

# Computer model calibration as a method of design

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## 1 Introduction

### 1.1 Computer experiments

### 1.2 Computer model calibration

#### 1.2.1 Gaussian processes

#### Background

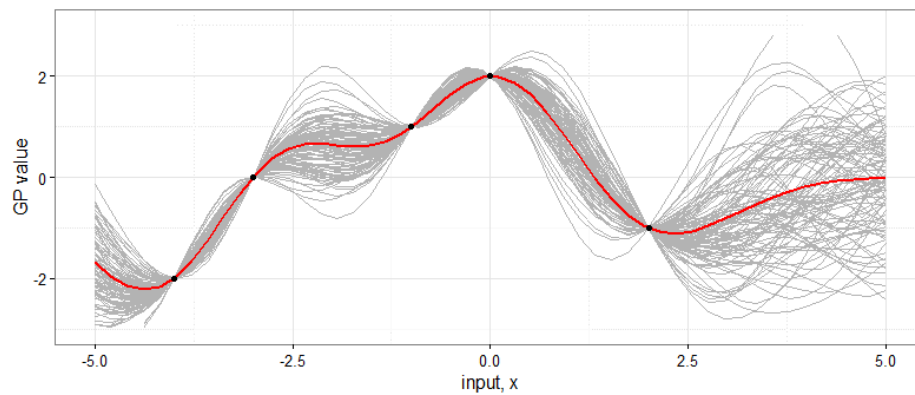


Figure 1: Example of a Gaussian process trained to interpolate five data points (black dots).

#### Gaussian process regression

#### Gaussian processes in computer model calibration

#### 1.2.2 Markov chain Monte Carlo methods

#### Background

#### Metropolis-Hastings algorithm

#### Elimination of boundary constraints

#### 1.2.3 Normalization of inputs and standardization of outputs

#### Blah

#### **1.2.4 Computational difficulties**

Blah

**Likelihoods** Blah

**Ill-conditioned covariance matrices**

## **2 Calibration for design**

## **3 Application**

### **3.1 Project background**

### **3.2 Emulation of finite element simulator**

Blah

#### **3.2.1 Wind turbine blade simulator**

Blah

#### **3.2.2 Mathematical basis for the emulator**

Blah

#### **3.2.3 Experimental design**

Blah

#### **3.2.4 Covariance parameters**

Blah

**Finding covariance parameters via MCMC** Blah

**Grid optimization** Blah

**Gradient method** Blah

## **4 MCMC using the emulator**

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### **4.1 MCMC methods**

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### **4.2 The model**

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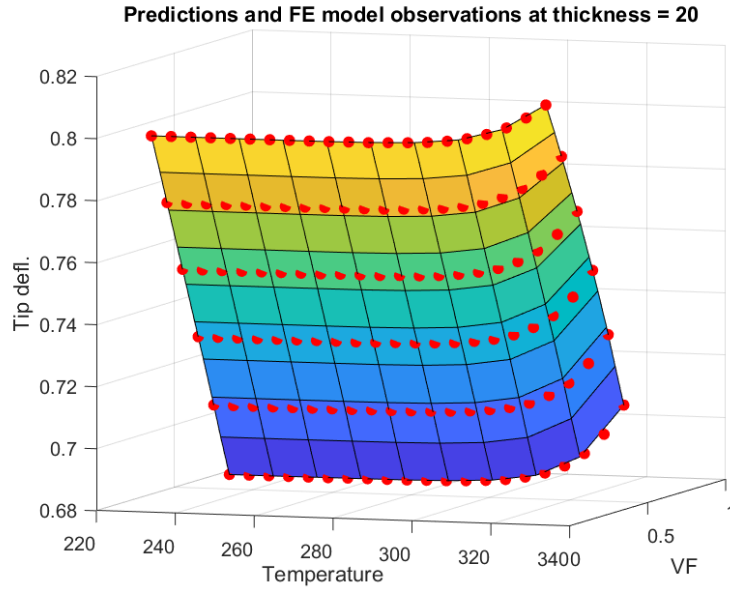


Figure 2: A slice of the GP emulator (restricted to the output for tip deflection) at thickness = 20mm. Red dots are observations from the simulator.

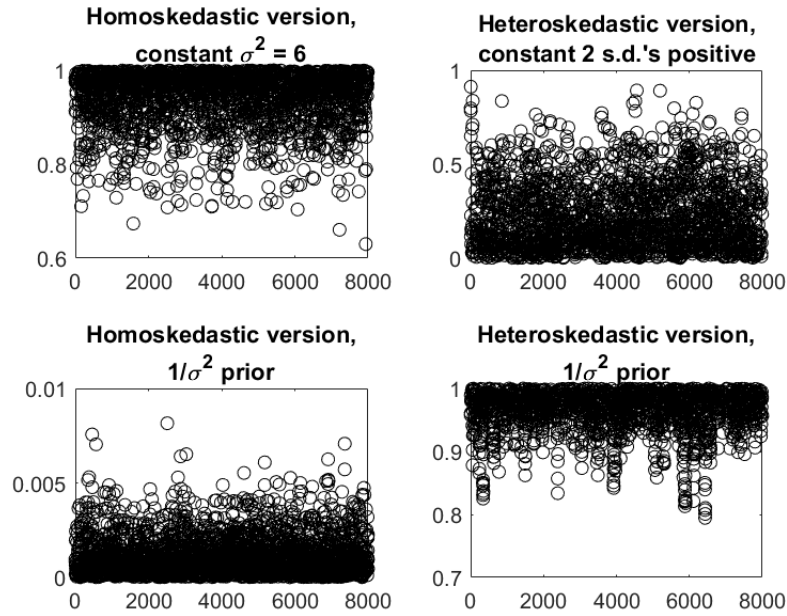


Figure 3: MCMC results at various observation variance settings.

	Heteroskedastic, constant	Homoskedastic, constant	Heteroskedastic, prior	Homoskedastic, prior
Deflection	0.749	0.729	0.659	0.709
Rotation	0.0904	0.0865	0.0773	0.0843
Cost	276.16	236.11	350.80	233.95

Table 1: Comparison of model outputs, where the desired data outputs are assumed to be either homoskedastic or heteroskedastic, with either a specified constant variance or a  $1/\sigma^2$  prior.

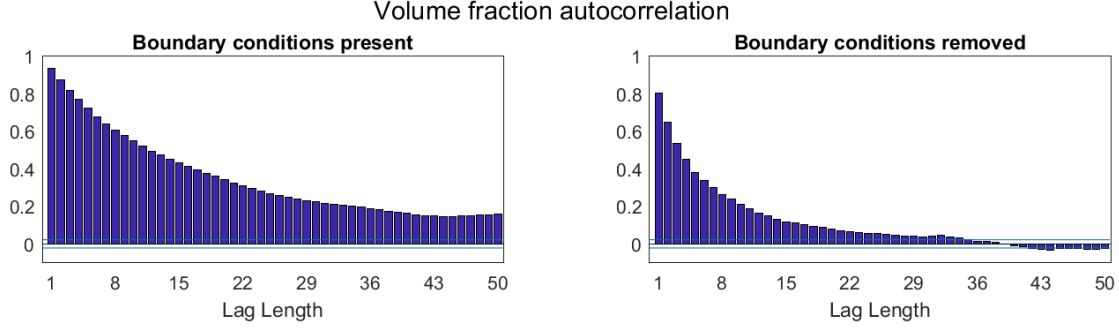


Figure 4: Auto-correlation for draws both with and without the elimination of boundary conditions.

#### 4.2.1 Desired observation variance

#### 4.2.2 Full model and likelihood

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#### 4.2.3 Convergence difficulties

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#### 4.2.4 Implementation of the Metropolis-Hastings algorithm

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### 4.3 Which data to desire?

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#### 4.3.1 Motivations behind the choice of desired data

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#### 4.3.2 Differing results

Desired data $d$	$\sigma_{defl}^2$	$\sigma_{rot}^2$	$\sigma_{cost}^2$	$\mu_{v d}$	$\mu_{h d}$	$\sigma_{v d}^2$	$\sigma_{h d}^2$
(0, 0, 0)	375.45	277.69	2.62	0.215	$4.01 \cdot 10^{-2}$	$4.41 \cdot 10^{-2}$	$1.92 \cdot 10^{-3}$
(0.65, 0.077, 96)	16.74	15.25	$4.62 \cdot 10^{-7}$	$1.09 \cdot 10^{-3}$	$3.36 \cdot 10^{-4}$	$1.02 \cdot 10^{-5}$	$9.97 \cdot 10^{-6}$

Table 2: Comparison of results for two different (low) values of  $d$ . Values listed are, respectively, the posterior means for the observation variance of each model output, posterior means for volume fraction ( $v$ ) and thickness ( $h$ ), and posterior variance of volume fraction and thickness.

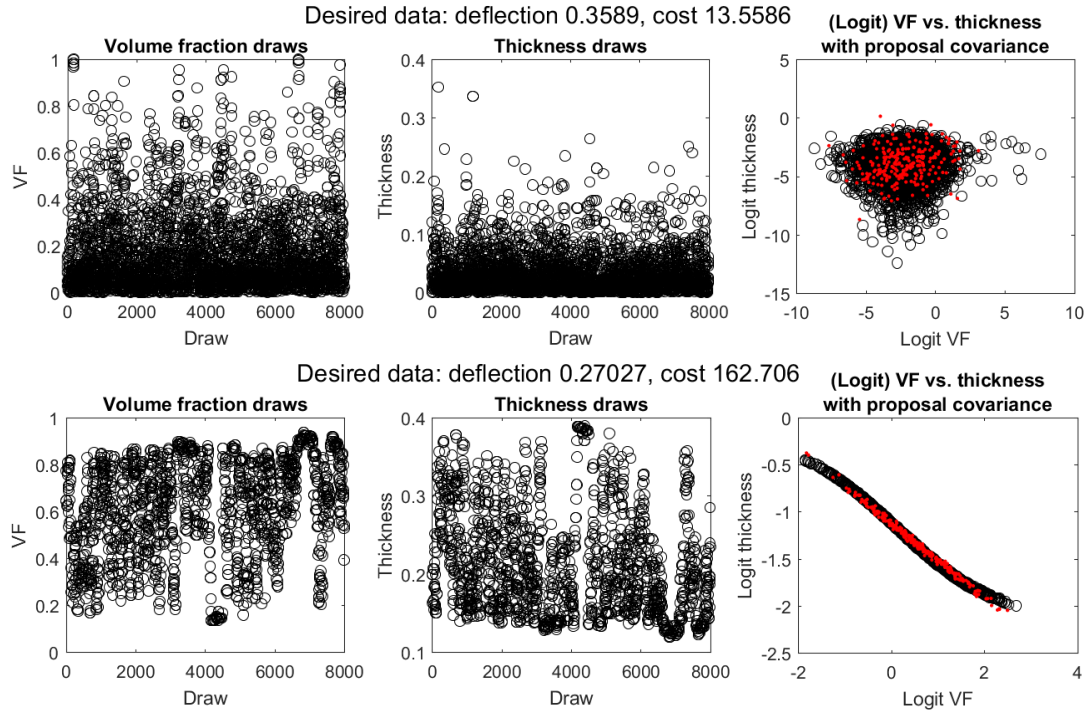


Figure 5: MCMC results for low deflection and cost (top row) and low deflection with easily achievable cost (bottom row).

#### 4.4 Exponentially distributed desired data

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##### 4.4.1 Motivation

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##### 4.4.2 Implementation and results

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#### 4.5 Identifiability issues

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### 5 Future work

Blah

#### 5.1 Alternative means of handling cost

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##### 5.1.1 Removing cost from the model

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### **5.1.2 Alternative priors for controlling cost**

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## **5.2 Building a desired data response surface**

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## **5.3 Implementing Hamiltonian Monte Carlo**

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### **5.3.1 Hamiltonian Monte Carlo**

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### **5.3.2 Benefits**

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## **5.4 Model discrepancy**

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## **6 Conclusion**

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