Complex systems: Accounting for model limitations

Jonathan Rougier

Department of Mathematics University of Bristol, UK

Research Students' Conference, Warwick, Monday 12 April 2010

Illustration: the Greenland ice-sheet



Simplest interesting example

Conditional on θ :

$$egin{aligned} x_0 &\sim \pi_{x_0}(\cdot; heta) & ext{(init. cond. unc.)} \ x_t &= g(x_{t-1}, \omega_t; heta) & ext{(state eqn.)} \ y_t &= f(x_t; heta) +
u_t & ext{(obs. eqn.)} \end{aligned}$$

where

$$\omega_t \stackrel{ ext{iid}}{\sim} \mathsf{N}(0,I)$$
 (structural uncertainty) $u_t \stackrel{ ext{iid}}{\sim} \mathsf{N}(0,v^2)$ (measurement unc.)

and then let $\theta \sim \pi_{\theta}(\cdot)$, to account for parametric uncertainty. The functions f and g are given, likewise the measurement uncertainty standard deviation, v.

Sampling from $\{x_0, x_1, \dots, x_T, \theta\} \mid \{y_1, \dots, y_T\}$ "intractable and unsolved" (C. Andrieu)



The calibration problem

To learn about θ , typically by summarising samples from the distribution $\pi(\theta \mid \mathbf{y})$, where $\mathbf{y} = (y_1, \dots, y_T)$. We'll treat x_0 as known, for simplicity.

▶ Ideally, we would run an MCMC chain with proposal $q(\theta \rightarrow \theta')$ and acceptance probability

$$lpha(heta, heta') = 1 \wedge rac{\pi(\mathbf{y} \mid heta') \, \pi(heta')}{\pi(\mathbf{y} \mid heta) \, \pi(heta)} \, rac{q(heta'
ightarrow heta)}{q(heta
ightarrow heta')}.$$

The calibration problem

To learn about θ , typically by summarising samples from the distribution $\pi(\theta \mid \mathbf{y})$, where $\mathbf{y} = (y_1, \dots, y_T)$. We'll treat x_0 as known, for simplicity.

ldeally, we would run an MCMC chain with proposal q(heta o heta') and acceptance probability

$$\alpha(\theta, \theta') = 1 \wedge \frac{\pi(\mathbf{y} \mid \theta') \, \pi(\theta')}{\pi(\mathbf{y} \mid \theta) \, \pi(\theta)} \, \frac{q(\theta' \to \theta)}{q(\theta \to \theta')}.$$

▶ The catch is that we need to integrate out ω in order to evaluate $\pi(\mathbf{y} \mid \theta)$:

$$\pi(\mathbf{y} \mid heta) = \int \pi(\mathbf{y} \mid oldsymbol{\omega}, heta) \, \pi(oldsymbol{\omega}) \, \mathbf{d}oldsymbol{\omega}$$

where
$$\boldsymbol{\omega} = (\omega_1, \dots, \omega_T)$$
 — ouch!!



The calibration problem (cont.)

In a picture . . .

 $(\omega \mid \theta)$ -space (high-dimensional)

 θ -space (low-dimensional)

The calibration problem (cont.)

We could approximate this tricky density with an Importance Sampler estimate

$$ilde{\pi}(\mathbf{y} \mid heta) = extstyle N^{-1} \sum_{i=1}^{N} rac{\pi(\mathbf{y} \mid oldsymbol{\omega}^i, heta) \, \pi(oldsymbol{\omega}^i \mid heta)}{q_{\omega}(oldsymbol{\omega}^i; \mathbf{y}, heta)} \quad oldsymbol{\omega}^i \stackrel{ ext{iid}}{\sim} q_{\omega}(\cdot; \mathbf{y}, heta),$$

but how would this affect the MCMC chain?

The calibration problem (cont.)

 We could approximate this tricky density with an Importance Sampler estimate

$$ilde{\pi}(\mathbf{y} \mid heta) = N^{-1} \sum_{i=1}^{N} rac{\pi(\mathbf{y} \mid \omega^{i}, heta) \, \pi(\omega^{i} \mid heta)}{q_{\omega}(\omega^{i}; \mathbf{y}, heta)} \quad \omega^{i} \stackrel{ ext{iid}}{\sim} q_{\omega}(\cdot; \mathbf{y}, heta),$$

but how would this affect the MCMC chain?

- ▶ Mark Beaumont's (2003) result. The θ -marginal of the MCMC equilibrium distribution with $\pi(\mathbf{y} \mid \theta)$ replaced by $\tilde{\pi}(\mathbf{y} \mid \theta)$ is $still\ \pi(\theta \mid \mathbf{y})$, for all $N \geq 1$.
 - 1. One has to accept/reject $\{\omega^i\}$ along with θ .
 - 2. Small *N* normally implies a sticky chain.
- ► The general result was stated by Andrieu et al (2007): the θ -marginal is $\pi(\theta \mid \mathbf{y})$ for any unbiased estimator of $\pi(\mathbf{y} \mid \theta)$.



The stochastic van der Pol oscillator

Has a 'slow' response x and a 'fast' response x', related as

$$x'' + x' + (\alpha - x^2)x = \sigma x dW,$$

where W is a Brownian motion. It is the basis for several phenomenological models of glacial cycles, where x is 'ice volume' and x' is 'temperature' (or, effectively, 'CO₂'). Here $\theta = (\alpha, \sigma)$.

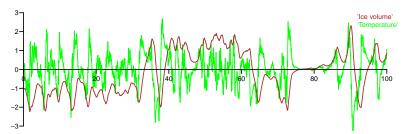
The stochastic van der Pol oscillator

Has a 'slow' response x and a 'fast' response x', related as

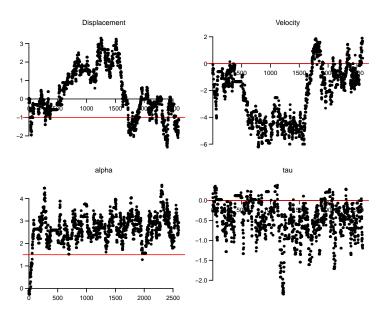
$$x'' + x' + (\alpha - x^2)x = \sigma x dW,$$

where W is a Brownian motion. It is the basis for several phenomenological models of glacial cycles, where x is 'ice volume' and x' is 'temperature' (or, effectively, 'CO₂'). Here $\theta = (\alpha, \sigma)$.

One realisation:



The evidence (24 hours)



Summary

- In inference for environmental systems, model limitations require us to account for both parametric and structural uncertainty.
- The generic problem for dynamical systems is therefore non-linear data assimilation with uncertain static parameters.
- ▶ Learning about the parameters involves integrating out the high-dimensional state vector; this can be done 'exactly' (in the MCMC sense) using Beaumont's result.
- ▶ Recent developments not mentioned here have generalised this approach (e.g. pseudo-marginal approach, particle-MCMC).
- ► This is an exciting time to be working as a statistician in environmental science!