Robust Design of Optimal Experiments Considering Consecutive Re-designs

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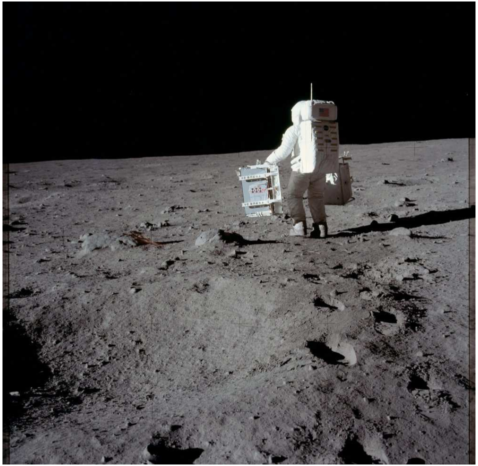
Modeling is . . .

. . . exploring behavior of the system → model structure

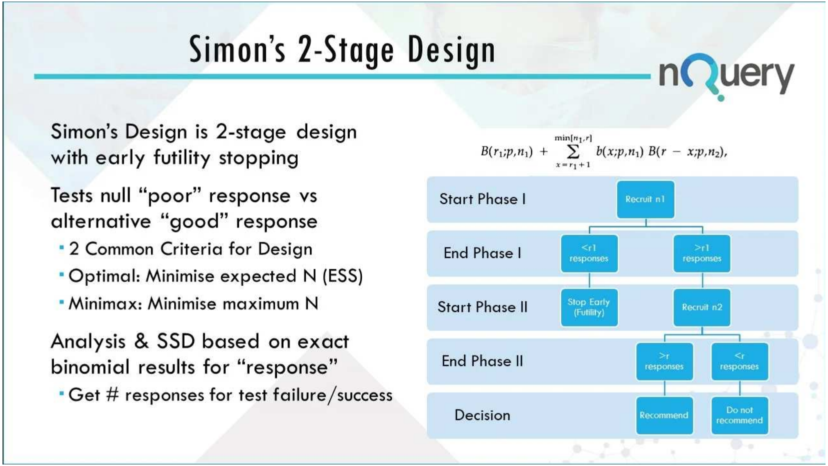


Modeling is . . .

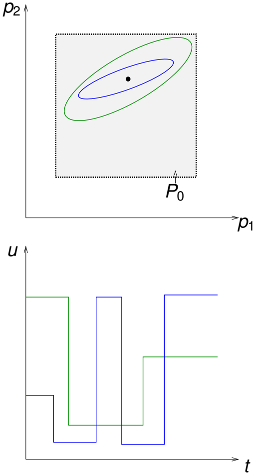
. . . conducting **good** experiments $\rightarrow$ accurate model parameters

Modeling is . . .

. . . a continuous (and eternal) struggle.

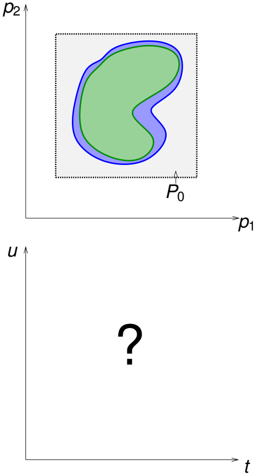


Linear Confidence Regions



Design of Optimal Experiments

Exact Confidence Regions



Design of Optimal Experiments

Motivation

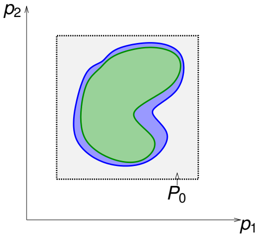
- Design of Optimal Experiments (DoE) with exact confidence regions presented in

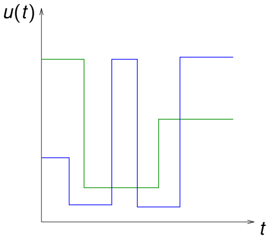
  Gottu Mukkula & Paulen: Optimal Experiment Design in Nonlinear Parameter Estimation with Exact Confidence Regions, Journal of Process Control 2019

- Inherent to DoE with linear confidence regions, the optimal design strongly depends on the expected values of parameters

- **How to find robust design of experiments?**
- **How to ideally use consecutive re-designs?**

Exact Confidence Regions





Design of Optimal Experiments

From Data to Model

1. Select the model structure.

Dynamic model or spatially discretized PDEs:

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

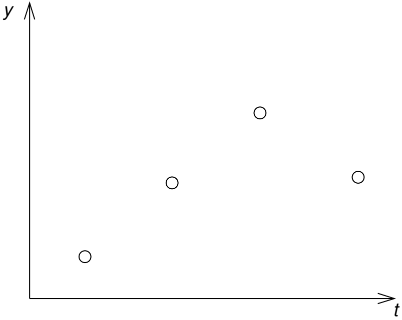
Steady-state or discretized model:

$$\hat{y} = F(u,p) \begin{cases} \text{state equation:} & 0 = f(x,u,p) \\ \text{output equation:} & \hat{y} = h(x,p) \end{cases}$$

$\hat{y}$ - outputs; p - parameters; u - experimental conditions; x - states

From Data to Model

2. Perform experiments. Gather data.

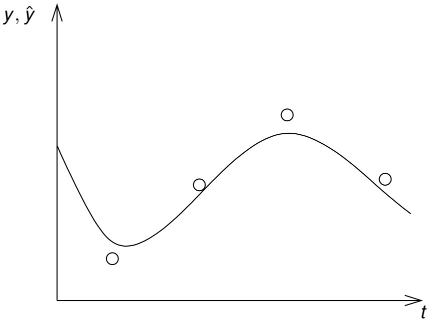


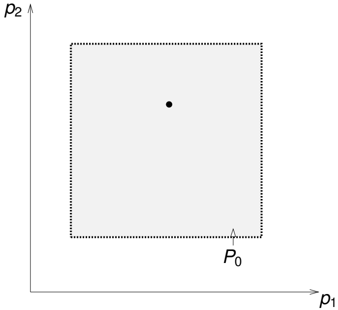
From Data to Model

3. Estimate unknown parameters.

$$\hat{p} = \arg\min_{p \in P_0} J(p) = \arg\min_{p \in P_0} \|y - \hat{y}\|_2^2$$

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



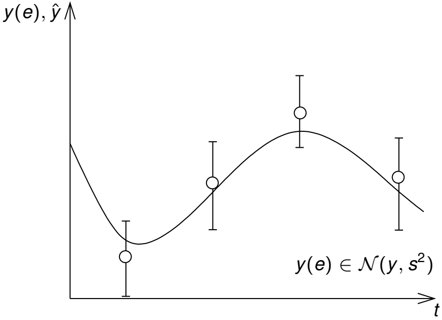


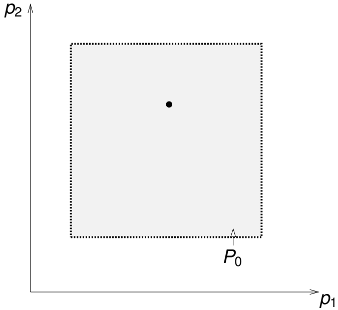
From Data to Model

4. Analyze the quality of estimates.

$$\hat{p} = \arg\min_{p \in P_0} J(p) = \arg\min_{p \in P_0} \|y(e) - \hat{y}\|_2^2$$

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





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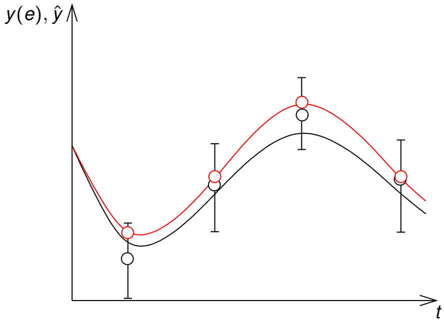
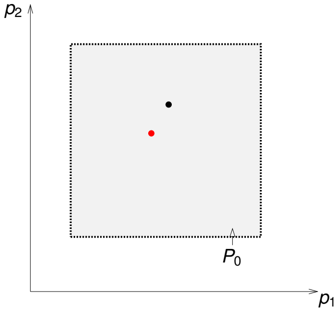
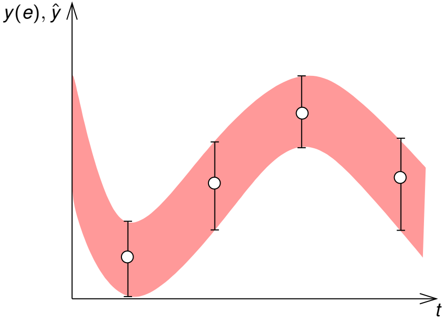


