OTTO VON GUERICKE UNIVERSITÄT MAGDEBURG

ADMIT

Tutorial – Concepts and Methods

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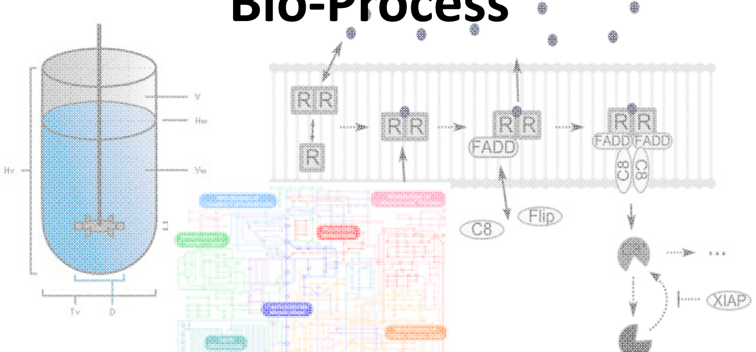
Introduction

Main issues:

- Model invalidation
- Parameter estimation
- State estimation

Bio-Process

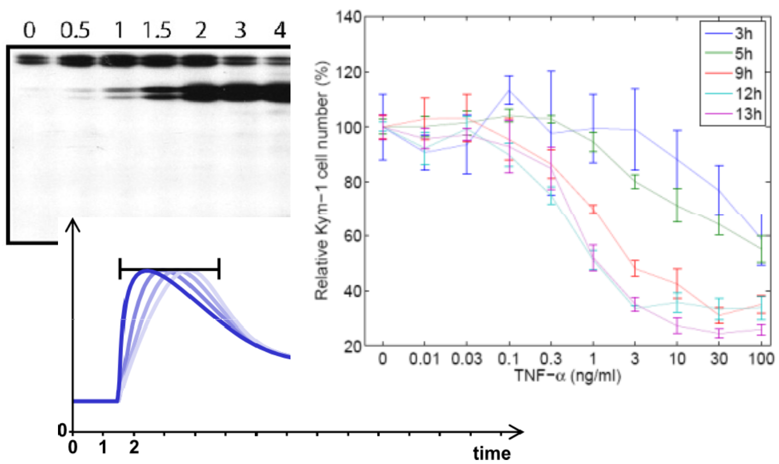


limited knowledge and measurement capacities

Challenges:

- uncertain data
- qualitative information
- nonlinear models
- competing hypotheses

Data



uncertain, sparse, erroneous, qualitative or quantitative

Invalidation →

Estimation →

Dynamical Models

$\Sigma_1 \quad \Sigma_2 \quad \Sigma_3$

competing hypotheses

$$\Sigma_i = \begin{cases} \dot{x} = f_i(x, p, u) \\ \dot{y} = g_i(x, p) \end{cases}$$

nonlinear

Premises and Concepts

Model

$$\Sigma = \begin{cases} f_i^k(x_{k+1}, x_k, p, u_k) = 0 \\ g_i^k(y_k, x_k, p) = 0 \end{cases}$$

- **discrete-time (discretization)**
- **polynomial model**

✓ outputs
✓ also discrete variables
✓ conservation relations

Data

- **bounded uncertainties**
- true (unknown) measurements covered

✓ measurement data
✓ a priori data
✓ **qualitative** data

Invalidation:

Is the model consistent with the available data?

