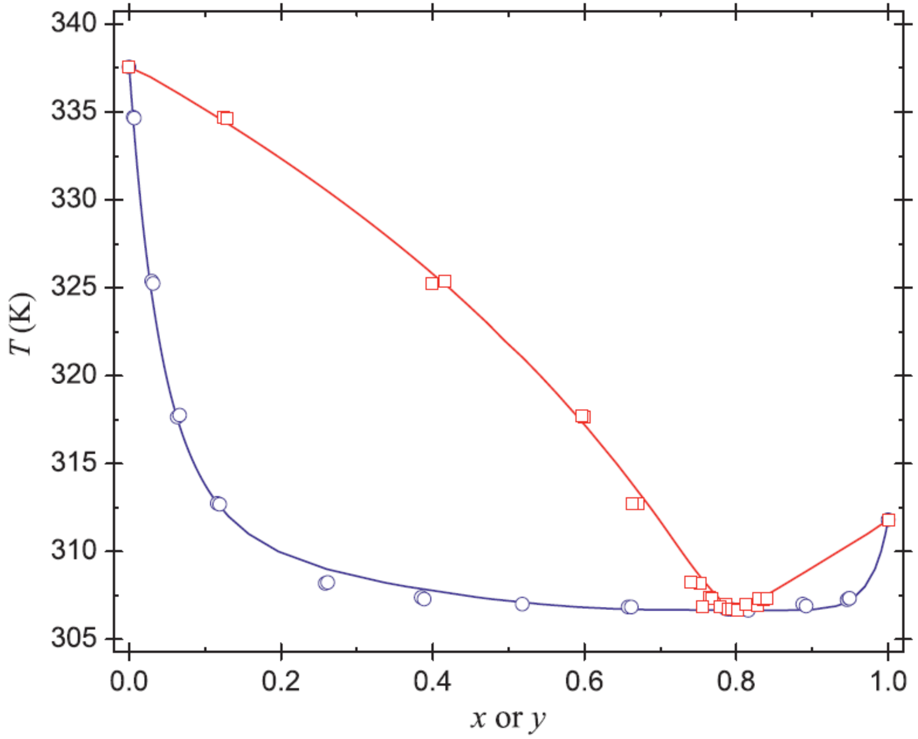
Parameter Estimation: VLE of 2-methyl-2-butene – methanol

- Experimental data shows homogeneous azeotrope

$\gamma - \phi$ method predicts heterogeneous azeotrope (spurious LLE split).



Bilevel formulation gives qualitatively and quantitatively correct fit.

