Návrh robustního experimentu založený na globální citlivosti

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**Experiment design problem**

Material parameters to be identified:
- \( m \) - values of thermal conductivity, heat capacity or water vapour resistance

Design variables to be optimised:
- \( d \) - loading types (e.g. prescribed temperature, moisture flux or heat transfer at a boundary) and loading magnitude as well as positions of sensors (thermometers, hygrometers etc.)

Noise variables to be considered:
- \( b = (b_d, b_r) \)
  - \( b_r \) - measurement errors,
  - \( b_d \) - inaccurate positioning of sensors or imperfections in prescribed loading conditions
Inverse analysis

\[ r(d) = f(d, b_d, m) + b_r \]

After realisation of an experiment according to selected values of \( d \).

**Nonlinear regression with random parameters \( b_d \)**

\[
\hat{m} = \arg \min_{m \in \mathcal{M}} \sum_i (r_i - f_i(d, b_d, m))^2
\]

- random = noise parameters follow prescribed probability distribution corresponding to distribution of their values in a set of repeated experiments
- assumption of more repeated experiments

**Bayesian inference**

\[
p(m, b_d | r) \approx p(r | m, b_d)p(m, b_d) = L(r - f(d, m, b_d))p(m, b_d)
\]

- distribution of noise parameters is updated along with the distribution of material properties
- assumption of only one realisation of the experiment, no repetitions
Goals of experiment design

- **Maximise information content on the investigated material parameters**
- **Minimise influence of experimental errors**

\[
\begin{align*}
\max_d S_m, & \quad \text{(sensitivity of observations to material properties)} \\
\min_d S_b, & \quad \text{(sensitivity of observations to noise variables)} \\
\text{s.t. } \quad m \in M, b \in B, d \in D
\end{align*}
\]

(\begin{itemize}
  \item expert on material model specifies feasible intervals
  \item expert on experimentation specifies feasible intervals for design variables and mean and variance of noise variables
\end{itemize})

**Bayesian approach**

- maximising Kullback-Leibner divergence
- quantifying information content of experiment by comparing prior and posterior distribution
- computationally very exhaustive
Nonlinear regression with random parameters

Local sensitivity matrix - 1st order derivatives in Taylor development of the model:

\[ f_{b_d, \widehat{m}}(d, b_d, m) = f(d, \overline{b_d}, \widehat{m}) + S_{b_d}(b_d - \overline{b_d}) + S_m(m - \widehat{m}) \]

Explicit solution of a least square problem:

\[ \widehat{m}(d, b_d, b_r) = (S_m^T S_m)^{-1} S_m^T [r(d) - f(d, \overline{b_d}, \widehat{m}) - S_{b_d}(b_d - \overline{b_d}) + S_m \widehat{m}] \]

\[ \text{cov}(\widehat{m}) = (S_m^T S_m)^{-1} S_m^T \text{cov}(b_r) + S_{b_d} \text{cov}(b_d) S_{b_d}^T S_m \]

With neglecting \( b_d \) and considering measurement errors to be i.i.d. variables with variance \( \sigma_{b_r}^2 \):

\[ \text{cov}(\widehat{m}) = \sigma_{b_r}^2 (S_m^T S_m)^{-1} \]

Optimality criterion:

F-optimality:

\[
\begin{align*}
F(d, \widehat{m}, \overline{b}) &= \sqrt{\text{trace} \left( (\text{cov}(\widehat{m}) \text{diag}(\widehat{m})^{-1})^T (\text{cov}(\widehat{m}) \text{diag}(\widehat{m})^{-1}) \right)} \\
&= \sqrt{\sum_i \left( \frac{\sigma_{m_i}}{\widehat{m}_i} \right)^2}
\end{align*}
\]
Robustness of solution

\[ f_{\overline{b_d}, \overline{m}}(d, b_d, m) = f(d, \overline{b_d}, \overline{m}) + S_{b_d}(b_d - \overline{b_d}) + S_m(m - \overline{m}) \]

