Análise Estatística de Simuladores
Lecture 4: Calibration

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Contents

This lecture is all about calibration.

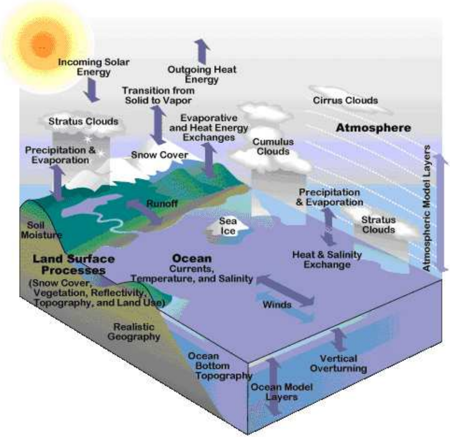
1. Calibration
   - What, why, when
   - Approaches
2. The concept of model error
   - Kennedy and O'Hagan 2001 framework,
   - Toy example: freefall
3. Example: UVic climate model

Calibration

For forwards models we specify parameters θ and i.c.s and the model generates output $\mathcal{D}_{sim}$. Usually, we are interested in the inverse-problem, i.e., observe data $\mathcal{D}_{field}$, want to estimate parameter values.

Different terminology:

- Calibration
- Parameter estimation
- Inverse-problem
- Bayesian inference



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1. Scientific knowledge captured by the model, η
2. Empirical information contained in the data, $\mathcal{D}_{field}$
3. Expert opinion based upon experience.

We want to combine all three sources to produce the 'best' parameter estimates we can.

Calibration - why?

In physical experiments nature controls all the model parameters.

- e.g., if we drop a ball of the leaning tower of Piza, we do not have to specify what acceleration due to gravity is, nature sets $g = 9.81\text{ms}^{-2}$ for us.

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- It is only if we run the model at a 'true' (or optimal) value $\hat{\theta}$ that we will predict the behaviour of the physical system being modelled.
- For example, if we model an object falling from the tower of Piza, but use $g = 1\text{ms}^{-2}$ in our computer model, we will produce very poor predictions.

Calibration - when?

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- an error model relating the model to the system.

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We may wish to calibrate if we want to

- Predict future behaviour
- Find physical values of unknown parameters
- Reduce and estimate the appropriate degree of uncertainty about our predictions

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     $$\mathcal{D}_{field} = \eta(\hat{\theta}) + e$$

     where $e \sim N(0, \sigma^2_{obs})$ then

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3. General ad hoc approaches
    - For example, choosing θ to minimize the sum of squares difference between the data and the model prediction, i.e., minimize

      $$S = \sum_i (D_i - \eta_i(\hat{\theta}))^2$$

      or some other measure.

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- All uncertainty quantities θ can be given distributions $\pi(\theta)$ that represent our (an experts?) uncertainty about the value - this doesn't mean that they are random quantities, just that we don't know their value.
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  - Even unknown function will be described by probability distributions across a class of unknown functions
- Bayesian approach uses the principle of conditionality, and always (where possible) conditions on our data.

Bayesian Inference

The basics of Bayesian inference are very simple.

- If quantity θ is unknown we describe our uncertainty by prior distribution $\pi(\theta)$.
- Suppose we have data D from model $\pi(D|\theta)$
- Then conditional on observing this data, our posterior distribution is

$$\pi(\theta|D) = \frac{\pi(\theta)\pi(D|\theta)}{\pi(D)}$$

In general we just use the relationship

$$\text{posterior } \propto \text{prior} \times \text{likelihood (model)}$$

Given a model and prior the entire Bayesian statistical approach is fully specified. In practice, computational difficulties make life difficult, and we must resort to Monte Carlo methods.

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- i.e., there is 95% posterior probability that $\theta \in [\theta_l, \theta_u]$ with θ_{MAP} the most likely value.

Model error

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This type of calibration is assuming a **perfect model hypothesis** - i.e.,

that our model is capable of exactly reproducing reality.

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When can we interpret the value found for θ as a physical value?

- If the model is a perfect representation of the system
- When the model is imperfect, but we have a description (that we believe) of the discrepancy between model and system.

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  - y is our data

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- solving the inverse problem $y = \eta(\theta) + e$ may not give sensible results.
  - e is measurement error
  - $\eta(\theta)$ is our computer model
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- If the model is imperfect, the residuals $D - \eta(\theta)$ will be correlated, even if the real measurement error process is iid.

Can we

- account for the error?
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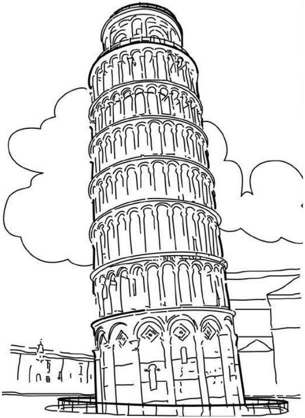
Kennedy and O'Hagan (2001) suggested we introduce reality ζ into our statistical inference

- Reality $\zeta = \eta(\hat{\theta}) + \delta$, the best model prediction plus model error $\delta(x)$.
- Data $y = \zeta + e$ where e represents measurement error

Toy Example: Freefall



Consider an experiment where we drop a weight from a tower and measure its position x_t every Δt seconds.

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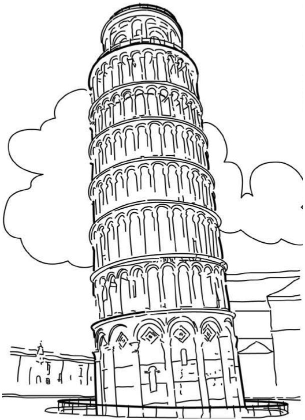

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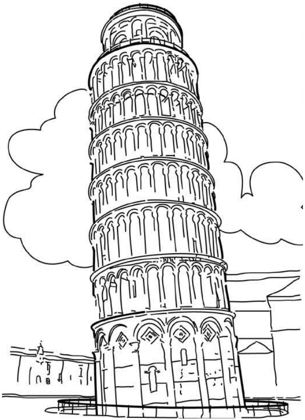

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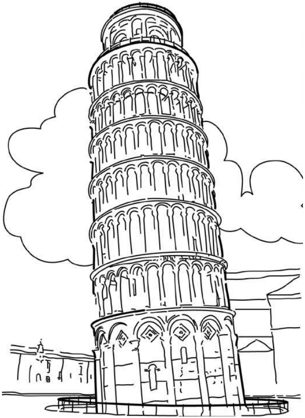

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$$\frac{\mathrm{dv}}{\mathrm{dt}} = g - kv$$

gravity minus a Stokes' drag term for air-resistance.

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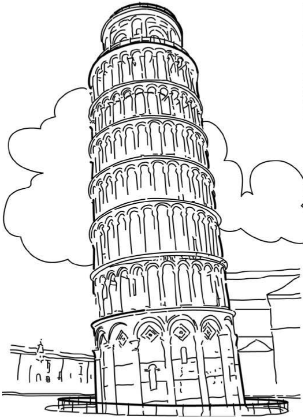

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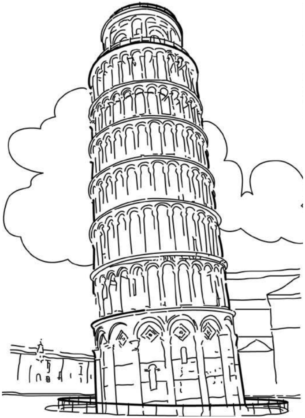
This gives single time step updates

$$\begin{aligned}
x_{t+1} &= \zeta_x(x_t, v_t) \\
&= x_t + \frac{1}{k}(\frac{g}{k} - v_t)(\mathrm{e}^{-\mathrm{k}\Delta \mathrm{t}} - 1) + \frac{\mathrm{g}\Delta \mathrm{t}}{\mathrm{k}} \\
v_{t+1} &= \zeta_x(x_t, v_t) \\
&= (v_t - \frac{g}{k})\mathrm{e}^{-\mathrm{k}\Delta \mathrm{t}} + \frac{\mathrm{g}}{\mathrm{k}}
\end{aligned}$$

Toy Model Error Example: Freefall



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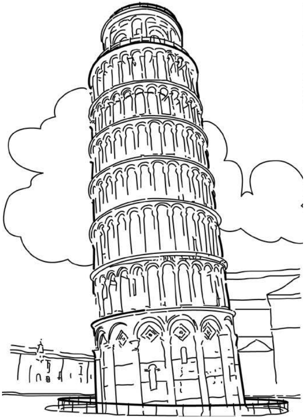

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Which gives predictions at the observations of

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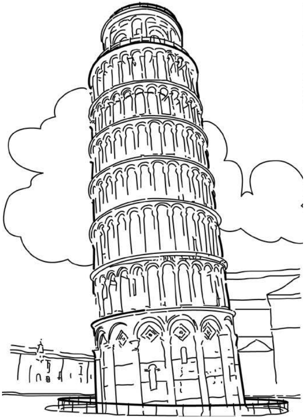

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Because we have ignored air-resistance in our model, we have model error!

Model Error Term

In this toy problem, the true discrepancy function can be calculated.

- It is a two dimensional function

  $$\delta = \begin{pmatrix} \delta_x \\ \delta_v \end{pmatrix} = \zeta - \eta$$

  giving the difference between the reality and the prediction from our model.

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If we expand $\mathrm{e}^{-\mathrm{k}\Delta\mathrm{t}}$ to second order we find

$$\delta(x, v, t) = \begin{pmatrix} \delta_x \\ \delta_v \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{-gk(\Delta t)^2}{2} \end{pmatrix} - v_t \begin{pmatrix} \frac{k(\Delta t)^2}{2} \\ k\Delta t(1 - \frac{k\Delta t}{2}) \end{pmatrix}$$

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This is solely a function of v.

- Note, to learn δ we only have the observations $D_1, \ldots, D_T$ of $x_1, \ldots, x_T$ - we do not observe v.

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We could use something very flexible and generic, such as a Gaussian process (which can fit any functional form)

$$\delta(x, v, t) \sim GP(m(v), \sigma^2 c(v, v'))$$

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- See Wilkinson and Oakley 2010 for a method to estimate a functional form for δ.

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- Argue that $\eta(\cdot, \hat{\theta})$ and $\delta(\cdot)$ are independent. Kennedy and O'Hagan 2001 use Gaussian processes to model both the model η and the error δ.

Calibrating the UVic Climate Model

Example: UVic Earth System Climate Model

With Nathan Urban (Penn State)

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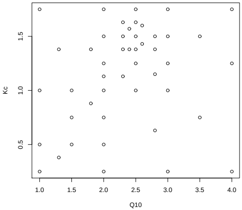
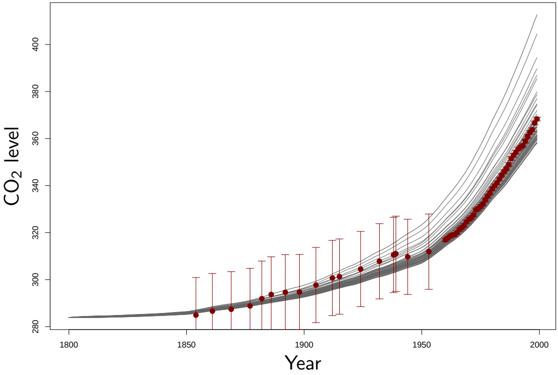
- Output: time-series of CO_2 values, cumulative carbon flux measurements, ...
- 48 member ensemble, grid design D, output $\mathcal{D}_{sim}$ ($48 \times n$).



The U.Vic Model

- 60 field measurements, $\mathcal{D}_{field}$:
  - 40 instrumental CO_2 measurements from 1960-1999
  - 17 ice core CO_2 measurements
  - 3 cumulative ocean carbon flux measurements