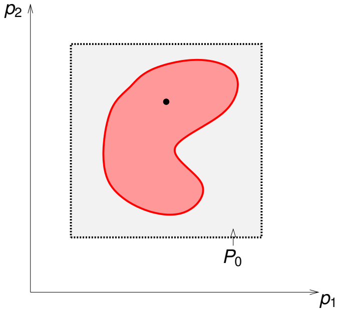


From Data to Model

4. Analyze the quality of estimates. (Exact confidence regions)

$$J(p) - J(\hat{p}) \leq n_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}$$





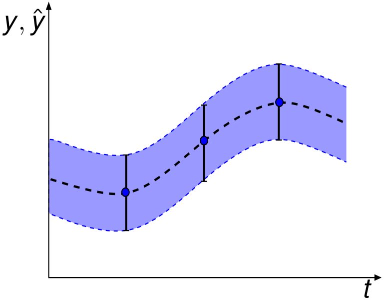
Design of Optimal Experiments (DoE)

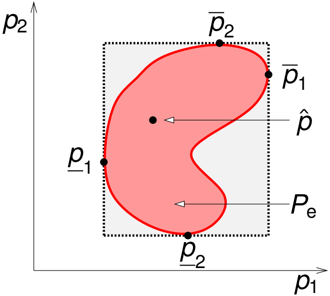
1. Find an over-approximation of the exact confidence region

$$\max_{\underline{p},\overline{p}} \sum_{j=1}^{n_p} \overline{p}_j - \underline{p}_j$$

$$\text{s.t. } \hat{y} = F(u, \pi), \quad \forall \pi \in \{\hat{p}, \underline{p}, \overline{p}\}$$

$$J(\pi) - J(\hat{p}) \leq n_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}, \quad \forall \pi \in \{\underline{p}, \overline{p}\}$$





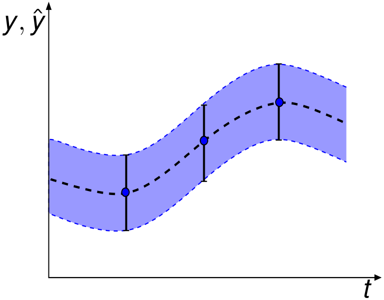
Design of Optimal Experiments (DoE)

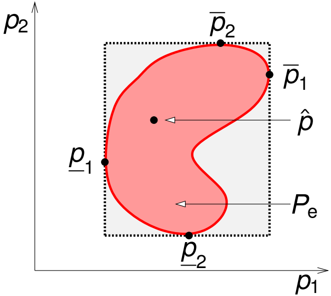
2. Optimize over the over-approximation of the exact confidence region

$$\min_{u} \max_{\underline{p},\overline{p}} \sum_{j=1}^{n_p} \overline{p}_j - \underline{p}_j$$

$$\text{s.t. } \hat{y} = F(u,\pi), \quad \forall \pi \in \{\hat{p}, \underline{p}, \overline{p}\}$$

$$J(\pi) - J(\hat{p}) \leq n_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}, \quad \forall \pi \in \{\underline{p}, \overline{p}\}$$





Robust DoE

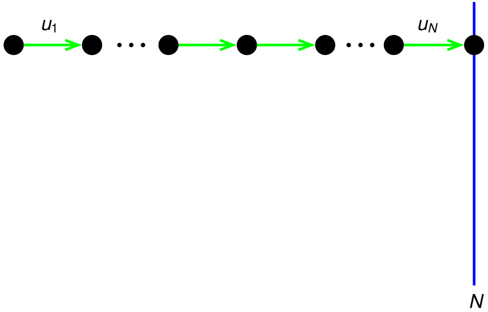
- Nominal design (Pronzato & Walter, 1989, Gottu Mukula & Paulen, 2019)

Robust DoE: Nominal Approach

$$\min_{u} \max_{\underline{p},\overline{p}} \sum_{j=1}^{n_p} \overline{p}_j - \underline{p}_j$$

$$\text{s.t. } \hat{y} = F(u,\pi), \quad \forall \pi \in \{\hat{p}, \underline{p}, \overline{p}\}$$

$$J(\pi) - J(\hat{p}) \leq n_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}, \quad \forall \pi \in \{\underline{p}, \overline{p}\}$$



Robust DoE

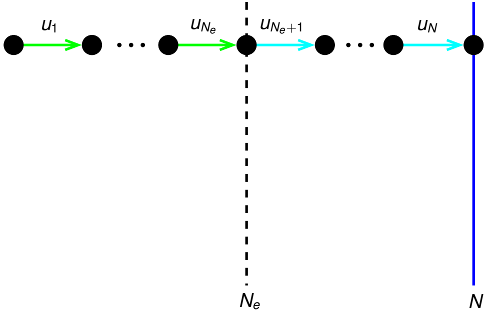
- Nominal design (Pronzato & Walter, 1989, Gottu Mukula & Paulen, 2019)
- Sequential design (Barz et al., 2010)
  1. Calculate and apply the nominal design for current $\hat{p}$.
  2. Take measurements, obtain new $\hat{p}$ and go to step 1.