\[ S_{b_d} = S_{b_d}(d, \overline{b_d}, \overline{m}) = \begin{bmatrix} \frac{\partial f_1(\cdot)}{\partial b_{d,1}} & \frac{\partial f_1(\cdot)}{\partial b_{d,2}} & \cdots \\ \frac{\partial f_2(\cdot)}{\partial b_{d,1}} & \frac{\partial f_2(\cdot)}{\partial b_{d,2}} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \]

and

\[ S_m = S_m(d, \overline{b_d}, \overline{m}) = \begin{bmatrix} \frac{\partial f_1(\cdot)}{\partial m_1} & \frac{\partial f_1(\cdot)}{\partial m_2} & \cdots \\ \frac{\partial f_2(\cdot)}{\partial m_1} & \frac{\partial f_2(\cdot)}{\partial m_2} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \]

Requires starting guess about \( \overline{m} \) which is apriori unknown!

Worst case approach

- Noise parameters \( b \) fixed at mean (zero) values
- Material parameters \( m \) evaluated in central star design points

\[ F_M(d) = \max \{ F(\overline{m}, d), F(\overline{m} - \delta m_i e_i, d), F(\overline{m} + \delta m_i e_i, d) : 1 \leq i \leq N_m \} \]

Robust optimisation of \( F_M(d) \) by particle swarm optimisation algorithm.
Formulation of using global sensitivity matrix

Polynomial chaos-based approximation of the model

\[ r(d) = f(d, b, m) \]

All problem variables need to be transformed into the standardised variables of a chosen family via linear or nonlinear transformation

\[ (d, b, m) = g(\xi = (\xi_d, \xi_b, \xi_m)) \]

According to Doob-Dynkin lemma (Bobrovski, 2005), model response is also random vector expressed as a function of the same random variables.

\[ \tilde{f}(\xi) = \sum_{\alpha \in J} f_{\alpha} H_{\alpha}(\xi) \]

According to (Xiu and Karniadakis, 2002, SIAM JSC), orthogonal polynomials w.r.t. given probability measures are the most suitable choice for the approximation.

- Hermite polynomials for Gaussian variables
- Legendre polynomials for uniform variables etc.
Formulation of using global sensitivity matrix

Construction of PCE-based approximation - computation of PC coefficients

- Linear regression
- Stochastic collocation method
- Stochastic Galerkin method

We use linear regression based on Latin Hypercube sampling derived from Halton sequence - very easy to implement

Global sensitivity matrix - variance-based Sobol' indices

\[
S_{f_k, \xi_i}^{*} = \frac{\sum_{\alpha \in \mathcal{I}_i} f^2_{k, \alpha} \mathbb{E}[H^2_{\alpha}(\mathbf{\xi})] + \sum_{\alpha \in \mathcal{I}_i^*} 1/n_i^* f^2_{k, \alpha} \mathbb{E}[H^2_{\alpha}(\mathbf{\xi})]}{\sum_{\alpha \in \mathcal{J}\setminus\{0\}} f^2_{k, \alpha} \mathbb{E}[H^2_{\alpha}(\mathbf{\xi})]}
\]

\[
\mathcal{I}_i^* = \{\alpha \in \mathbb{N}^s : 0 \leq \sum_{j=1}^{s} \alpha_j \leq p, \alpha_i \neq 0 \land \alpha_l \neq 0 \iff l \neq i, \forall l = 1, \ldots, s\}
\]

\[
\mathbb{E}[H^2_{\alpha}(\mathbf{\xi})] = \int H^2_{\alpha}(\mathbf{\xi})d\mathbb{P}(\mathbf{\xi}) = \int \cdots \int \prod_{j=1}^{s} (H^2_{\alpha,j}(\xi_j)) d\mathbb{P}(\xi_1) \cdots d\mathbb{P}(\xi_s) = \prod_{j=1}^{s} p_{\alpha,j}!
\]
Formulation of using global sensitivity matrix

