Computer model calibration as a method of design

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1 Introduction

1.1 Computer experiments

Suppose that one wishes to improve one's understanding of, say, the movement of people in a crowd escaping from a building in a crisis situation. This is an example of an area in which field data are extremely difficult to acquire. Merely assembling a crowd of research subjects in one place is costly and difficult. Asking them to flee a building may result in behaviors which are unlike those in real crisis situations – but which may nonetheless present unacceptable physical risk to the subjects. Inducing them to flee through the generation of a (real or apparent) crisis is similarly infeasible. Observational data are likewise scarce here, since panic-inducing crises are by their nature difficult to predict and chaotic in ways that hinder the reliable collection of data.

In the face of these difficulties, computer models offer an alternative to the choice between attempting field data collection and giving up on the hope of progress. Using existing theory concerning human psychology and movement, it is possible to construct a computer model simulating the behavior of people evacuating from a large building. For example, the SIMULEX model described by Thompson and Marchant [3] allows one to observe simulated evacuation behaviors in any specified building layout, using any desired distribution of individuals, whose individual relevant characteristics (walking speed, initial bodily orientation, etc) may be controlled by the researcher. Thus, computer models provide a means to collect data which might otherwise be largely inaccessible.

1.2 Computer model calibration

Consider again the SIMULEX model. Suppose that we wish to use this model to compare two different proposed building codes to be enforced in, say, St. Louis, Missouri. We may use average walking speed and average interpersonal distance as input parameters for this model. It is well-established that average walking speed [1] and interpersonal distance [2] vary across locales. These values may be unknown. Thus we may wish to find the true values for average walking speed and interpersonal distance in St. Louis; we may wish, in other words, to *calibrate* these parameters in the model.

Broadly, in model calibration, we may consider a model to be of the form $\eta(x, \theta)$, where (x, θ) comprise all inputs to the model. Control inputs — inputs under the control of the researcher (in the evacuation example, this would include the building layout) comprise x, whereas θ is the set of calibration inputs — parameters the values of which are not under researcher control, but rather are unknown values which must be estimated for successful simulation. Thus where f describes the true system, we consider the model to be

$$f(x, \theta) = f(x) = \eta(x, \theta) + \delta(x) \tag{1}$$

where δ is some form of model discrepancy. Notice that we may write $f(x) = f(x, \theta)$ since θ does not vary in reality. To undertake model calibration, we must have access to at least some observations of the real system; it is to these real observations that we calibrate the computer model.

Much interest in the past two decades has centered on Bayesian methods for model calibration. The appeal of a Bayesian approach to model calibration lies in the fact that the calibration parameters are a source of uncertainty for the model. This uncertainty should be quantified so that its effect on the model can be made explicit. We can thus use Bayesian methods to arrive at a posterior distribution on the calibration parameters which balances our prior knowledge about the calibration parameters with what can be learned from the available data, and which also allows for accurate uncertainty quantification on the model outputs.

1.2.1 Gaussian processes

Background

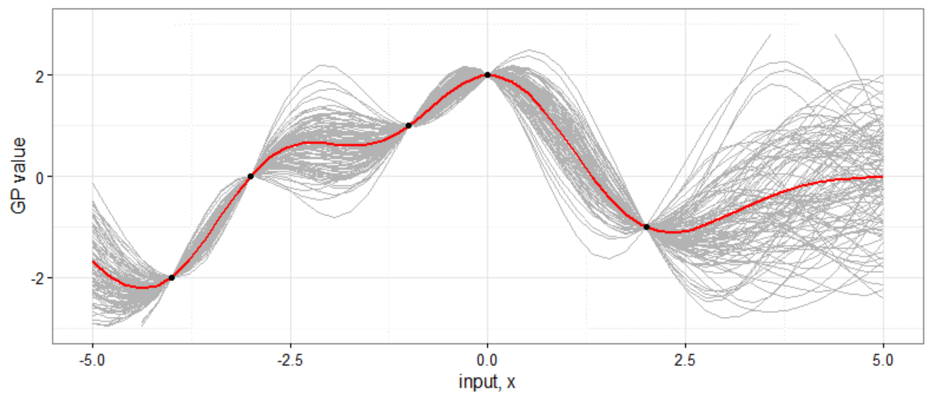

Figure 1: Example of a Gaussian process trained to interpolate five data points (black dots).

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

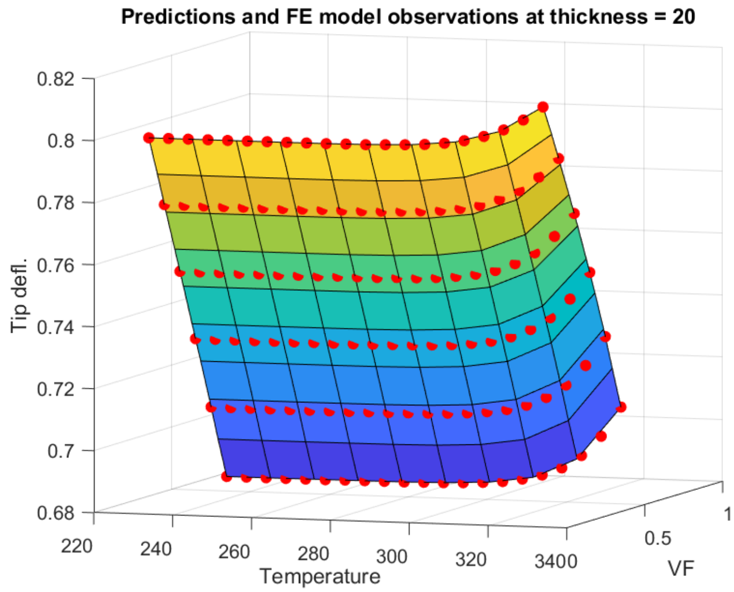

Figure 2: A slice of the GP emulator (restricted to the output for tip deflection) at thickness =20mm. Red dots are observations from the simulator.

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

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3.2.3 Experimental design

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3.2.4 Covariance parameters

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Finding covariance parameters via MCMC Blah

Grid optimization Blah

Gradient method Blah

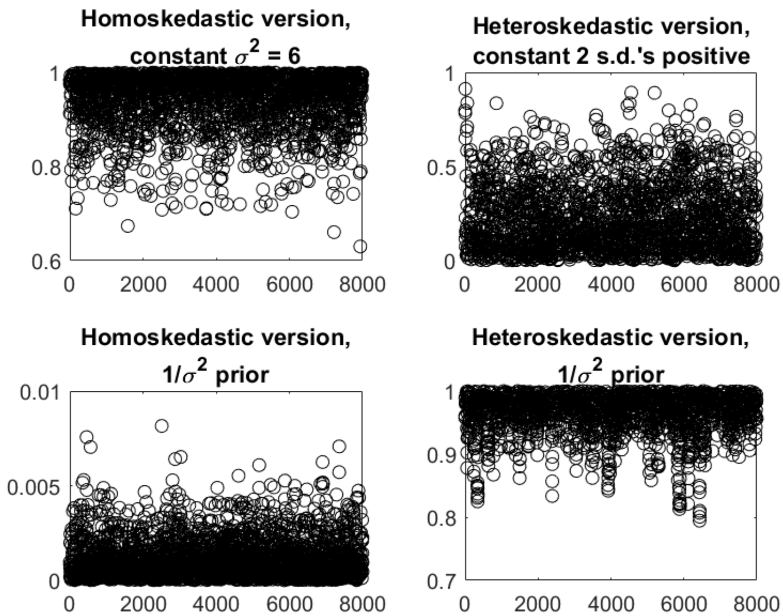

Figure 3: MCMC results at various observation variance settings.

4 MCMC using the emulator

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4.1 MCMC methods

Blah

4.2 The model

Blah

4.2.1 Desired observation variance

	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.

4.2.2 Full model and likelihood

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4.2.3 Convergence difficulties

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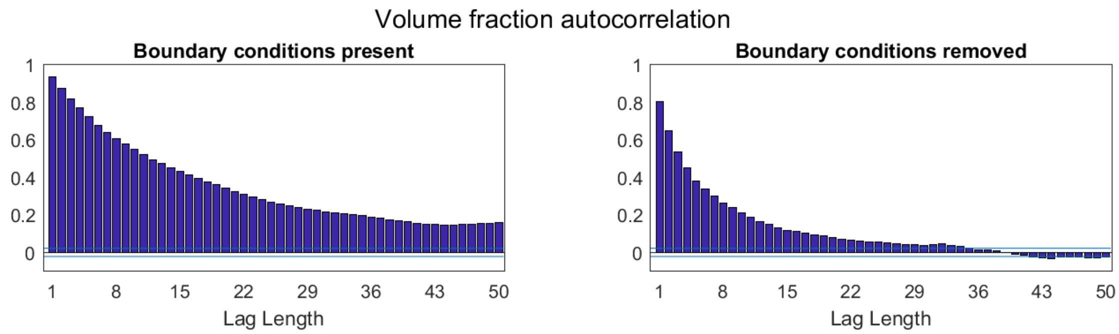

Figure 4: Auto-correlation for draws both with and without the elimination of boundary conditions.

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	σ^2_{defl}	σ^2_{rot}	σ^2_{cost}	$\mu_{v\|d}$	$\mu_{h\|d}$	$\sigma^2_{v\|d}$	$\sigma^2_{h\|d}$
$(0, 0, 0)$	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.

