Model-Based Optimal Experiment Design for Nonlinear Parameter Estimation Using Exact Confidence Regions

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July 13, 2017
Motivation

Linearized Confidence Regions

Optimal Experiment Design
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Exact Confidence Regions

Optimal Experiment Design

Optimal Experiment Design
1. Select the model structure.

Dynamic model or spatially discretized PDEs:

\[ \hat{y} = F(u, p) \]

\[ \begin{align*}
\text{state equation:} & \quad \dot{x} = f(x, u, p), \quad x(0) = g(u, p) \\
\text{output equation:} & \quad \hat{y} = h(x, p)
\end{align*} \]

Steady-state or discretized model:

\[ \hat{y} = F(u, p) \]

\[ \begin{align*}
\text{state equation:} & \quad 0 = f(x, u, p) \\
\text{output equation:} & \quad \hat{y} = h(x, p)
\end{align*} \]

\( \hat{y} \) - outputs; \( u \) - experimental conditions
2 Perform experiments. Gather data.
Estimate unknown parameters.

\[ \hat{p} = \arg \min_{p \in P_0} J = \arg \min_{p \in P_0} \| y - \hat{y} \|^2_2 \]

subject to \( \hat{y} = F(u, p) \)
Analyze the quality of estimates.

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

s.t. \( \hat{y} = F(u, p) \)
4. Analyze the quality of estimates.

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

\[ \text{s.t. } \hat{y} = F(u, p) \]
Analyze the quality of estimates.

\[ J(p) - J(\hat{p}) \leq n_p s^2 F_{n_p, N-n_p, \alpha} \]
Analyze the quality of estimates.

\[(p - \hat{p})^T \sum_{k=1}^{N} \frac{\partial \hat{y}(k)}{\partial p^T} \frac{\partial \hat{y}(k)}{\partial p} (p - \hat{p}) \leq n_p s^2 F_{n_p, N-n_p, \alpha}\]

(Fisher Inform. Mtx. (FIM))
Linearized Optimal Experiment Design (OED)

- Idea: Improve the reliability of parameter estimates by optimizing some measure of Fisher Information Matrix (FIM).

\[
\min_{u(t)} \phi(FIM) \quad \text{s.t. } FIM = \sum_{k=1}^{N} \frac{\partial \hat{y}(k)}{\partial \rho^T} Q \frac{\partial \hat{y}(k)}{\partial \rho}, \quad \hat{y} = F(p, u)
\]

A design: \( \phi(FIM) = \text{tr}(FIM) \), D design: \( \phi(FIM) = \text{det}(FIM) \), ...
The linearized and exact confidence regions are different in general.

How to find OED using the exact confidence region?
Example

- Benchmark nonlinear problem (biological oxygen demand (BOD))

\[ \hat{y} = p_1(1 - \exp(-p_2 u)), \quad u \in [0, 20], \]

with \( y \) measured at the incubation times \( u \).

- Random normally distributed measurement noise with standard deviation \( \sigma = 0.1 \).

- True values of parameters \( p^* = (p_1, p_2)^T = (2.5, 0.5)^T \).

- \( N = 4 \), e.g. \( u := (2, 2, 20, 20)^T \) (linearized D design)
Example: $2\sigma(95\%)$-confidence regions

- Ellipsoidal over-approximation
- Orthotopic over-approximation
- Linearized confidence ellipsoid
- True values of parameters

$p_1$ vs. $p_2$
Over-approximation of exact confidence regions

Ellipsoidal over-approximation

$$\max_{p,k} \quad k$$

s.t.  $$J(p) - J(\hat{p}) = n_p s^2 F_{n_p, N-n_p, \alpha}$$

$$(p - \hat{p})^T FIM(p - \hat{p}) =$$

$$k n_p s^2 F_{n_p, N-n_p, \alpha}$$
Ellipsoidal over-approximation

$$\max_{p,k} k$$

s.t. $$J(p) - J(\hat{p}) = np s^2 F_{np,N-np,\alpha}$$

$$(p - \hat{p})^T \text{FIM}(p - \hat{p}) =$$

$$knp s^2 F_{np,N-np,\alpha}$$

Orthotopic over-approximation

$$\max_{\pi} \sum_{j=1}^{np} p_j^U - p_j^L$$

s.t. $$J(\pi_j) - J(\hat{p}) = np s^2 F_{np,N-np,\alpha}$$
Optimal Experiment Design

