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Surrogate-based Bayesian Inversion for the Model Calibration of Fire Insulation Panels

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Motivation

Efficient inversion

Timber engineering relies on accurate model calibration for:

- simulation of fire hazards (component additive method)
- code based design

Experiments are carried out under standardized conditions for different insulation materials.

Breu (2016), Isofloc Insulation
Motivation

**Efficient inversion**

Timber engineering relies on accurate model calibration for:

- simulation of fire hazards (component additive method)
- code based design

Experiments are carried out under standardized conditions for different insulation materials.
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Experiments are carried out under standardized conditions for different insulation materials.
Outline

1 Introduction
   Problem formulation
   Bayesian inversion

2 Inversion with surrogate forward modelling

3 Inversion with surrogate likelihood

4 Conclusion
Experimental data $y$

Huge variations in measurements due to:
- cracking
- inhomogeneous insulation material

Forward model $\mathcal{M}(X)$

1D heat transfer problem with temperature dependent effective material parameters solved with FEM.
**Experimental data and forward model**

**Experimental data \( y \)**

Huge variations in measurements due to:
- **cracking**
- **inhomogeneous insulation material**

**Forward model \( M(X) \)**

1D heat transfer problem with temperature dependent effective material parameters solved with FEM.
Experimental data \( y \)

Huge variations in measurements due to:
- cracking
- inhomogeneous insulation material

Forward model \( \mathcal{M}(X) \)

1D heat transfer problem with temperature dependent effective material parameters solved with FEM.
Bayes’ theorem

With observed data regarded as \( Y \mid x \sim \pi(y \mid x) \)

\[
\pi(x \mid y) \propto \pi(y \mid x) \pi(x)
\]

with the Posterior \( \pi(x \mid y) \), the Prior \( \pi(x) \) and the Likelihood \( \pi(y \mid x) \)

Black-Box model
Prior in insulation problem

Parametrization

Define prior \( \pi(\mathbf{x}) \) on temp. dependent parameter curve parameters:

\[ \mathbf{x} \sim \mathcal{U}(\mathbf{x}_l, \mathbf{x}_u) \]
Likelihood in insulation problem

Likelihood function $\pi(y|x)$

Pdf of the data $y$ conditioned on the parameters $x$ as a function of these parameters:

$$Y|x \sim \mathcal{N}(M(x) - y, \Sigma(x))$$

Normal distribution describes the discrepancy between the model predictions $M(x)$ and the observed data $y$. 

Experimental curve vs. predictions
Outline

1. Introduction

2. Inversion with surrogate forward modelling
   - Surrogate forward modelling
   - MCMC
   - Results

3. Inversion with surrogate likelihood

4. Conclusion
Inversion with surrogate forward modelling

Method

**Two-stage procedure:**

- build a sufficiently accurate surrogate model of $\mathcal{M}(X)$
  1. run $N$ forward runs of $y = \mathcal{M}(x)$
  2. construct $\mathcal{M}^{PC}(X) \approx \mathcal{M}(X)$

- perform inference
  1. set up a standard method (MAP, MLE, MCMC, etc.)
  2. use $\mathcal{M}^{PC}(X)$ instead of $\mathcal{M}(X)$
PCE + PCA

Principal Component Analysis

The $N = 235$ output dimensions of $Y = M(X)$ are compressed to $N' = 7$ dimensions of a set of principal components $Z$ through PCA:

$$\log(Y) \approx \bar{\mu}_Y + \sum_{p=1}^{N'} \tilde{z}_p(X) \bar{\phi}_p$$

with the empirical mean $\bar{\mu}_Y$ and a set of $N'$ eigenvectors of the empirical covariance matrix $\bar{\phi}_p$ of $\log(Y)$.

Polynomial Chaos Expansion

The $N'$ retained principal components are expanded using an orthogonal polynomial basis $\Psi_\alpha(X)$:

$$\tilde{z}_p(X) = \sum_{\alpha \in \mathbb{N}^M} a_{p,\alpha} \Psi_\alpha(X) \approx \sum_{\alpha \in \mathcal{A}_\gamma} a_{p,\alpha} \Psi_\alpha(X)$$
Inversion with surrogate forward modelling

**Surrogate model** $\mathcal{M}^{PC}(\boldsymbol{x})$

- After computing the coefficients the response random vector can be represented as:

$$Y \approx \exp \left[ \bar{\mu}_Y + \sum_{p=1}^{N'} \left( \sum_{\alpha \in \mathcal{A}_\gamma} a_p, \alpha \Psi(\boldsymbol{x}) \right) \bar{\phi}_p \right]$$

which can be used as a metamodel for $\mathcal{M}(\boldsymbol{x})$.

- The transformation to the log-space assures:

$$\mathcal{M}^{PC}(\boldsymbol{x}) \in \mathbb{R}_+^N$$

**Comparison of $\mathcal{M}$ and $\mathcal{M}^{PC}$**

The surrogate model is accurate enough!
Solution of the inverse problem

We are interested in sampling from the posterior distribution $\pi(x|y)$:

$$X | y \sim \pi(x | y)$$

AIES

We use the affine-invariant ensemble sampler (AIES) presented in Goodman, Weare (2010)

+ invariant under affine transformations of the target distribution
+ multiple parallel chains simultaneously explore the target distribution
+ little tuning necessary
− slow (no parallelization)
Posterior distribution $\pi(x|y)$
Posterior curves

Posterior Parameters

Conductivity

Specific Heat

$T(\degree C)$

$T(\degree C)$

$T(\degree C)$
Outline

1. Introduction

2. Inversion with surrogate forward modelling

3. Inversion with surrogate likelihood
   Surrogate likelihood (SLE)
   Results

4. Conclusion
Inversion with surrogate likelihood

Method

One-stage procedure:
- build sufficiently accurate surrogate model of \( \pi(y|x) \)
  1. run \( N \) forward runs of \( \mathcal{L}(x) = \pi(y|x) \)
  2. construct \( \mathcal{L}^{PC}(X) \approx \mathcal{L}(X) \)
  3. inference is merely post-processing of \( \mathcal{L}^{PC}(X) \)

Spectral likelihood expansion

directly build a surrogate model for the likelihood:

\[
\mathcal{L}(X) \approx \mathcal{L}^{PC}(X) = \sum_{\alpha \in \mathcal{A}_\gamma} a_\alpha \Psi_\alpha(X)
\]

### Inference

- By post-processing the coefficients $a_\alpha$, an approximation to the posterior distribution can be derived easily:

$$
\pi(x|y) \approx \frac{1}{a_0} L^{PC}(x) \pi(x)
$$

- The posterior moments of the marginals can be derived analytically:

$$
E[X_j|y] \approx \frac{1}{a_0} \left\langle x_j, L_j^{PC} \right\rangle_{L^2_{\pi_j}}
$$

$$
\text{Var}[X_j|y] \approx \frac{1}{a_0} \left\langle (x_j - E[X_j|y])^2, L_j^{PC} \right\rangle_{L^2_{\pi_j}}
$$
Posterior distribution $\pi(x|y)$ SLE vs. MCMC

Large model error assumed!
Posterior moments of $\pi(\mathbf{x}|\mathbf{y})$ SLE vs. MCMC

<table>
<thead>
<tr>
<th></th>
<th>$X_1$</th>
<th>$X_2$</th>
<th>$X_3$</th>
<th>$X_4$</th>
<th>$X_5$</th>
<th>$X_6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E[X_j</td>
<td>\mathbf{y}]_{\text{MCMC}}$</td>
<td>427.4</td>
<td>$3.308 \cdot 10^{-4}$</td>
<td>0.016</td>
<td>$5.12 \cdot 10^4$</td>
<td>142</td>
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<tr>
<td>$E[X_j</td>
<td>\mathbf{y}]_{\text{SLE}}$</td>
<td>446.5</td>
<td>$3.708 \cdot 10^{-4}$</td>
<td>0.015</td>
<td>$4.431 \cdot 10^4$</td>
<td>144</td>
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<td>$\varepsilon$ (%)</td>
<td>4.47</td>
<td>12.09</td>
<td>6.25</td>
<td>13.46</td>
<td>1.41</td>
<td>1.58</td>
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<tr>
<td>$\text{Var}[X_j</td>
<td>\mathbf{y}]_{\text{MCMC}}$</td>
<td>$5.667 \cdot 10^3$</td>
<td>$1.669 \cdot 10^{-9}$</td>
<td>$6.616 \cdot 10^{-5}$</td>
<td>$1.118 \cdot 10^9$</td>
<td>628.1</td>
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<tr>
<td>$\text{Var}[X_j</td>
<td>\mathbf{y}]_{\text{SLE}}$</td>
<td>$4.707 \cdot 10^3$</td>
<td>$9.242 \cdot 10^{-9}$</td>
<td>$6.265 \cdot 10^{-5}$</td>
<td>$8.855 \cdot 10^8$</td>
<td>475.3</td>
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<tr>
<td>$\varepsilon$ (%)</td>
<td>20.4</td>
<td>81.94</td>
<td>5.6</td>
<td>26.26</td>
<td>32.15</td>
<td>16.14</td>
</tr>
</tbody>
</table>

**Correlation matrices**

- $\rho_{X_iX_j,\text{MCMC}}$
- $\rho_{X_iX_j,\text{SLE}}$
Posterior curves

SLE pros/cons

+ sampling free
+ deterministic approach for inversion
+ only one source of error (Quality of PCE)

− does not work with spiked likelihood functions (yet!)
− high dimensions (PCE based)
Outline

1. Introduction
2. Inversion with surrogate forward modelling
3. Inversion with surrogate likelihood
4. Conclusion
Conclusion & outlook

- Bayesian inversion is suitable for calibrating transient heat conduction models of fire experiments
- Classical MCMC can be used together with advanced surrogate models (principal component analysis + polynomial chaos expansion)
- Spectral likelihood expansion is a promising, sampling free approach that requires some further tuning
- Multiple experiments shall be combined using hierarchical Bayesian models

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Thank You!

Questions?