Multivariate Models

Wilkinson 2010

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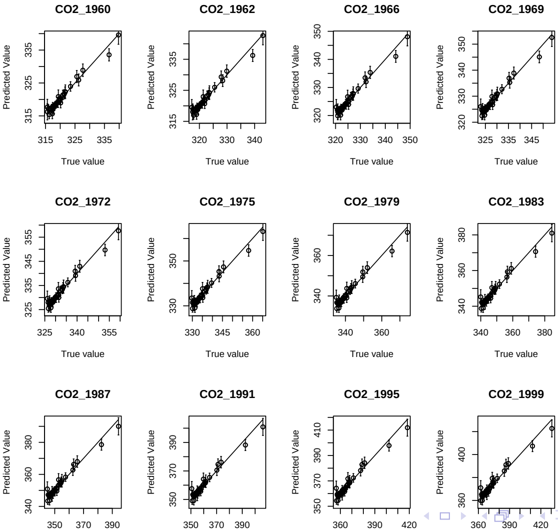
$$
\begin{tikzcd}
\Theta \arrow[rr, "\eta(\cdot)"] \arrow[dr, "\eta^{pc}(\cdot)"'] & & \mathcal{Y} \arrow[dl, shift right, "\mathrm{PCA}"'] \\
& \mathcal{Y}^{pc} \arrow[ur, shift right, "\mathrm{PCA}^{-1}"'] &
\end{tikzcd}
$$

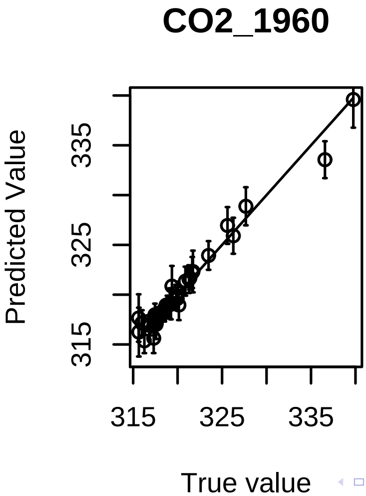
Emulator Diagnostics

Cross-validation plots, instrumental data only (1960:1999), using 3PCs (99.2% of variance explained)



Emulator Diagnostics

Cross-validation plots, instrumental data only (1960), using 3PCs (99.2% of variance explained)

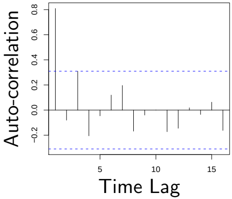


UVic Model Discrepancy

The calibration framework used is:

$$\mathcal{D}_{field}(t) = \eta(\theta, t) + \delta(t) + e(t)$$

The model predicts the underlying trend, but real climate fluctuates around this. We model



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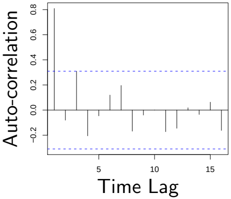

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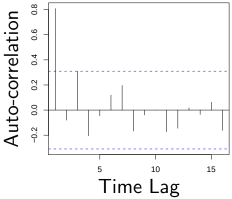
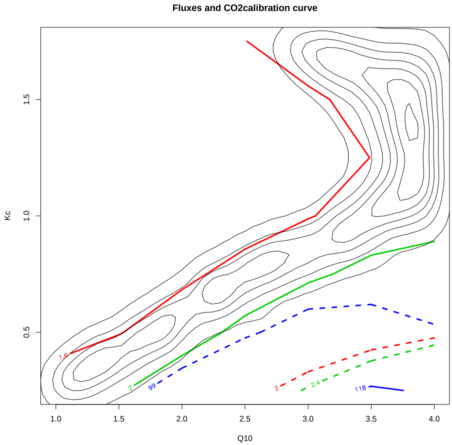
- Measurement error as heteroscedastic independent random noise $e(t) \sim N(0, \lambda(t))$.



Results

After several hours of MCMC (Metropolis-within-Gibbs - see lecture 6) we find



The data are equally well explained by a range of parameter values.

Summary

- Calibration is the process of estimating parameters from empirical observations
- The Bayesian approach is ideal for measuring and summarizing any uncertainties.
- When calibrating models it is important to account for the existence of model error
  - we need a statistical relationship between the computer simulator output and the physical system.
- Accounting for model error is a relatively new idea in statistics. See Goldstein *et al.* 2009, Beven 2006, and Poole *et al.* 2000, for a selection of other approaches to calibration and model error.

References

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- MUCM toolkit, available at `http://mucm.aston.ac.uk/MUCM/MUCMToolkit/`