Ellipsoidal over-approximation

\[
\min_u \phi(FIM/k) \quad \text{s.t.}
\]

\[
\max_{p,k} k
\]

\[
\text{s.t. } J(p) - J(\hat{p}) = n_p s^2 \mathcal{F}_{n_p,N-n_p,\alpha}
\]

\[
(p - \hat{p})^T FIM(p - \hat{p}) = kn_p s^2 \mathcal{F}_{n_p,N-n_p,\alpha}
\]
Optimal Experiment Design

Ellipsoidal over-approximation

\[
\min_u \phi(\text{FIM}/k) \quad \text{s.t.}
\max_{p,k} k
\]

\[
\text{s.t. } J(p) - J(\hat{p}) = n_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}
\]

\[
(p - \hat{p})^T \text{FIM}(p - \hat{p}) = kn_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}
\]

Orthotopic over-approximation

\[
\min_u \sum_{j=1}^{n_p} p_j^U - p_j^L \quad \text{s.t.}
\max_{\pi} \sum_{j=1}^{n_p} p_j^U - p_j^L
\]

\[
\text{s.t. } J(\pi_j) - J(\hat{p}) = n_p s^2 \mathcal{F}_{n_p, N-n_p, \alpha}
\]
Solving bi-level program

\[
\begin{align*}
\min_x f(y) \\
\text{s.t. } \max_y g(y) \\
\text{s.t. } 0 = h(x, y)
\end{align*}
\]

- Using KKT-based reformulation of the lower-level problem

\[
\begin{align*}
\min_{x, y, \lambda} f(y) \\
\text{s.t. } 0 &= \nabla_y g(y) + \nabla_y h(x, y) \lambda \\
0 &= h(x, y)
\end{align*}
\]

- Using nested approach

\[
\begin{align*}
\min_x f(y^*(x)) &\quad \leftrightarrow \quad x^*, y^* \\
\max_y g(y) &\quad \text{s.t. } 0 = h(x^*, y)
\end{align*}
\]
Solving bi-level program

\[
\begin{align*}
&\min_x f(y) \\
&\text{s.t. } \max_y g(y) \\
&\text{s.t. } 0 = h(x, y)
\end{align*}
\]

Using KKT-based reformulation of the lower-level problem

\[
\begin{align*}
&\min_{x,y,\lambda} f(y) \\
&\text{s.t. } 0 = \nabla_y g(y) + \nabla_y h(x, y)\lambda \\
&\quad 0 = h(x, y)
\end{align*}
\]

Using nested approach

\[
x_{k+1} = x_k - \frac{\partial f}{\partial y}\Big|_{y^*} \frac{\partial y^*}{\partial x}\Big|_{x_k}
\]

\[
\begin{align*}
&\max_y g(y) \\
&\text{s.t. } 0 = h(x^*, y)
\end{align*}
\]
Example: Simulation results

\[ \hat{y} = p_1(1 - \exp(-p_2u)), \quad u \in [0, 20] \]

Linearized \iff \text{Confidence Regions} \implies \text{Exact}

- Linearized design: \( u_A = (1.6855, 1.6855, 20, 20)^T \), 
  \( u_D = (2, 2, 20, 20)^T \)

- Orthotope-based design: \( u_{A/D} = (1.3685, 1.3685, 20, 20)^T \)
Conclusions

- Problem of optimal experiment design formulated as a bilevel program.
- A tight over-approximation of a joint-confidence region realized as an orthotope.
- Computationally intensive problem but tractable for small-scale cases.
- Classical optimal experiment design does not cope well with model nonlinearity → Optimal experiment designed using the exact confidence region can differ greatly from the (classical) linearized counterpart.

Acknowledgement: