Computer Model Calibration… part 2
Some comments on model calibration and an approach for unbiased computer models

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How do we feel about this set-up?

$$
\begin{aligned}
y_s(x,t) &= \eta(x,t) \\
y_f(x,\theta) &= \eta(x,\theta) + \delta(x) + \varepsilon
\end{aligned}
$$

- Where,
  - x model or system inputs;
  - y_f system response
  - y_s simulator response
  - θ calibration parameters
  - ε random error

Comments/questions

- Suppose that the computer model does not perfect reflect the mean of the physical process

- What can go wrong?

- What does the discrepancy function do?

Toy example - Chemical Kinetics example

- Field design with 11 equally spaced (time) points in [0,3] with 3 replicates for the model

$$y_f(x) = 1.5 + 3.5e^{-1.7x} + \epsilon;\ \ \epsilon \sim N(0, 0.36)$$

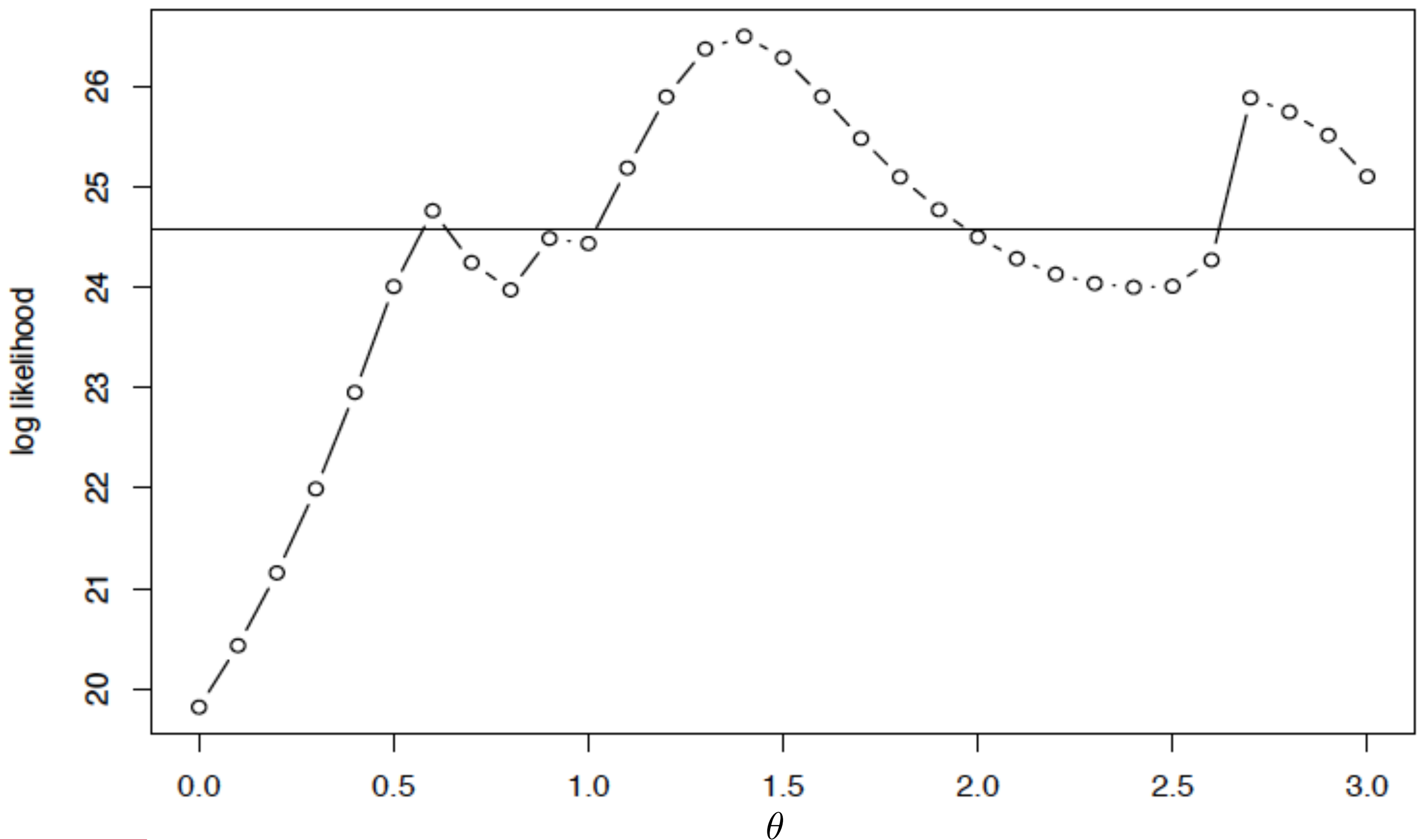
- Computer model run design: 21-point random Latin hypercube design