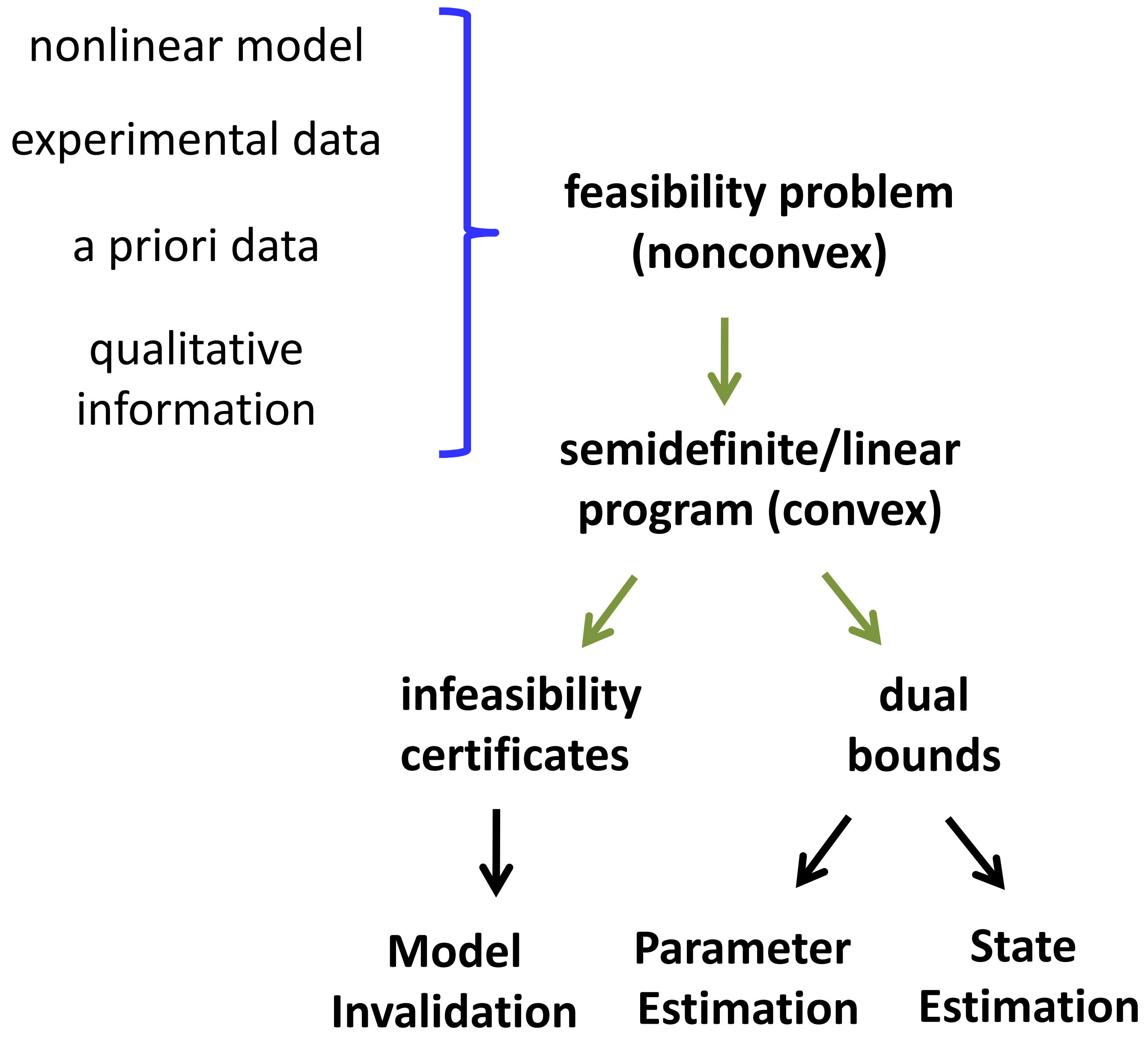
- **constraint satisfaction/feasibility problem**

Parameter/State Estimation:

The set of all parameters/states such that the model is consistent with the available data.