| Global sensitivity matrix for given values of design variables: |
|$	ilde{f}_{\xi_d}^\chi(\xi_m, \xi_b) = \tilde{f}(\xi)|_{\xi_d=\xi_d}^\chi$|
| Complete global sensitivity matrix: |
|$
\begin{bmatrix}
\cdots & S_{f_1,\xi_m}^* (\xi_d^\chi) & \cdots & S_{f_1,\xi_b}^* (\xi_d^\chi) & \cdots \\
\cdots & S_{f_2,\xi_m}^* (\xi_d^\chi) & \cdots & S_{f_2,\xi_b}^* (\xi_d^\chi) & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots 
\end{bmatrix}$|
| Global sensitivity to material properties: |
|$
\begin{bmatrix}
\cdots & S_{f_1,\xi_m}^* (\xi_d^\chi) & \cdots \\
\cdots & S_{f_2,\xi_m}^* (\xi_d^\chi) & \cdots \\
\vdots & \vdots & \vdots 
\end{bmatrix}$|

Optimality measures:

$A^*(S_m^*) = \text{trace} \left( (S_m^*)^T S_m^* \right)^{-1}$,

$D^*(S_m^*) = \text{det} \left( (S_m^*)^T S_m^* \right)$,

$E^*(S_m^*) = \text{cond} \left( (S_m^*)^T S_m^* \right)$,
Illustrative example – physical problem

**Linear non-stationary heat problem**

**Energy balance equation**

\[ C \frac{d\theta}{dt} = \nabla \cdot [\lambda \nabla \theta], \]

+ Boundary conditions
+ Initial conditions

**Discretized system of equations**

\[ C \frac{dr}{dt} + Kr = q, \]

**Solution at time step i+1**

\[ (C + \xi \Delta \tau K)r^{i+1} = \xi \Delta \tau q + C[r^i + \Delta \tau (1 - \xi)r^i], \]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta )</td>
<td>[°C]</td>
<td>temperature</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>[Wm(^{-1})K(^{-1})]</td>
<td>thermal conductivity</td>
</tr>
<tr>
<td>( C = \rho c )</td>
<td>[Jm(^{-3})K(^{-1})]</td>
<td>capacity term</td>
</tr>
<tr>
<td>( c )</td>
<td>[Jkg(^{-1})K(^{-1})]</td>
<td>specific heat capacity</td>
</tr>
<tr>
<td>( \rho )</td>
<td>[kgm(^{-3})]</td>
<td>mass density</td>
</tr>
</tbody>
</table>

**Initial scheme**

- Material parameters: \( C, \lambda_x, \lambda_y \)
- Initial temperature: \( \theta(0) = 0 [°C] \)
- Other properties: \( \Delta \tau = 1 [s] \)
- Time duration = 60 [s]

- Heat flux: \( q = 0 [Wm^{-2}] \)
- Length: \( l_x = 0.05 [m] \)
- Height: \( l_y = 0.05 [m] \)
- \( q = 25 \cdot 10^3 [Wm^{-2}] \)
Illustrative example – physical problem

Linear non-stationary heat problem, numerical example

\[ C = 1.7 \cdot 10^6 \text{ [J m}^{-3}\text{K}^{-1}] \], \( \lambda_x = 0.6 \text{ [W m}^{-1}\text{K}^{-1}] \), \( \lambda_y = 4.7 \text{ [W m}^{-1}\text{K}^{-1}] \)

Evolution of temperature
Polynomial chaos – error analysis

- Polynomial degree $p=5$
- $x=y=0$
- $t=60$

$\theta_{0,0}$ [°C] ($t = 60$ [s])

$\lambda_x$ [Wm$^{-1}$K$^{-1}$]

$\lambda_y$ [Wm$^{-1}$K$^{-1}$]

$\epsilon_{rel,pce}(\theta)$ [%]

$\epsilon_{rel,pce}(\theta) = \frac{|\theta_{pce} - \theta_{MC}|}{\theta_{pce}} \times 100$

- Polynomial degree $p=5$
- $x=y=0$
- $t=60$

$\theta_{0,0}$ [°C] ($t = 60$ [s])

$C$ [Jm$^{-3}$K$^{-1}$] ($x = 10^6$)
Material parameters to be identified:

- \( m \) - values of thermal conductivities and heat capacity (3 variables):
  \[ m = (\lambda_x, \lambda_y, C) \]
  \[
  \begin{align*}
  \lambda_x & \in [0.3; 0.7] \quad \text{Wm}^{-1}\text{K}^{-1} \\
  \lambda_y & \in [3.0; 7.0] \quad \text{Wm}^{-1}\text{K}^{-1} \\
  C & \in [1.4 \times 10^6; 1.8 \times 10^6] \quad \text{Jm}^{-3}\text{K}^{-1}
  \end{align*}
  \]

Design variables to be optimised:

- \( d \) - positions of 3 sensors (6 variables):
  \[ d = (d_{x1}, d_{y1}, d_{x2}, d_{y2}, d_{x3}, d_{y3}) \]

Noise variables to be considered:

- all zero-mean normal variables
- \( b_r \) - measurement errors - at 3 sensors at 60 time steps: 180 i.i.d. variables, \( \sigma_r = 0.1^\circ\text{C} \)
- \( b_x \) - inaccurate positions of sensors, 6 i.i.d. var., \( b_x = (b_{x1}, b_{y1}, b_{x2}, b_{y2}, b_{x3}, b_{y3}) \), \( \sigma_{x_i} = \sigma_{y_i} = 0.5\text{mm} \)
- \( b_q \) - imperfection in loading \( \sigma_q = 50\text{W/m}^2 \)
• design variables: sensor positions \( d = (d_x, d_y) = g_d(\xi_d) \)

• noise variables: error in sensor positions \( b_d = (b_x, b_y) = g_b(\xi_b) \)

FE discretisation of model response

\[
A(\xi_m)u = q \\
\hat{u}(\xi_m) = \sum_{\alpha \in I} \beta_\alpha \psi_\alpha(\xi_m)
\]

• localisation of k-th element

\[
\hat{u}_k(\xi_m) = (\hat{u}_1(\xi_m), \hat{u}_2(\xi_m), \hat{u}_3(\xi_m))^T
\]

\[
N_k(d(\xi_d)) = (N_1(d(\xi_d)), N_2(d(\xi_d)), N_3(d(\xi_d))) = \left( \frac{A_1(\xi_d)}{A}, \frac{A_2(\xi_d)}{A}, \frac{A_3(\xi_d)}{A} \right)
\]

\[
\nabla = (\nabla x, \nabla y)^T
\]

\[
f_k(\xi_m, \xi_d, \xi_b) = N_k(\xi_d)\hat{u}_k(\xi_m) + b_d(\xi_b) \left[ \nabla N_k(\xi_d) \right] \hat{u}_k(\xi_m) = [N_k(\xi_d) + b_d(\xi_b) \left[ \nabla N_k(\xi_d) \right]] \hat{u}_k(\xi_m)
\]

\[
f_k(\xi_m, \xi_d, \xi_b) = \sum_{\alpha \in I} \beta_\alpha \psi_\alpha(\xi_m, \xi_d, \xi_b)
\]
Experiment design problem definition

Material parameters to be identified:
- \(m\) - values of thermal conductivities and heat capacity (3 variables): \(m = (\lambda_x, \lambda_y, C)\)

Design variables to be optimised:
- \(d\) - positions of 3 sensors (6 variables):

Noise variables to be considered:
- \(b_r\) - measurement errors,
- \(b_x\) - inaccurate positions of sensors,
- \(b_q\) - imperfection in loading

\[\tilde{u}(\cdot) = \sum_{\alpha \in I} \beta_\alpha \psi_\alpha(\xi_m, \xi_{br_k})\]

\[f_k(\cdot) = [N_k(\xi_d) + \xi_{bx} \nabla N_k(\xi_d)] \tilde{u}_k(\xi_m, \xi_{bq}) + \xi_{br_k}\]