Robust DoE: Sequential Approach

$$\min_{u} \max_{\underline{p},\overline{p}} \sum_{j=1}^{n_p} \overline{p}_j - \underline{p}_j$$

$$\text{s.t. } \hat{y} = F(u,\pi), \quad \forall \pi \in \{\hat{p}, \underline{p}, \overline{p}\}$$

$$J(\pi) - J(\hat{p}) \leq n_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}, \quad \forall \pi \in \{\underline{p}, \overline{p}\}$$



Robust DoE

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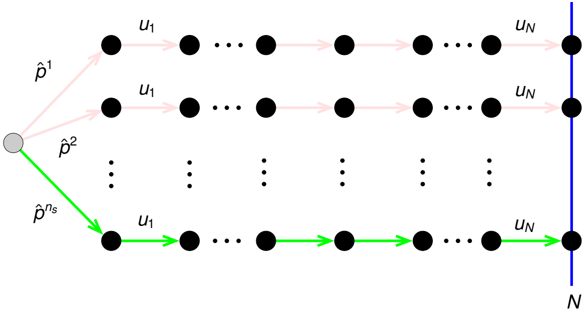
  1. Calculate and apply the nominal design for current $\hat{p}$.
  2. Take measurements, obtain new $\hat{p}$ and go to step 1.
- Min-max design (Walter & Piet-Lahanier, 1990)
  - Find the best design for the possibly worst-case realization of $\hat{p}$.

Robust DoE: Min-max Approach

$$\min_{u} \max_{\underline{p},\overline{p}} {\color{red}\max_{k}} \sum_{j=1}^{n_p} \overline{p}_j^k - \underline{p}_j^k$$

$$\text{s.t. } \hat{y} = F(u,\pi), \quad \forall \pi \in \{\hat{p}^k, \underline{p}^k, \overline{p}^k\}, \forall k$$

$$J(\pi) - J(\hat{p}^k) \leq n_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}, \quad \forall \pi \in \{\underline{p}^k, \overline{p}^k\}, \forall k$$



Robust DoE

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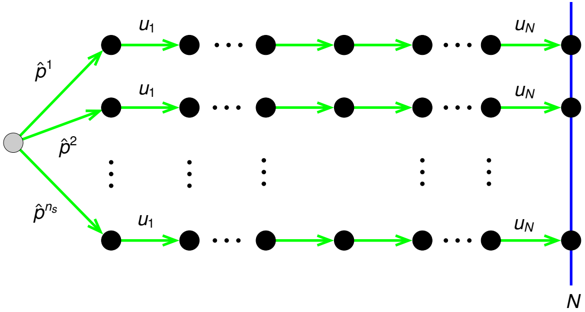
- Min-max design (Walter & Piet-Lahanier, 1990)
  - Find the best design for the possibly worst-case realization of $\hat{p}$.
- Scenario-based design (Telen et al., 2014)
  - Find the best design for the mean of possible realizations of $\hat{p}$.

Robust DoE: Scenario-based Design

$$\min_{u} \max_{\underline{p},\overline{p}} \sum_{k=1}^{n_s} \sum_{j=1}^{n_p} \overline{p}_j^k - \underline{p}_j^k$$

$$\text{s.t. } \hat{y} = F(u,\pi), \quad \forall \pi \in \{\hat{p}, \underline{p}^k, \overline{p}^k\}, \forall k$$

$$J(\pi) - J(\hat{p}^k) \leq n_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}, \quad \forall \pi \in \{\underline{p}^k, \overline{p}^k\}, \forall k$$



Robust DoE

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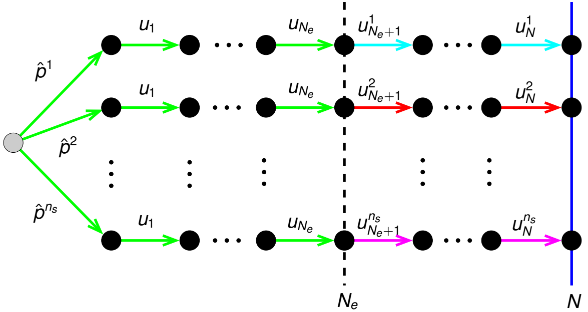
- Min-max design (Walter & Piet-Lahanier, 1990)
  - Find the best design for the possible worst-case realization of $\hat{p}$.
- Scenario-based design (Telen et al., 2014)
  - Find the best design for the mean of possible realizations of $\hat{p}$.
- Multi-stage design (this talk, idea from Garstka and Wets, 1974)
  - Find the best design for the mean realization of $\hat{p}$, but take the future estimation into account.

Robust DoE: Multi-stage Approach

$$\min_{u} \max_{\underline{p},\overline{p}} \sum_{k=1}^{n_s} \sum_{j=1}^{n_p} \overline{p}_j^k - \underline{p}_j^k$$

$$\text{s.t. } \hat{y} = F(u, \pi), \quad \forall \pi \in \{\hat{p}^k, \underline{p}^k, \overline{p}^k\}, \forall k$$

$$J(\pi) - J(\hat{p}^k) \leq n_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}, \quad \forall \pi \in \{\underline{p}^k, \overline{p}^k\}, \forall k$$

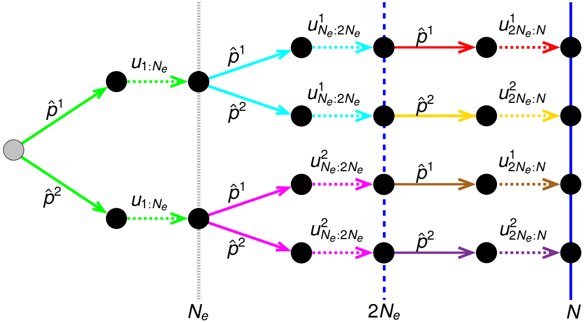


Robust DoE: Multi-stage Approach

$$\min_{u} \max_{\underline{p},\overline{p}} \sum_{k=1}^{n_s} \sum_{j=1}^{n_p} \overline{p}_j^k - \underline{p}_j^k$$

$$\text{s.t. } \hat{y} = F(u,\pi), \quad \forall \pi \in \{\hat{p}^k, \underline{p}^k, \overline{p}^k\}, \forall k$$

$$J(\pi) - J(\hat{p}^k) \leq n_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}, \quad \forall \pi \in \{\underline{p}^k, \overline{p}^k\}, \forall k$$



Robust DoE: 1D Toy Example

- Model

$$\hat{y}(p, u) = 1 - \exp(-pu)$$

- Uncertainty Level

$$\Delta p = 0.5$$

- Experiment Setup

$$N_e = 1, N = 2$$

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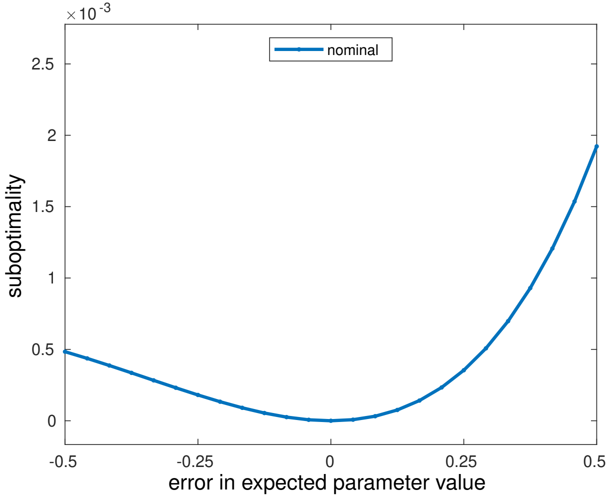

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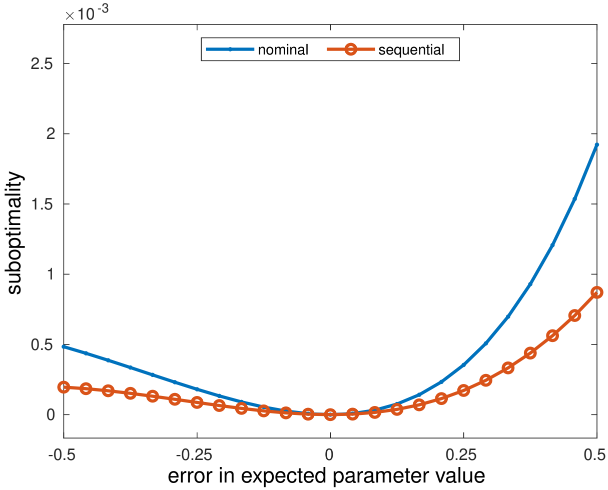

