Bayesian Linear Uncertainty Analysis for complex computer models

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Camila’s talk (following) will apply these ideas, for a climate model which is simple but has interesting behaviour.
Examples

**Oil reservoir** Simulator inputs are properties of the reservoir (permeabilities, porosities, faults). Outputs are behaviour at wells (gas/oil production, water cut). The aim is to develop efficient production schedules, determine whether and where to sink new wells, and so forth.
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**Climate change**  Global climate simulators are used to assess likely effects of human intervention upon future climate behaviour. Inputs are physical constants describing the evolution of climate in response to properties like CO2 forcing. Outputs are features of global future climate. Aims are scientific - to learn about large scale interactions which determine climate - and practical, as such simulators provide evidence for the need to change our behaviour before irreversible changes are set into motion.
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(ix) **decision uncertainty** (to use the model to influence real world outcomes, we need to relate things in the world that we can influence to inputs to the simulator and through outputs to actual impacts. These links are uncertain.)
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- the optimal assignment of any decision inputs, $d$, in the model.

[In a climate model, $y_h$ might correspond to historical climate outcomes over space and time, $y$ to current and future climate, and the “decisions” might correspond to different policy relevant choices such as carbon emission scenarios.]
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If observations, \( z \), are made without error and the model is perfect reproduction of the system, we can write \( z = f_h(x^*) \), invert \( f_h \) to find \( x^* \), learn about all future components of \( y = f(x^*) \) and choose decision elements of \( x^* \) to optimise properties of \( y \).
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In practice, the observations $z$ are made with error, and model is not the same as physical system so we must separate the uncertainty representation into two relations and carry out statistical inversion/optimisation:

$$z = y_h \oplus e, \ y = f(x^*) \oplus \epsilon$$

where $e, \epsilon$ have some appropriate probabilistic specification, possibly involving parameters which require estimation.

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RAPID-WATCH

What are the implications of RAPID-WATCH observing system data and other recent observations for estimates of the risk due to rapid change in the MOC? In this context risk is taken to mean the probability of rapid change in the MOC and the consequent impact on climate (affecting temperatures, precipitation, sea level, for example). This project must:

* contribute to the MOC observing system assessment in 2011;
* investigate how observations of the MOC can be used to constrain estimates of the probability of rapid MOC change, including magnitude and rate of change;
* make sound statistical inferences about the real climate system from model simulations and observations;
* investigate the dependence of model uncertainty on such factors as changes of resolution;
* assess model uncertainty in climate impacts and characterise impacts that have received less attention (eg frequency of extremes).

The project must also demonstrate close partnership with the Hadley Centre.
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The adjusted or Bayes linear expectation and variance for $B$ given $D$ are

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E_D[B] = E(B) + \text{Cov}(B, D)\text{Var}(D)^{-1}(D - E(D)),
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In practice, we may choose a mix of expectation and probability based methods. Here our focus is on the expectation based methodology.
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Problems arise when we forget these simplifications and confuse the analysis of the model with the corresponding analysis for the physical system itself.
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One of the simplest, and most popular, approaches is to suppose that there is an appropriate choice of system properties $x^*$ (currently unknown), so that $f(x^*)$ contains all the information about the system:

$$y = f(x^*) \oplus \epsilon$$

where $\epsilon$, the model or structural discrepancy, has some appropriate probabilistic specification, possibly involving parameters which require estimation, and is taken to be independent of $f, x_0, e$. 
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Careful structural uncertainty assessment is crucial. Two aspects:

(i) **Internal discrepancy**: aspects we assess by simulator experiments
(ii) **External discrepancy**: inherent limitations of modelling process
Reification

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We can’t evaluate $f^*$, but we can “emulate” it.
## Relating the model and the system

<table>
<thead>
<tr>
<th>Model evaluations</th>
<th>Actual system</th>
<th>System observations</th>
</tr>
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</table>

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3. We link the ‘best’ evaluation to the actual system
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2. We link the evaluations to the notion of a ‘best’ evaluation.

3. We link the ‘best’ evaluation to the actual system.

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In such cases, $f$ must be treated as uncertain for all input choices except the small subset for which an actual evaluation has been made.
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Therefore, we must construct a description of the uncertainty about the value of $f(x)$ for each $x$.

Such a representation is often termed an emulator of the function - the emulator both suggests an approximation to the function and also contains an assessment of the likely magnitude of the error of the approximation.
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Such a representation is often termed an emulator of the function - the emulator both suggests an approximation to the function and also contains an assessment of the likely magnitude of the error of the approximation.

We use the emulator either to provide a full joint probabilistic description of all of the function values (full Bayes) or to assess expectations variances and covariances for pairs of function values (Bayes linear).
Form of the emulator

We may represent beliefs about component $f_i$ of $f$, using an emulator:

$$f_i(x) = \sum_j \beta_{ij} g_{ij}(x) \oplus u_i(x)$$
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where $B = \{\beta_{ij}\}$ are unknown scalars, $g_{ij}$ are known deterministic functions of $x$, $u_i(x)$ is a weakly second order stationary stochastic process, with (for example) correlation function

$$\text{Corr}(u_i(x), u_i(x')) = \exp\left(-\left(\frac{\|x-x'\|}{\theta_i}\right)^2\right)$$

$Bg(x)$ expresses global variation in $f$. $u(x)$ expresses local variation in $f$. 
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We fit the emulators, given a collection of carefully chosen model evaluations, using our favourite statistical tools - generalised least squares, maximum likelihood, Bayes - with a generous helping of expert judgement.
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We need careful (multi-output) experimental design to choose informative model evaluations, and detailed diagnostics to check emulator validity.
Linked emulators

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\[
f'_i(x) = \sum_j \beta'_{ij} g_{ij}(x) \oplus u'_i(x)
\]

We use this form as the prior for the emulator for \( f_i(x) \).

Then a relatively small number of evaluations of \( f'_i(x) \), using relations such as

\[
\beta_{ij} = \alpha_i \beta'_{ij} + \gamma_{ij}
\]

lets us adjust the prior emulator to an appropriate posterior emulator for \( f_i(x) \).
History matching

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A conceptually simple alternative is “history matching”, i.e. finding the collection
of all input choices \(x\) for which you judge the match of the model to the data,
\[\|z - f_h(x)\|\] to be acceptably small, using some “implausibility measure”
\(I(x)\) based on a natural probabilistic metric, accounting for emulator
uncertainty, condition uncertain, structural discrepancy, observational error etc.
Using the emulator we can obtain, for each set of inputs $x$, the mean and variance, $E(f_h(x))$ and $\text{Var}(f_h(x))$. 
History matching via Implausibility

Using the emulator we can obtain, for each set of inputs $x$, the mean and variance, $E(f_h(x))$ and $\text{Var}(f_h(x))$.

As $z_i = y_i + \epsilon_i$, $y_i = f_i(x^*) + \epsilon_i$,

if $x = x^*$, then

$\text{Var}(z_i - E(f_i(x))) = \text{Var}(f_i(x)) + \text{Var}(\epsilon_i) + \text{Var}(\epsilon_i)$. 
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$\text{Var}(z_i - E(f_i(x))) = \text{Var}(f_i(x)) + \text{Var}(\epsilon_i) + \text{Var}(\epsilon_i)$.

We can therefore calculate, for each output $f_i(x)$, the “implausibility” if we consider the value $x$ to be the best choice $x^*$, which is the standardised distance between $z_i$ and $E(f_i(x))$, which is

$$I_{(i)}(x) = |z_i - E(f_i(x))|^2 / [\text{Var}(f_i(x)) + \text{Var}(\epsilon_i) + \text{Var}(\epsilon_i)]$$

[Large values of $I_{(i)}(x)$ suggest that it is implausible that $x = x^*$.]
Using Implausibility measures

The implausibility calculation can be performed univariately, or by multivariate calculation over sub-vectors. The implausibilities are then combined, such as by using $I_M(x) = \max_i I_i(x)$, and can then be used to identify regions of $x$ with large $I_M(x)$ as implausible, i.e. unlikely to be good choices for $x^*$. 
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over such sub-regions and repeating the analysis.
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This process is a form of iterative global search aimed at finding all choices of $x^*$ which would give good fits to historical data.
The mean and variance of $f(x)$ are obtained from the mean function and variance function of the emulator $f$ for $F$. Using these values, we compute the mean and variance of $f^* = f(x^*)$ by first conditioning on $x^*$ and then integrating out $x^*$ (over the space remaining after the history match).
Forecasting

The mean and variance of $f(x)$ are obtained from the mean function and variance function of the emulator $f$ for $F$. Using these values, we compute the mean and variance of $f^* = f(x^*)$ by first conditioning on $x^*$ and then integrating out $x^*$ (over the space remaining after the history match). Given $\mathbb{E}(f^*)$, $\text{Var}(f^*)$, and the model discrepancy, $\epsilon$ and sampling error $e$ variances, it is now straightforward to compute the joint mean and variance of the collection $(y, z)$ (as $y = f^* + \epsilon$, $z = y_h + e$).
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We now evaluate the adjusted mean and variance for $y_p$ adjusted by $z$ using the Bayes linear adjustment formulae. This analysis is tractable even for real time control of large systems under complex forms of reification.
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(When the forecast variance is large, then we have methods to improve forecast accuracy.)
Concluding comments

To assess our uncertainty about complex systems, it is enormously helpful to have an overall (Bayesian) framework to unify all of the sources of uncertainty.
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In particular, Bayes (linear) multivariate, multi-level, multi-model emulation, careful structural discrepancy modelling, iterative history matching and forecasting gives a great first pass treatment for most large modelling problems.
Concluding comments

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In particular,
Bayes (linear) multivariate, multi-level, multi-model emulation,
careful structural discrepancy modelling
iterative history matching and forecasting
gives a great first pass treatment for most large modelling problems.

Great resource: the Managing Uncertainty in Complex Models web-site http://www.mucm.ac.uk/ (for references, papers, toolkit, etc.)

[MUCM is a consortium of U. of Aston, Durham, LSE, Sheffield, Southampton - with Basic Technology funding. Now mutated into the MUCM community.]
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