- Computer model:

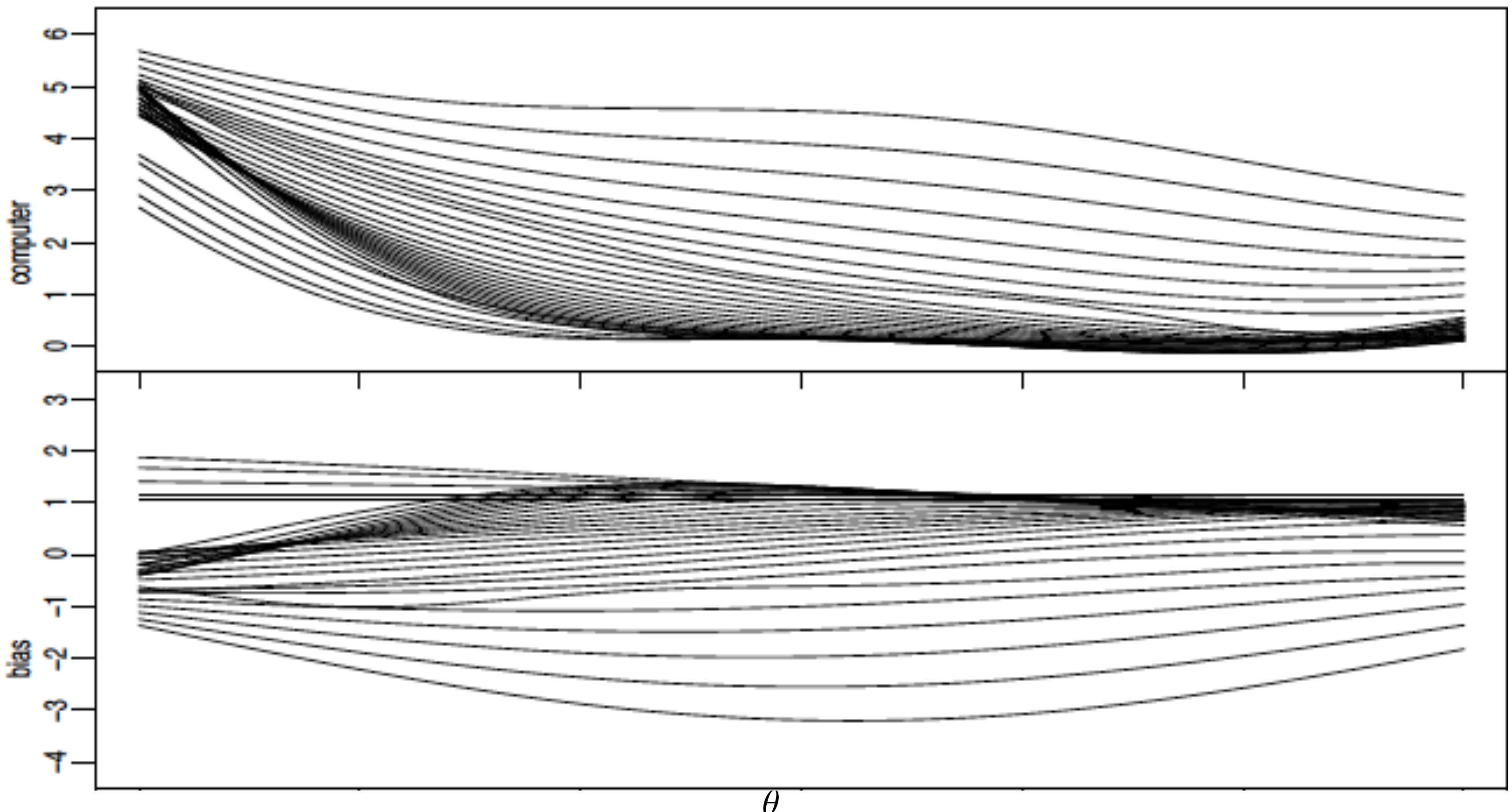
$$y_s(x) = 5e^{-\theta x}$$

- Note: $\theta = 1.7$

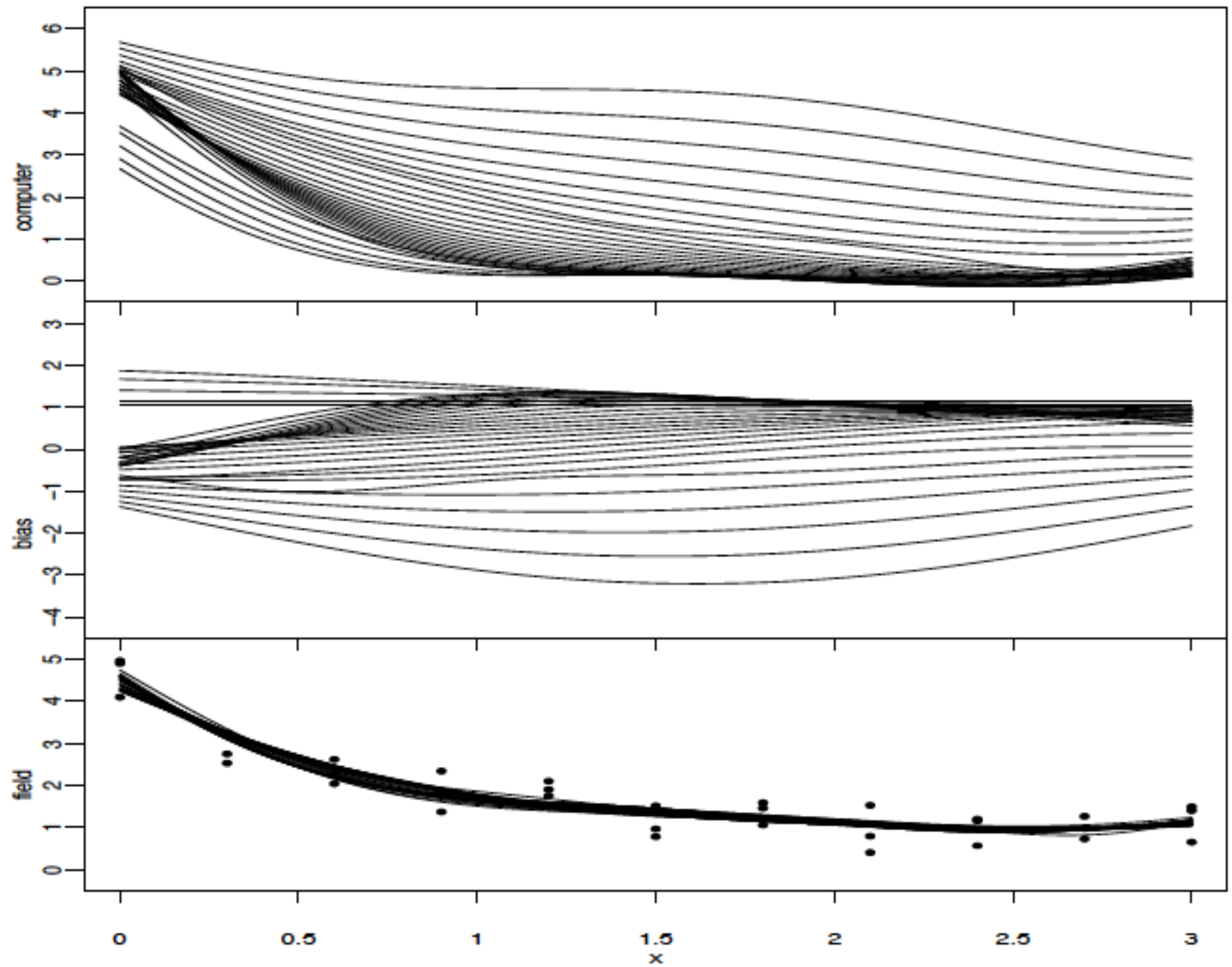
Profile likelihood for θ is multi-modal



Computer model output and bias function for different values of θ



Predictive distribution appears relatively unaffected by changes in θ



Questions

- What is a good value of the calibration parameter?
- How should this be interpreted?

Back to CRASH example

- We have just looked at issues related to the calibration parameter
- What about the discrepancy?
- Where does the information come from?

CRASH data summary

- Have observations from 1-D CRASH model and experiments
- Experiment data:
  - 9 experiments
  - experiment variables: Be thickness, Laser Energy, Xe pressure and Time
  - responses: Shock location
- 1-D CRASH Simulations
  - 320 simulations, varied over 8 inputs
  - experiment variables: Be thickness, Laser Energy, Xe pressure and Time
  - calibration parameters: Be Gamma, Be OSF, Xe Gamma, Xe OSF
  - response: Shock location

What does this say about model calibration?

- Have to be thoughtful about what it can and cannot do