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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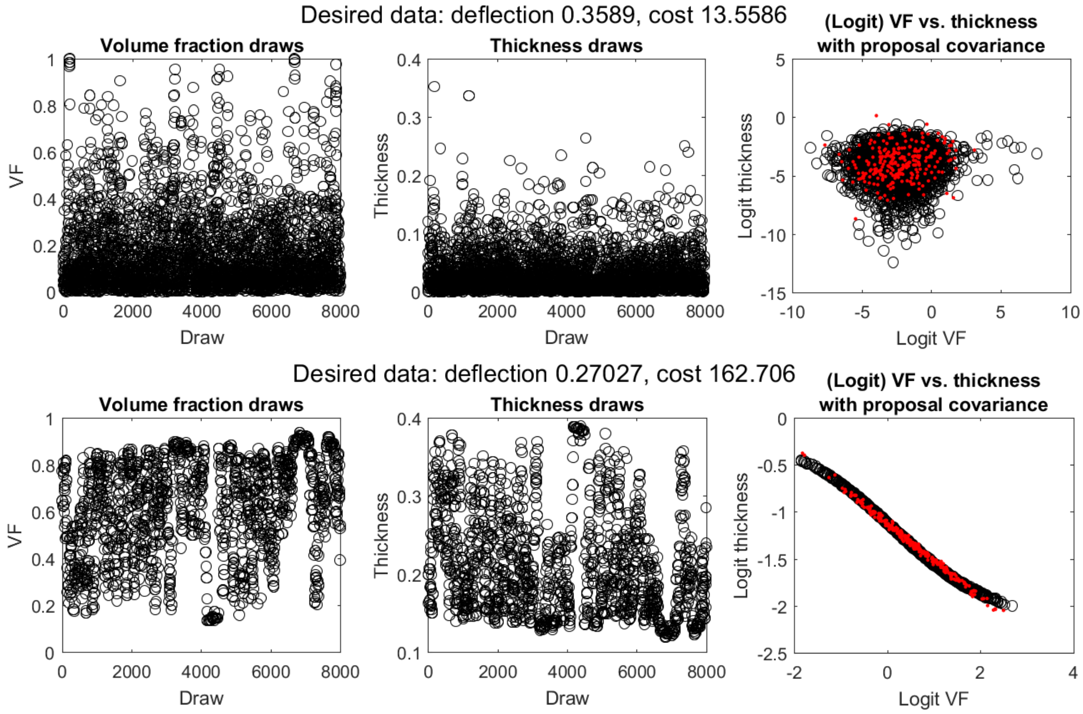

Figure 5: MCMC results for low deflection and cost (top row) and low deflection with easily achievable cost (bottom row).

5 Future work

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5.1 Alternative means of handling cost

Blah

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

Blah

6 Conclusion

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References

[1] Marc H. Bornstein and Helen G. Bornstein. The pace of life. *Nature*, 259(5544):557–559, feb 1976.

[2] Agnieszka Sorokowska, Piotr Sorokowski, Peter Hilpert, Katarzyna Cantarero, Tomasz Frackowiak, Khodabakhsh Ahmadi, Ahmad M. Alghraibeh, Richmond Aryeetey, Anna Bertoni, Karim Bettache, Sheyla Blumen, Marta Błażejewska, Tiago Bortolini, Marina Butovskaya, Felipe Nalon Castro, Hakan Cetinkaya, Diana Cunha, Daniel David, Oana A. David, Fahd A. Dileym, Alejandra del Carmen Domínguez Espinosa, Silvia Donato, Daria Dronova, Seda Dural, Jitka Fialová, Maryanne Fisher, Evrim Gulbetekin, Aslhan Hamamcolu Akkaya, Ivana Hromatko, Raffaella Iafrate, Mariana Iesyp, Bawo James, Jelena Jaranovic, Feng Jiang, Charles Obadiah Kimamo, Grete Kjelvik, Frat Koç, Amos Laar, Fívia de Araújo Lopes, Guillermo Macbeth, Nicole M. Marcano, Rocio Martinez, Norbert Mesko, Natalya Molodovskaya, Khadijeh Moradi, Zahrasadat Motahari, Alexandra Mühlhauser, Jean Carlos Natividade, Joseph Ntayi, Elisabeth Oberzaucher, Oluyinka Ojedokun, Mohd Sofian Bin Omar-Fauzee, Ike E. Onyishi, Anna Paluszak, Alda Portugal, Eugenia Razumiejczyk, Anu Realo, Ana Paula Relvas, Maria Rivas, Muhammad Rizwan, Svjetlana Salkičević, Ivan Sarmány-Schuller, Susanne Schmehl, Oksana Senyk, Charlotte Sinding, Eftychia Stamkou, Stanislava Stoyanova, Denisa Šukolová, Nina Sutresna, Meri Tadinac, Andero Teras, Edna Lúcia Tinoco Ponciano, Ritu Tripathi, Nachiketa Tripathi, Mamta Tripathi, Olja Uhryn, Maria Emília Yamamoto, Gyesook Yoo, and John D. Pierce. Preferred Interpersonal Distances: A Global Comparison. *Journal of Cross-Cultural Psychology*, 48(4):577–592, may 2017.

[3] Peter A Thompson and Eric W Marchant. A Computer Model for the Evacuation of Large Building Populations. *Fire Safety Journal*, 24:131–148, 1995.