\[f_k(\cdot) = \sum_{\alpha \in I} \beta_\alpha \psi_\alpha(\xi_m, \xi_d, \xi_{br_k}, \xi_{bx}, \xi_{bq})\]
Considering only measurement errors:
\[
\text{cov}(\tilde{m}) = \sigma_{br}^2 (S_m^T S_m)^{-1}
\]
Linearised inverse analysis, global sensitivity

\[
\tilde{m}(\cdot) = (S_m^T S_m)^{-1} S_m^T [r(d) - f(d, b_d, m) - S_{b_d} + S_m \tilde{m}]
\]

\[
\text{cov}(\tilde{m}) = (S_m^T S_m)^{-1} S_m^T \left[ \text{cov}(b_r) + S_{b_d} \text{cov}(b_d) S_{b_d}^T \right] S_m (S_m^T S_m)^{-1}
\]

\[
\text{cov}(\tilde{m}) = \text{diag} \left( \frac{\sigma_{\lambda_x}}{\lambda_x}, \frac{\sigma_{\lambda_y}}{\lambda_y}, \frac{\sigma_C}{C} \right)
\]

Considering only measurement errors:

\[
\text{cov}(\tilde{m}) = \sigma_{b_r}^2 (S_m^T S_m)^{-1}
\]

<table>
<thead>
<tr>
<th></th>
<th>A-opt.coarse</th>
<th>A-opt.fine</th>
<th>E-opt.fine</th>
<th>D-opt.fine</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\sigma_{\lambda_x}/\lambda_x)</td>
<td>20.6% (0.03%)</td>
<td>19.1% (0.03%)</td>
<td>12.1% (0.29%)</td>
<td>20.2% (0.03%)</td>
</tr>
<tr>
<td>(\sigma_{\lambda_y}/\lambda_y)</td>
<td>13.0% (0.05%)</td>
<td>16.2% (0.06%)</td>
<td>5.64% (0.20%)</td>
<td>13.7% (0.05%)</td>
</tr>
<tr>
<td>(\sigma_C/C)</td>
<td>9.92% (0.02%)</td>
<td>10.3% (0.02%)</td>
<td>5.10% (0.06%)</td>
<td>10.4% (0.02%)</td>
</tr>
</tbody>
</table>
Linearised inverse analysis

Global sensitivity

Local sensitivity

<table>
<thead>
<tr>
<th></th>
<th>Sawaf</th>
<th>E-opt.fine</th>
<th>U1-design</th>
<th>U2-design</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{x}/x$</td>
<td>125.2% (0.14%)</td>
<td>12.1% (0.29%)</td>
<td>4.61% (1.58%)</td>
<td>7.96% (1.70%)</td>
</tr>
<tr>
<td>$\sigma_{y}/y$</td>
<td>123.5% (0.11%)</td>
<td>5.64% (0.20%)</td>
<td>7.45% (6.18%)</td>
<td>2.91% (2.34%)</td>
</tr>
<tr>
<td>$\sigma_{C}/C$</td>
<td>110.9% (0.13%)</td>
<td>5.10% (0.06%)</td>
<td>2.94% (1.15%)</td>
<td>2.00% (1.26%)</td>
</tr>
</tbody>
</table>

[Sawaf et al., 1995, IJHMT]  
[Ruffio, Saury, Petit, 2012, IJHMT]
Testing of robustness:
- statistics over discretised space of material parameters

$$\begin{align*}
\lambda_x & \in [0.3; 0.7] \text{ Wm}^{-1}\text{K}^{-1} \\
\lambda_y & \in [3.0; 7.0] \text{ Wm}^{-1}\text{K}^{-1} \\
C & \in [1.4 \times 10^6; 1.8 \times 10^6] \text{ Jm}^{-3}\text{K}^{-1}
\end{align*}$$