- **set-membership problem**

Relaxation-based framework: Overview



Approach:

1. Reformulation
2. Relaxation/ Duality
3. Approximation

Reformulation

Model (discrete time)

$$f_i^k(x_{k+1}, x_k, p, u_k) = 0$$
$$g_i^k(y_k, x_k, p) = 0$$
$$(k \in [0:N])$$

Prior knowledge (interval bounds)

$$\underline{p}_i \leq p_i \leq \overline{p}_i \quad (i \in [1:n_p])$$

Measurements (interval bounds)

$$\underline{x}_k \leq x_k \leq \overline{x}_k$$
$$\underline{y}_k \leq y_k \leq \overline{y}_k$$
$$\underline{u}_k \leq u_k \leq \overline{u}_k \qquad (k \in [0:N])$$

Qualitative information

$$(x1 \geq 0) \text{ OR } (\text{x2} \leq 1) \ldots$$

Constraint satisfaction problem:

$$\begin{aligned}
&\text{find } \mathbf{p}, \text{ s.t.} \\
&f_l^k(x_k, x_{k-1}, p, u_{k-1}) = 0 && k \in [1:N] \\
&g_l^k(y_{k-1}, x_{k-1}, p) = 0 && k \in [1:N] \\
&\underline{x}_k \leq x_k \leq \overline{x}_k && k \in [0:N] \\
&\underline{y}_k \leq y_k \leq \overline{y}_k && k \in [0:N-1] \\
&\underline{u}_k \leq u_k \leq \overline{u}_k && k \in [0:N-1] \\
&\underline{p}_i \leq p_i \leq \overline{p}_i && i \in [1:n_p]
\end{aligned}$$

- discrete variables can be included
- conditional logic constraints
- **non-convex**

Relaxation

Relaxation approach:

- non-convex constraint satisfaction problem can be reformulated as quadratic optimization program (QOP) -> **quadrification**
- QOP can be relaxed into semidefinite (SDP)or linear program (LP) -> **convexifying relaxation**

Duality

- guaranteed **infeasibility certificates** can be derived from duality properties of general convex problems
- **dual bounds** provide guaranteed bounds for an objective function

Infeasibility certificate $\Rightarrow$ **Invalidation**

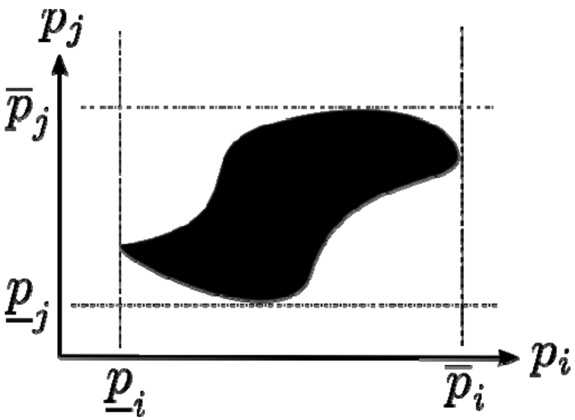
Dual bounds $\Rightarrow$ **Estimation**

Estimation (Guaranteed Approximation)

- Two possible **set-membership** approaches for **guaranteed estimation:**

Outer-bounding

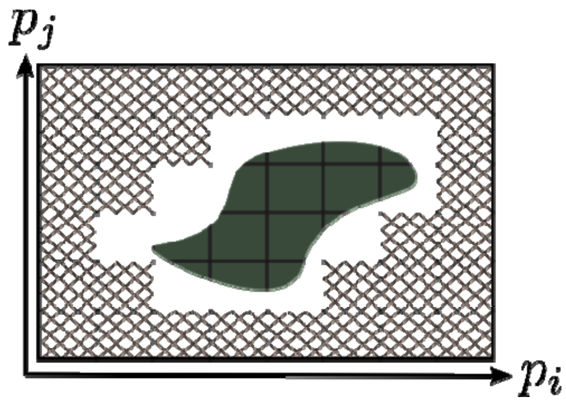
- consider dual bounds
- computationally advantageous (linear complexity)



(orthotopic bounding)

Bisectioning/partitioning

- use infeasibility certificates
- adjustable accuracy (exponential complexity)

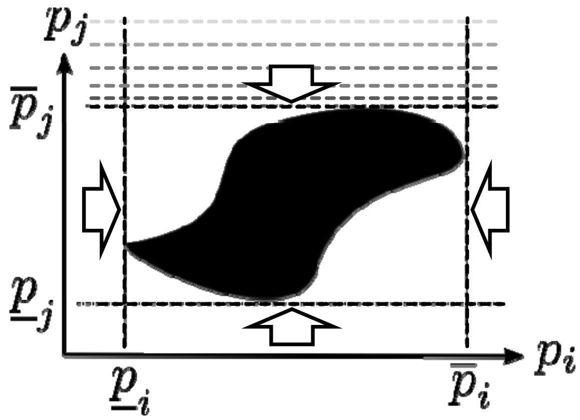


(axis-aligned partitioning)

Estimation: Outer-bounding

Description:

- one-dimensional projections of the feasible region
- obtained by iteratively tightening bounds of single variables over complete region



Performance:

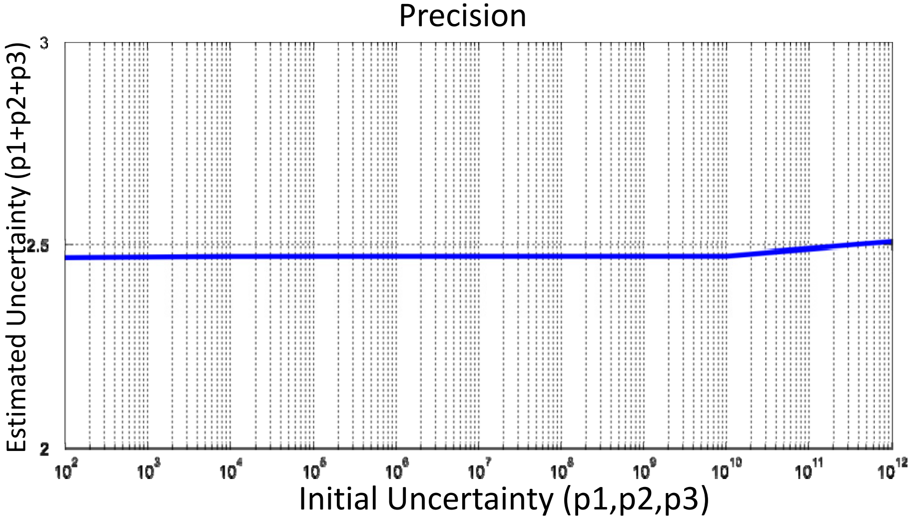
- **Low effort:** solve ***2n*** instances to bound ***n*** variables
- **Easy to use result:** estimated bounds on single parameters or states
- **Requires multiple iterations:** relaxation errors depend on initial region size
- **Poor estimation for interconnected variables:** see Bisectioning procedure

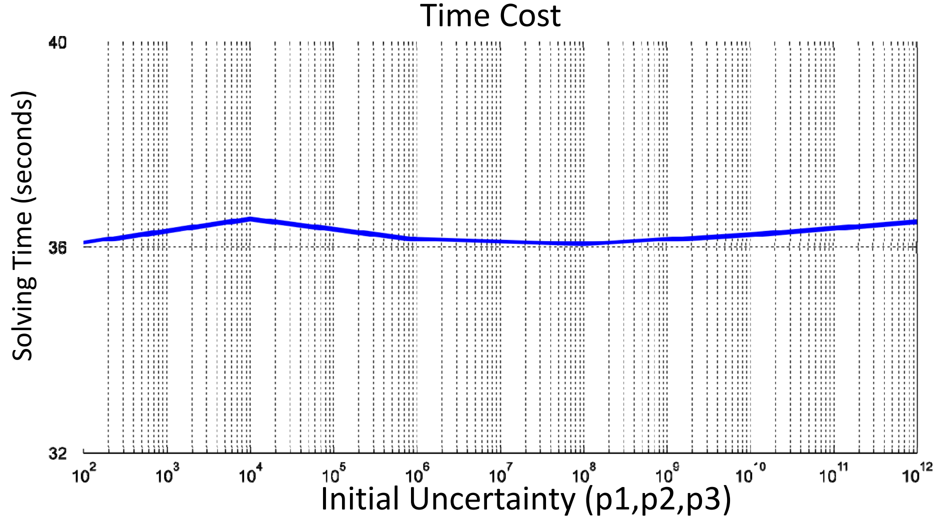
When to use Outer-bounding:

- ➢ should always be used first to estimate uncertainty bounds
- ➢ estimation of not interconnected parameters and states

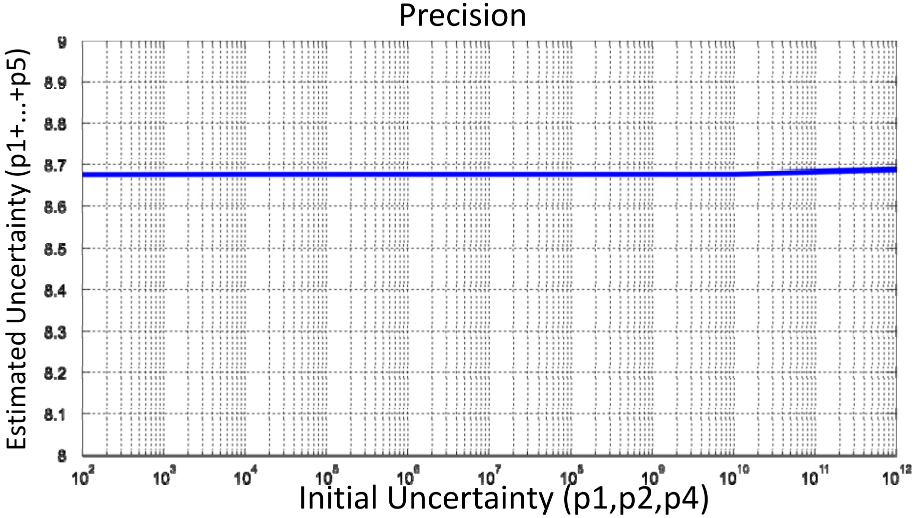
Estimation: Outer-bounding Performance

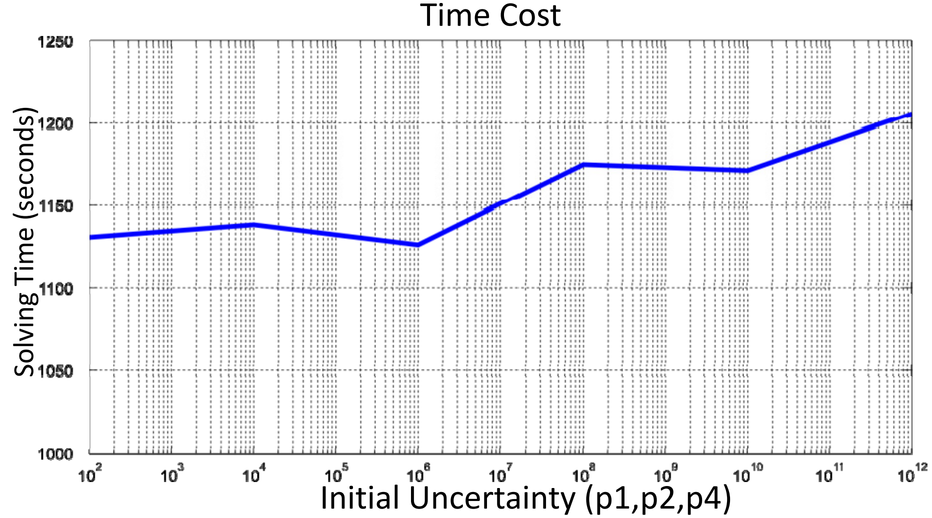
Michaelis-Menten Example (see examples tutorial)





Carnitine Shuttle Example (see examples tutorial)





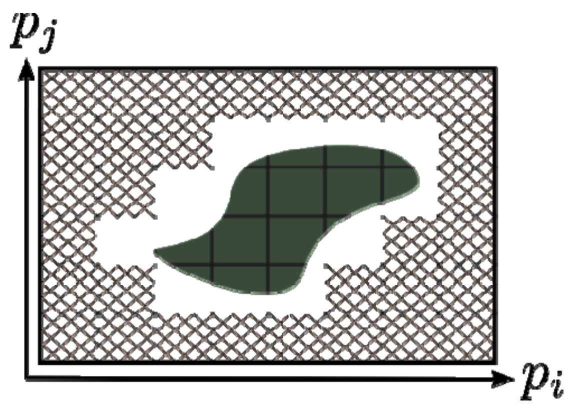
Performance for different initial uncertainty values:

- Time costs almost constant (Intel Core2Quad **Q6600 2.4Ghz**; 64-bit, MATLAB **R2010b**)
- Similar estimated uncertainty (sum of uncertainties for three parameters)

Estimation: Bisectioning

Description:

- full-dimensional subregions of the feasible region
- obtained by checking feasibility of every subregion



Performance:

- **Arbitrary precision:** user specifies spliting depth of the initial region
- **Reduced relaxation error:** due to small size of subregions
- **Highlights variable relation:** form of estimated region surfaces interconnections
- **High effort:** exponential number of solver calls in variable count and split depth
- **Hard to use results:** requires further interpretation by the user

When to use Bisectioning:

- highly dependent variables
- interested in the form of the feasible region
- numerical issues occurred during Outer-bounding due to large uncertainties

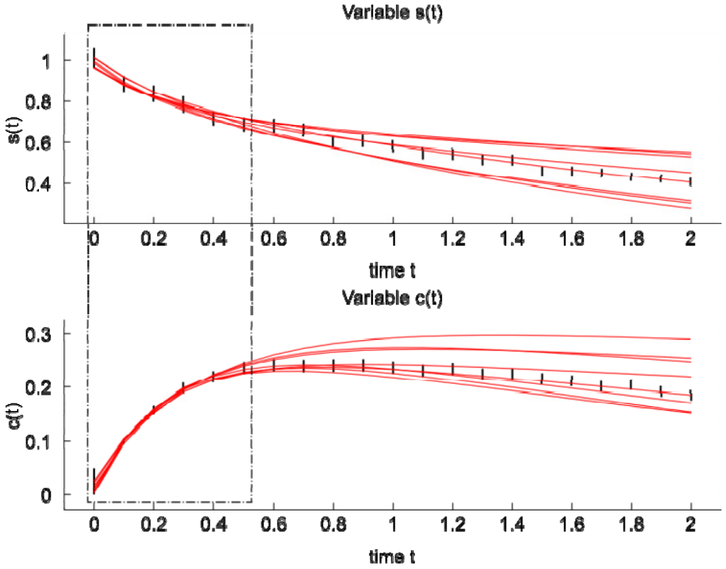
Estimation: Time Horizon

Discretized problem formulation:

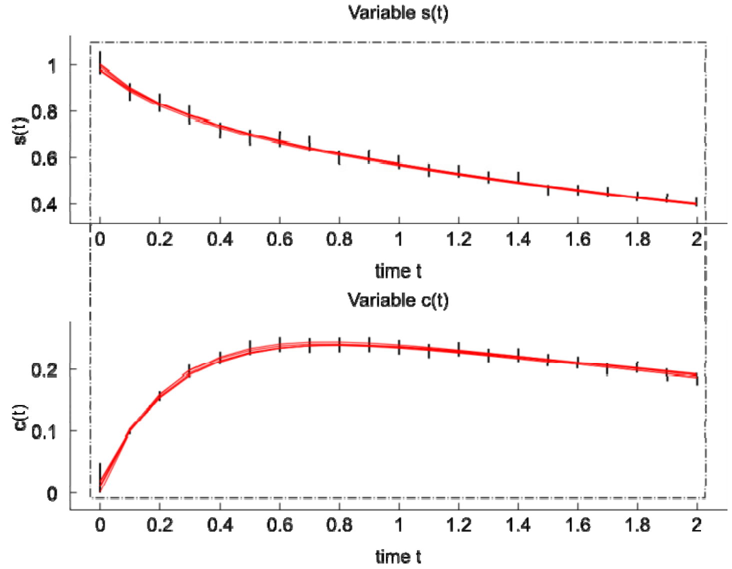
- variables connected through difference equations
- sequencing equations connects variables within a time window
- size of this time window affects solving time and estimation quality

Michaelis-Menten Example (Monte-Carlo samples for estimated parameter ranges)

Short time window (5 steps)



Full Time Window (20 steps)



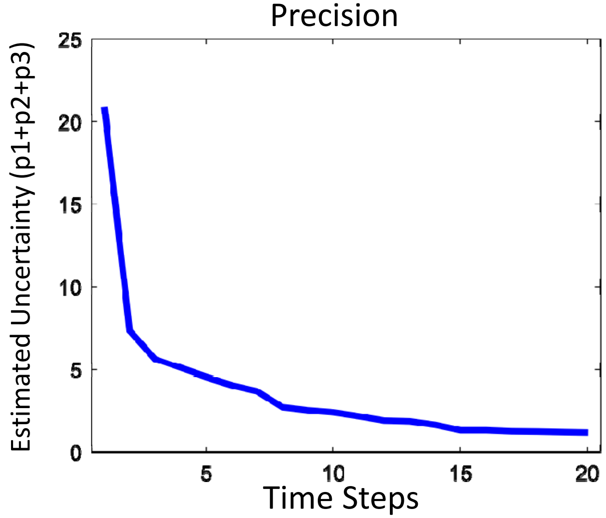
Precision of estimation for different time horizon length:

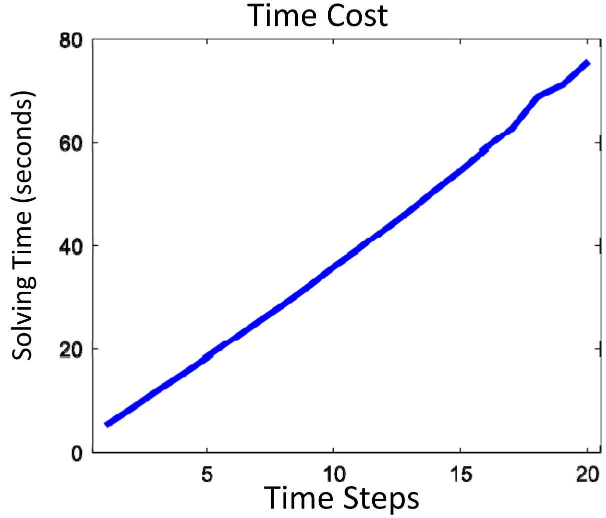
➢ State constraints are only satisfied within the time window

➢ Added bounds improve parameter estimates

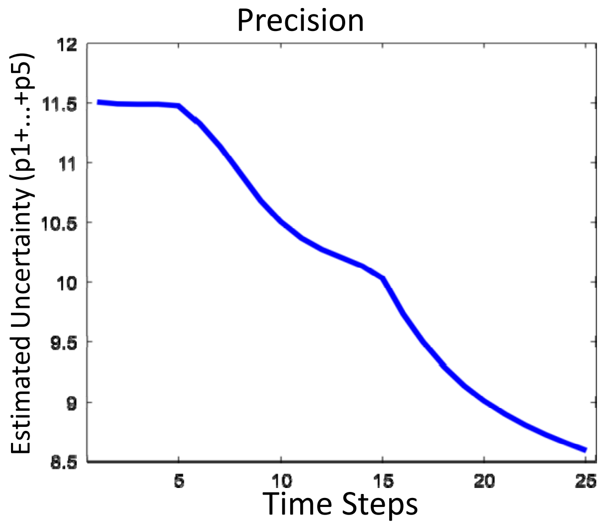
Estimation: Time Horizon Performance

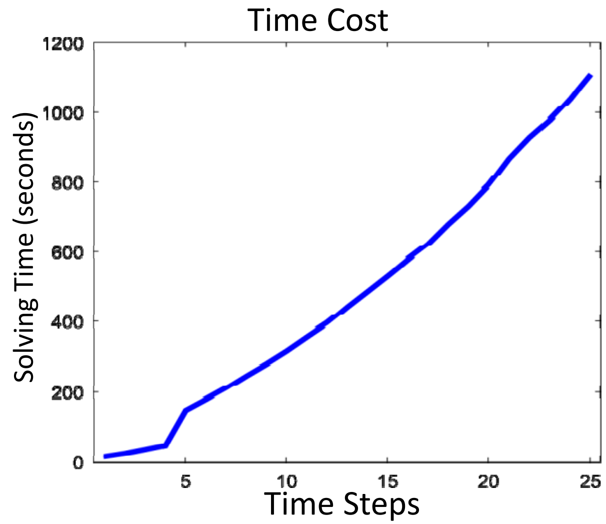
Michaelis-Menten Example





Carnitine Shuttle Example





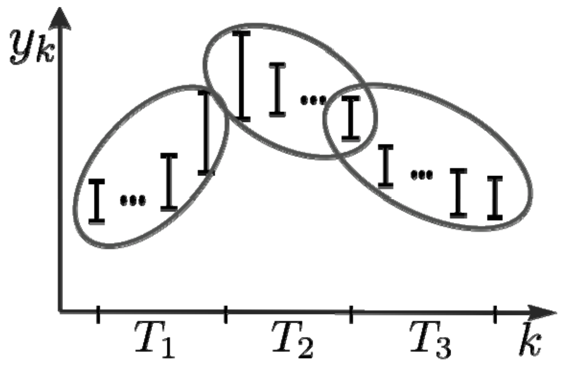
Performance for different time horizon length:

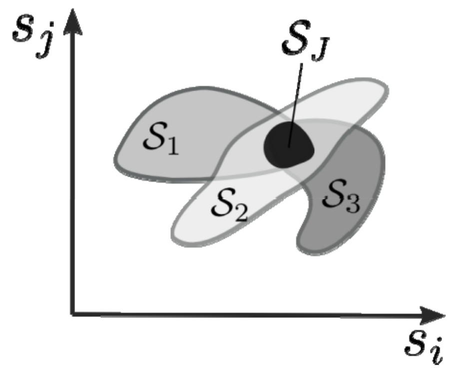
- Time costs grow almost linearly in the examples (for the considered range)
- Improved estimated uncertainty for larger horizon lengths

Estimation: Precision/Complexity Trade-off

Decomposition by time

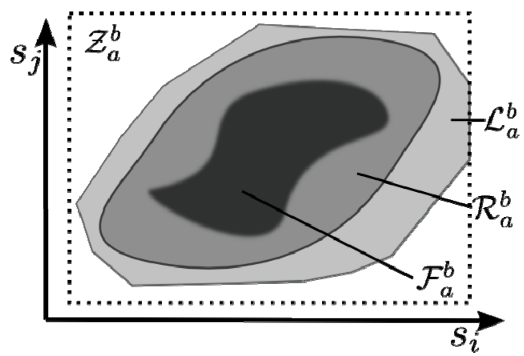
- split large estimation problem into a sequence of smaller ones
- infer overall estimate by intersection





Relaxation hierarchy

- use or relax additional constraints
- relax to SDP or LP
  - ➢ SDP solvers (e.g. SeDuMi) for small problem size/high precision
  - ➢ (MI)LP solvers (e.g. Gurobi, Cplex) for larger size/discrete variables



Applications

➡ Refer ADMIT Examples Tutorial

- parameter estimation
- state estimation
- model invalidation
- uncertainty analysis
- fault detection and analysis
- disorder diagnosis
- reachability analysis

References (selected)

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