- Generally very good at combining field and simulation data to make predictions in the physical system
- By very cautious about using the calibration parameters for any other purpose **if the discrepancy is important**
- Be even more cautious about the form of the discrepancy

Return to the classical inverse problem

$$y_s(t) = \eta(t)$$

$$y_f(\theta) = \eta(\theta) + \epsilon$$

- Where,
  - y_f system response
  - y_s simulator response at input t
  - θ calibration parameters
  - ε random error

Have data from 2 separate sources – computer model and field observations

Problem is to estimate the calibration parameters

Obvious solutions

- Just do the K-O approach
- Could emulate computer model and minimize the least squares deviation

$$L = \sum_{field\ obs} (y_f - \hat{\eta}(t))^2$$

- What if field data are complex data structures?

Example

- Field observations available from the Polar Ultraviolet Imager satellite
- Computer model is assumed to capture all salient features of the solar wind interactions, up to random error … model is unbiased
- However, the inputs ($\theta = (\alpha, \beta, R)$) are not known
- Scientific problem: estimate $\theta = (\alpha, \beta, R)$
- Computer model is slow to run... 4 runs ≈ 1 month

Data

- 20 simulations from the deterministic computer model
- Each simulation gives a space-time field on a 1,944 grid for each response variable
- Have one field observation from UVI for both responses on the same grid (i.e., have observed one storm)
- Leads to roughly $40,000 \times 40,000$ covariance matrix to calibrate one response


4 17 30

… and complicating matters

- LFM model output exhibits behaviour that is not well represented by a non-stationary GP as a function of the inputs

- Challenges: Large data structure and non-stationary covariance model is required

Approach (Pratola et al., 2013)

- Criterion-based approach
- Need a (well designed) collection of initial model runs
- Attempts to measure the discrepancy between the computer model run at a each input setting and the field observation
- **Model the criterion as a function of the calibration parameter**
- Estimate of the calibration parameter is where the criterion surface is minimized (can use expected improvement to pick future trials)

Basic set-up

- Recall,

$$y_s(t) = \eta(t)$$

$$y_f(\theta) = \eta(\theta) + \epsilon$$

- If ran the computer model at $t = \theta$, then the difference between the simulator output and the observations would be a vector (or matrix) of white noise

Discrepancy

- Let $\delta(t) = Y_f(\theta) - Y_c(t) = \eta(\theta) - \eta(t) + \epsilon$

- Idea:
  - Restricted model: if $t = \theta$, $\delta(\theta) \sim N(0, \sigma^2 I)$

  - Unrestricted Model: otherwise $\delta(t) \sim N(\mu_t, \sigma_t^2 R + \sigma^2 I)$

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Discrepancy criterion

- Define the discrepancy criterion:

$$\Delta(t_i) = -2log\left(\frac{L_r^*(\delta(t_i))}{L_u^*(\delta(t_i)}\right)$$

where L_r^* denotes the maximized likelihood for the restricted model, L_u^* denotes the likelihood for the unrestricted model

Idea

- If we are lucky enough to have run the computer model at the correct value of the calibration parameter, then criterion will be small (zero)

- Otherwise, the criterion will be relatively large

$$\Delta(t_i) = -2log\left(\frac{L_r^*(\delta(t_i))}{L_u^*(\delta(t_i)}\right)$$

- Will model this surface with a GP

Sequential design

- Criterion allows for simple sequential design strategy based on the Expected Improvement of Jones et al (1998) we have already covered
- Define the improvement as $I(t) = max(min\Delta(t) - \hat{\Delta(t)}, 0)$
- New trials are chosen so that $E(I(t))$ is maximized

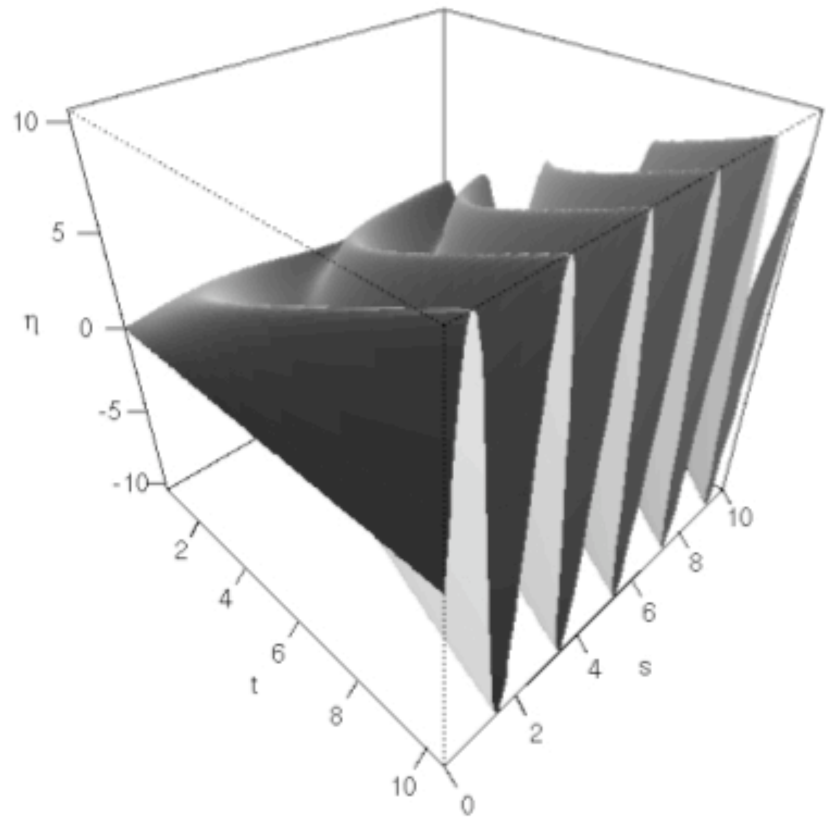
Toy example

- Consider the simple harmonic oscillator of an object with unit mass

- A simplified form of the solution to the differential equation is (*t* is the calibration parameter):