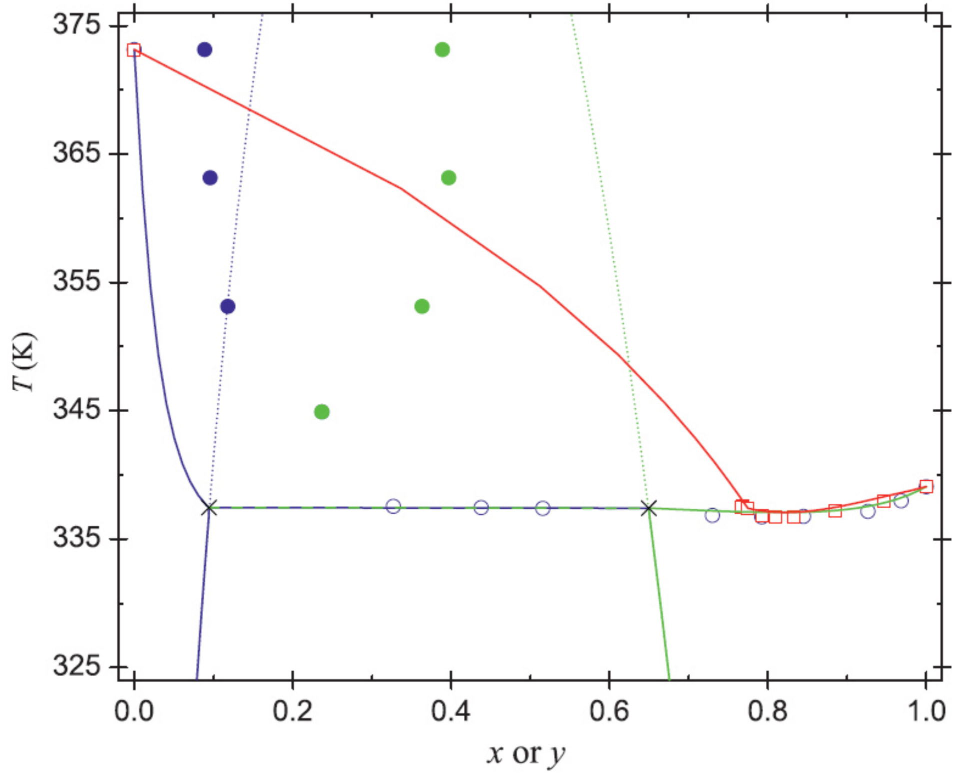


Bollas, Barton & Mitsos, *Chemical Engineering Science 2009*

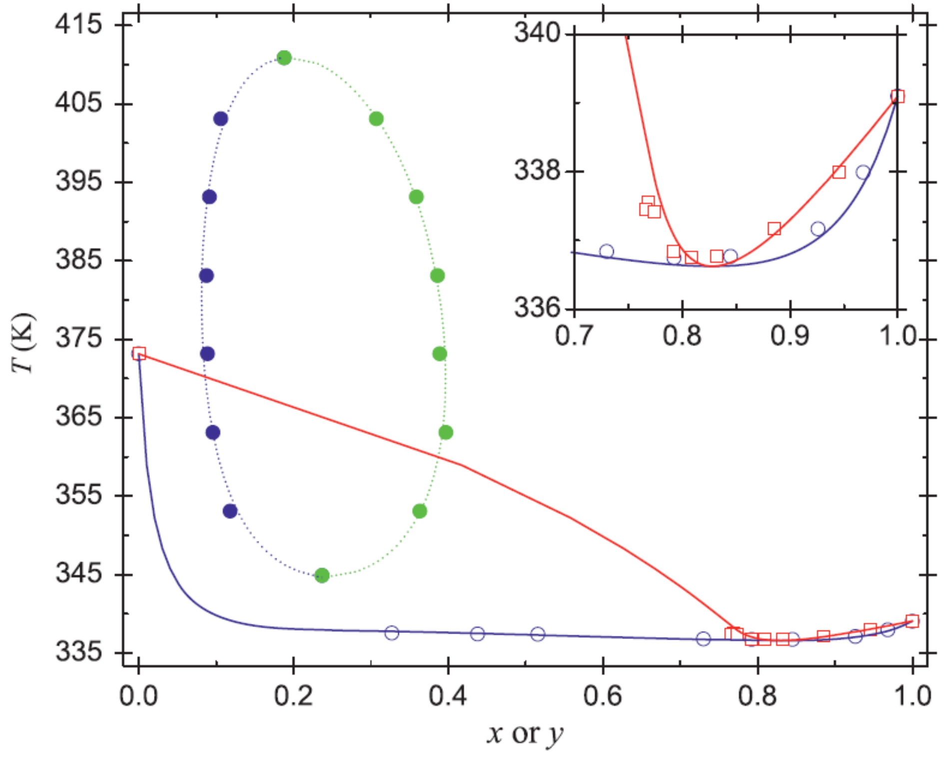
Parameter Estimation: VLE of tetrahydrofuran-water

- Experimental data shows homogeneous azeotrope, LCST, and UCST

$\gamma - \phi$ method predicts spurious liquid phase split. LCST is missed



Proposed formulation gives qualitatively and quantitatively correct fit.



Bollas, Barton & Mitsos, *Chemical Engineering Science 2009*

Check Yourself

- How does parameter estimation in thermodynamics work?