<table>
<thead>
<tr>
<th>Design</th>
<th>$\sigma_{\lambda_x}/\lambda_x$</th>
<th>$\sigma_{\lambda_y}/\lambda_y$</th>
<th>$\sigma_C/C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>U2-design</td>
<td>7.90-31.9% (0.54-15.2%)</td>
<td>1.73-6.34% (1.06-5.89%)</td>
<td>1.53-4.30% (0.42-3.83%)</td>
</tr>
<tr>
<td>A-opt.coarse</td>
<td>18.8-26.7% (0.02-0.03%)</td>
<td>10.2-18.6% (0.04-0.06%)</td>
<td>8.33-14.9% (0.02-0.03%)</td>
</tr>
<tr>
<td>A-opt.fine</td>
<td>17.6-22.0% (0.02-0.04%)</td>
<td>15.3-24.2% (0.04-0.07%)</td>
<td>8.63-17.3% (0.02-0.03%)</td>
</tr>
<tr>
<td>E-opt.fine</td>
<td><strong>10.6-14.4% (0.17-1.80%)</strong></td>
<td><strong>2.47-6.16% (0.15-0.28%)</strong></td>
<td><strong>3.26-7.18% (0.04-0.07%)</strong></td>
</tr>
<tr>
<td>D-opt.fine</td>
<td>18.5-25.2% (0.02-0.03%)</td>
<td>10.5-20.2% (0.04-0.07%)</td>
<td>8.55-16.4% (0.02-0.03%)</td>
</tr>
</tbody>
</table>
Wider bounds

\[ \theta_{0,0} \left( t = 60 \text{ [s]} \right) \]

\[ \lambda_x \left[ \text{Wm}^{-1}\text{K}^{-1} \right] \]

\[ \theta \left( ^\circ\text{C} \right) \]

\[ \lambda_y \left[ \text{Wm}^{-1}\text{K}^{-1} \right] \]

\[ \theta \left( ^\circ\text{C} \right) \]

\[ \theta \left( ^\circ\text{C} \right) \]
Linearised inverse analysis

Testing of robustness:
- statistics over discretised space of material parameters

\[
\begin{align*}
\lambda_x & \in [0.3; 0.7] \quad \text{Wm}^{-1}\text{K}^{-1} \\
\lambda_y & \in [3.0; 7.0] \quad \text{Wm}^{-1}\text{K}^{-1} \\
C & \in [1.4 \times 10^6; 1.8 \times 10^6] \quad \text{Jm}^{-3}\text{K}^{-1}
\end{align*}
\]

\[
\begin{array}{|c|c|c|c|}
\hline
& \sigma_{\lambda_x}/\lambda_x & \sigma_{\lambda_y}/\lambda_y & \sigma_C/C \\
\hline
S2 & 4.11-1664\% (0.05-1656\%) & 1.82-1521\% (0.06-1522\%) & 1.86-12.89\% (0.01-12.37\%) \\
E-opt.coarse & 9.36-46.31\% (0.008-0.11\%) & 6.56-35.14\% (0.01-0.13\%) & 4.49-24.16\% (0.005-0.09\%) \\
\hline
\end{array}
\]

| & \sigma_{\lambda_x}/\lambda_x, \lambda_x = 0.6 & \sigma_{\lambda_y}/\lambda_y, \lambda_y = 4.7 & \sigma_C/C, C = 1.7 \times 10^6 |
|---|---|---|---|
| S2 & 14.60\% (0.55\%) & 7.01\% (0.76\%) & 2.51\% (0.28\%) |
| E-opt.coarse & 20.48\% (0.033\%) & 12.66\% (0.059\%) & 7.71\% (0.0274\%) |

20\th June 2016
Janov nad Nisou
MCMC-based Bayesian inference

E-opt. design

S2 design

PDF

Std = 0.119%

Std = 1.097%

PDF

Std = 0.090%

Std = 0.541%

PDF

Std = 0.849%

Std = 0.103%
**Proposed method:**

- Global sensitivity matrix – no need for good guess about parameters to be identified, only wide intervals are sufficient
- Better suited for cases, where response is nonlinear w.r.t. material properties
- Involve two approximations: FEM & PCE & total Sobol
  - Cause inaccuracy
  - Decrease computational demands – allow to solve more complex tasks

**Future work:**

- Investigation of optimality criteria – multi-objective optimisation, minimisation of correlation among the identified parameters etc.
Thank you for your attention

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