$$\eta(t) = t \times sin(ts)$$

Toy example



Toy example

- Simulate from this system with $(n_f = 20; n_c=20)$

$$s \in [0, 10] \qquad\qquad t \sim U[0, 11]$$

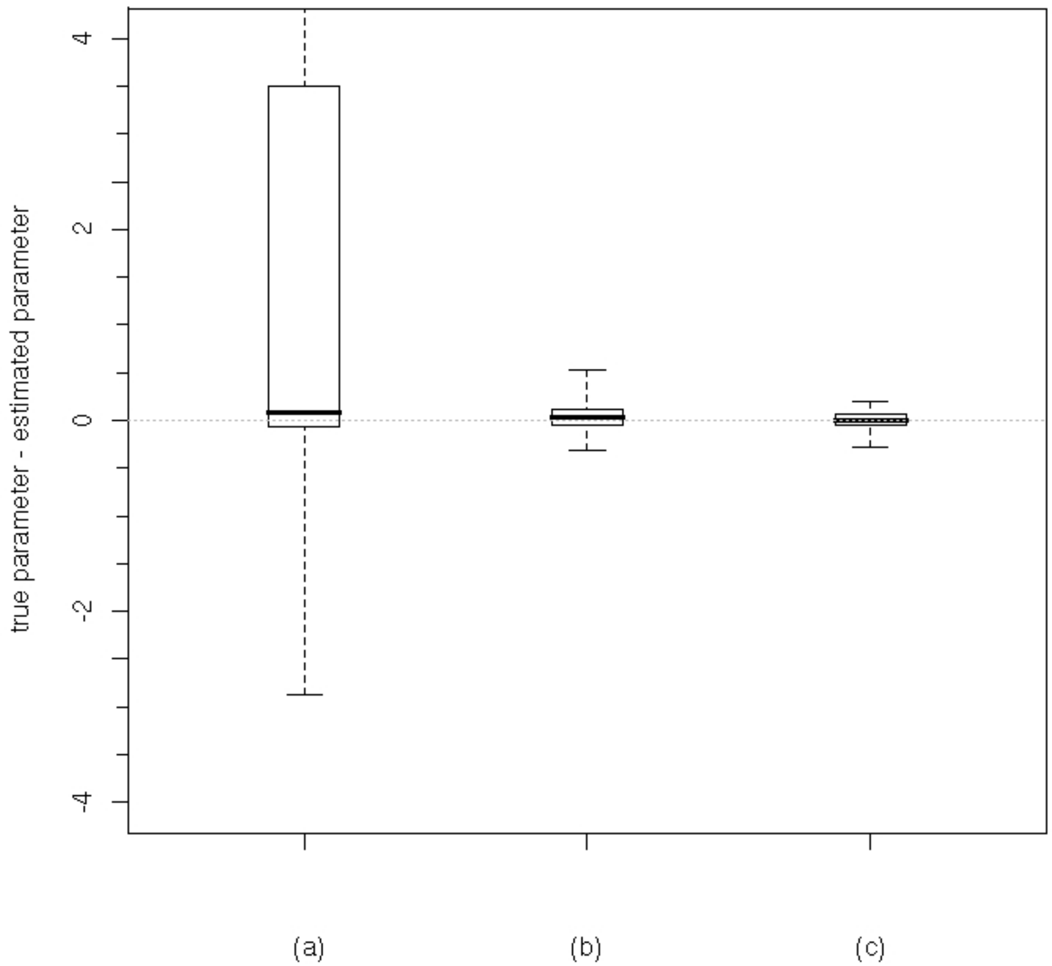
- Error for field observations:

$$\epsilon \sim N(0, \rho Var(\eta(\theta)))$$

- Did this 1000 times, each time applying the estimation method

$$\rho = 0.25$$

Toy example



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Back to LFM

- The LFM model has three inputs
- 20 simulations from the deterministic computer model
- Two output fields: flux and energy

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Back to LFM