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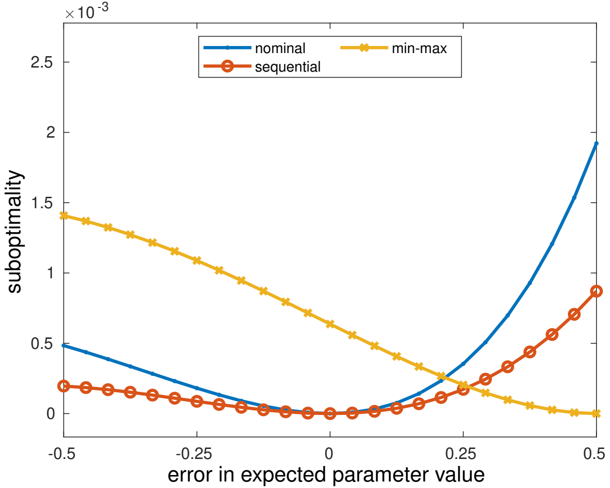

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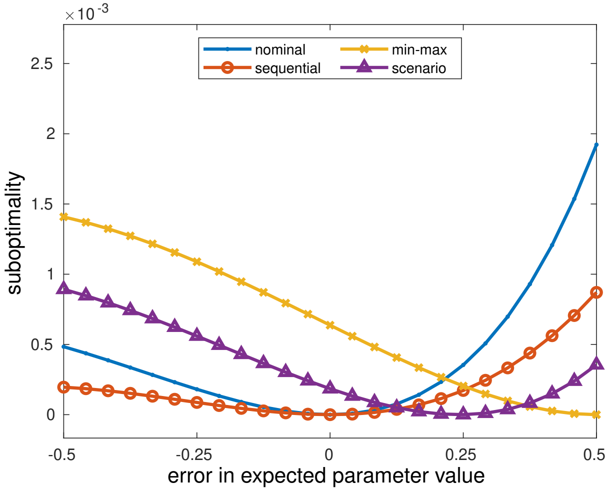

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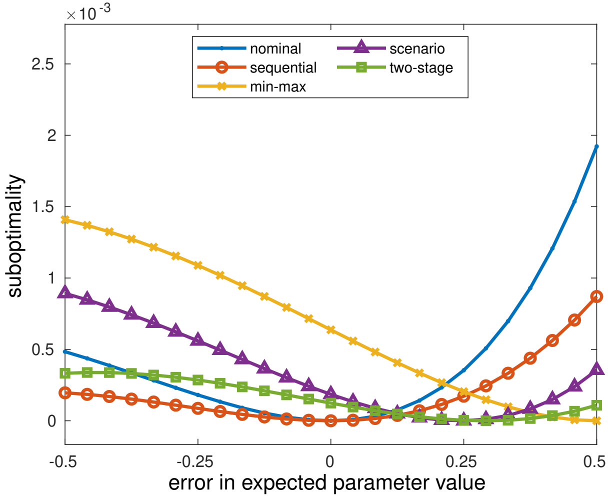


Robust DoE: 1D Toy Example

- Model

$$\hat{y}(p, u) = 1 - \exp(-pu)$$

- Uncertainty Level

$$\Delta p = 0.75$$

- Experiment Setup

$$N_e = 1, N = 2$$

Robust DoE: 1D Toy Example

- Model

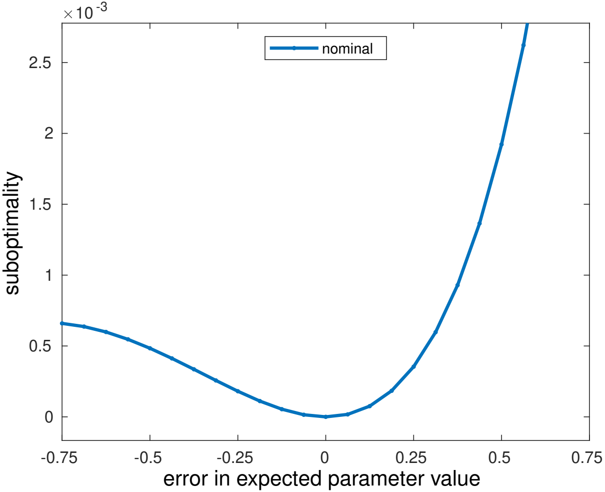
$$\hat{y}(p, u) = 1 - \exp(-pu)$$

- Uncertainty Level

$$\Delta p = 0.75$$

- Experiment Setup

$$N_e = 1, N = 2$$



Robust DoE: 1D Toy Example

- Model

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- Uncertainty Level

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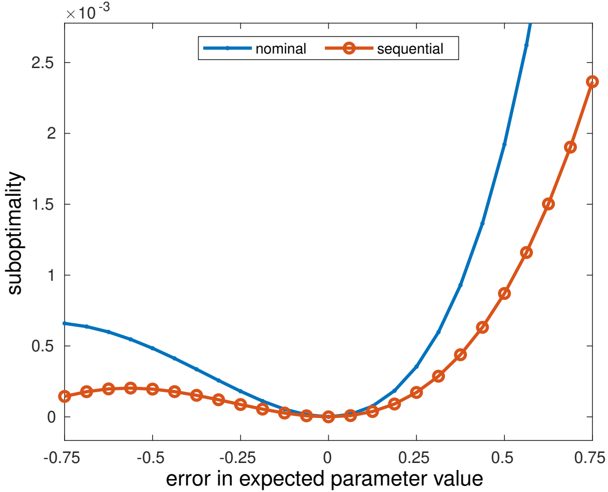
- Experiment Setup

$$N_e = 1, N = 2$$



Robust DoE: 1D Toy Example

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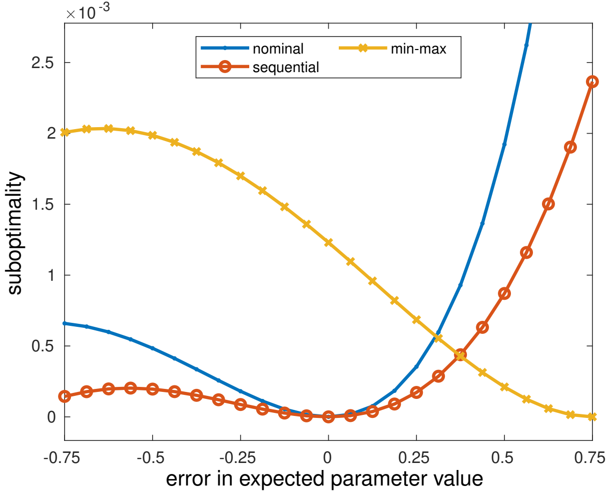

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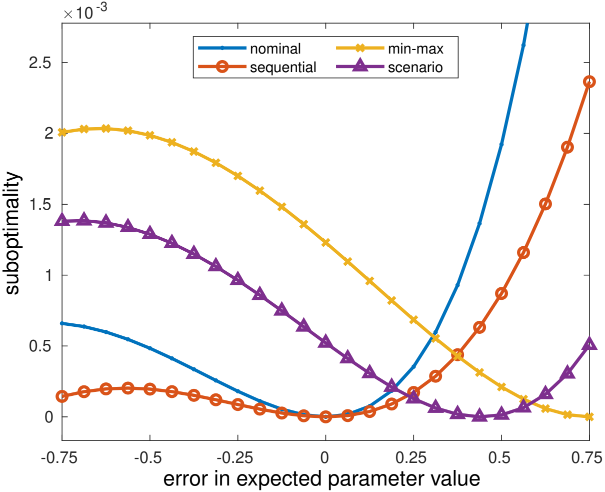

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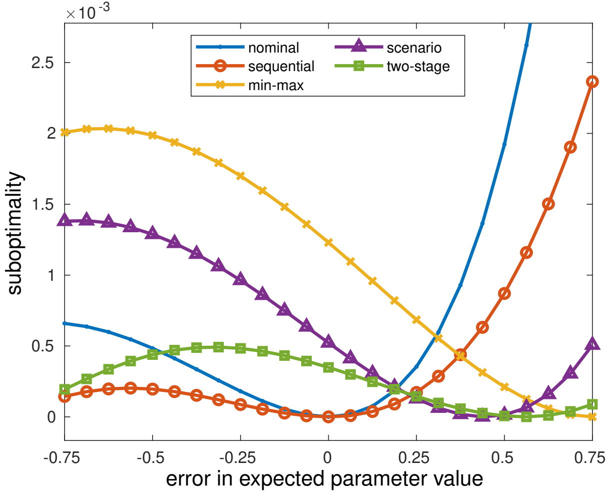


Robust DoE: 2D Example in Reaction Kinetics

- Model

$$\hat{y}(p, u) = \frac{p_1}{p_1 - p_2}\left(e^{-p_2 u} - e^{-p_1 u}\right)$$

- Uncertainty Level

$$\Delta p = 0.5$$

- Experiment Setup

$$N_e = 2, N = 4$$

Robust DoE: 2D Example in Reaction Kinetics

- Model

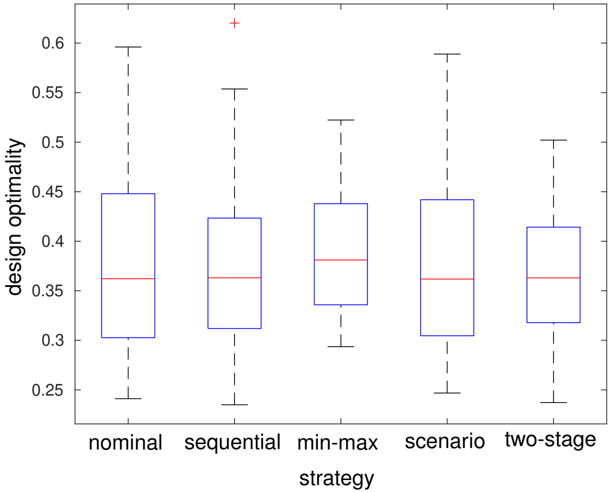
$$\hat{y}(p,u) = \frac{p_1}{p_1 - p_2}\left(e^{-p_2 u} - e^{-p_1 u}\right)$$

- Uncertainty Level

$$\Delta p = 0.5$$

- Experiment Setup

$$N_e = 2, N = 4$$



Robust DoE: 4D Example in Microbial Growth Kinetics

- Model

$$\hat{y}(p,\tau) = p_1 \left[1 - \frac{(u_\tau - p_2)^2}{(u_\tau - p_2)^2 + u_\tau(p_3 + p_4 - u_\tau) - p_3 p_4}\right]$$

- Uncertainty Level

$$\Delta p = 0.5$$

- Experiment Setup

$$N_e = 4, N = 6$$

Robust DoE: 4D Example in Microbial Growth Kinetics

- Model

$$\hat{y}(p,\tau) = p_1 \left[1 - \frac{(u_\tau - p_2)^2}{(u_\tau - p_2)^2 + u_\tau(p_3 + p_4 - u_\tau) - p_3 p_4} \right]$$

- Uncertainty Level

$$\Delta p = 0.5$$

- Experiment Setup

$$N_e = 4, N = 6$$

Approach	Suboptimality
nominal	614 %
sequential	179 %
min-max	134 %
scenario-based	148 %
two-stage	95 %

Conclusions

- Robust approaches for the design of optimal experiments using exact confidence regions
- Approach is based on bi-level programming
- Computationally intensive problem but tractable for small- to medium-scale cases
- The robust design based on multi-stage decision making proposed
- Modelling of possible re-design via multi-stage approach shows promising performance

- Future work: application to high-dimensional systems; modelling of dynamic problems
- Extension to classical linear confidence regions:

  A.R. Gottu Mukkula, M. Mateáš, M. Fikar, R. Paulen, Robust multi-stage model-based design of optimal experiments for nonlinear estimation, Computers & Chemical Engineering 155, 2021, pp. 107499

Solving the bi-level program

$$\min_{x} f(y)$$
$$\text{s.t. } \max_{y} g(y) \text{ s.t. } 0 = h(x, y)$$

- KKT-based reformulation in the lower level (non-convexity $\rightarrow$ infeasibility)

$$\min_{x,y,\lambda} f(y)$$
$$\text{s.t. } 0 = \nabla_y g(y) + \nabla_y h(x, y)\lambda, \; 0 = h(x, y)$$

- Using alternating approach (local optimality)

$$x_{k+1} = x_k - \frac{\partial f}{\partial y}\bigg|_{y^*} \frac{\partial y^*}{\partial x}\bigg|_{x_k} \quad \overset{x_{k+1}(y^*),y^*(x_k)}{\Longleftrightarrow} \quad y^* = \arg\max_{y} g(y) \text{ s.t. } 0 = h(x_k, y)$$