Methodology Panel

Development, Assessment and Utilization of Complex Computer Models

Kickoff Workshop

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Panelists

Michael Goldstein  (U. Durham)
Tony O’Hagan  (U. Sheffield)
Henry Wynn  (London School of Economics)
Susie Bayarri  (U. Valencia)
Calibration/Validation/Prediction

often for statisticians $\sim$ a CompMod can be treated as a black-box:

- feed it with inputs $z = (x, u)$ (large dimension):
  - $x \sim$ controllable
  - $u \sim$ unknown parameters (tuning, calibration)
- produces output $y^M(x, u)$ (expensive)
- CompMod $y^M(x, u) \sim$ surrogate of ‘reality’ $y^R(x)$
  (reality ‘knows’ $u$)
- Model is run at inputs $(x, u) \in D^M \sim y^M$
  Field data is collected at inputs $x \in D^F \sim y^F$
- Calibration $\sim$ learn about $u$
  Prediction $\sim$ learn about $y^R(x)$
- Most important: Take into account all uncertainties:
  - Give $\hat{u}$ and uncertainty (confidence) bands
  - Give $\hat{y}^R(x)$ and uncertainty (confidence) bands
(Laura Swiler’s talk)
• Validation $\leadsto$ is $y^M$ useful for the intended use ??
  (see also Wendy Parker and Laura Swiler’s talks)

  Note: Usual question “is the model correct?” not good

• Validation $\approx$ learn about $bias = reality - model$

• useful framework to achieve these goals:

$$y^R(x) = y^M(x, u) + b_u(x)$$
$$y^F(x) = y^R(x) + \epsilon$$

+ Bayes (incorporates uncertainties)
• function $b_u$ unknown $\sim$ a prior on it: $\pi(b_u \mid \theta^b)$

• often $y^M$ very slow $\sim$ unknown function (known only at some few inputs) $\sim$ a prior on it: $\pi(y^M \mid \theta^M)$ (when 'fitted' $\sim$ emulator, surrogator, fast simulator, meta-model, ...)

• from joint posterior one gets:
  – posterior of $y^M$ $\sim$ 'emulator'
  – posterior of $u$ $\sim$ calibration
  – posterior of $y^R$ $\sim$ prediction
  – posterior of $b_u$ $\sim$ validation

• basic framework seems simple; but lots of issues.
• **Design** \( \sim \) choose \( D^M, D^F \). Should ‘extreme’ values of \( u \) be used? How do we interpret run failures? can we identify ‘unfeasible’ regions of \((x, u)\) values?

• **Surrogator/fast simulator** (non parametric prior on \( y^M \)) usually \( \sim \) ‘fitted’ with little data
  – GASP (Gaussian separable processes) most popular
  – Other Processes: Lee, Morris, Wilkinson, Wolpert, ...
  – Other (statistical) possibilities? (looking inside the ‘black box’?) (D. Wilkinson talk)
  – Simpler/rougher models? (D. Wilkinson talk)

• What to do with **HUGE input spaces**? (GASP does not scale to large dimensions) more research needed.
• High correlation among parameters; **Confounding** between \( u \) and \( b_u \) (and others)
  – How to report individual inferences?
  – How to interpret them?
  – Note: Prediction of reality is not affected

• Problem aggravated when \( x \) is also uncertain \( \sim \) more parameters and more confounding

• Lots of hyperparameters \( (\theta^M, \theta^b, \text{variances, means, . . .}) \)
  – Which priors to use for *automatic* use?
  – Because of confounding, many will have to be proper: which ones should not be automatic? (incorporate external information)
• **Functional outputs:** a couple possibilities
  
  – Add (discretized) ‘time’ as another input (and do something clever with GASP)
  
  – Expand function (e.g. wavelet basis) and apply methodology independently to each coefficient $\sim$ correlated errors?
  
  – Tempor-spacial models?
- Multivariate outputs
  - Multivariate priors
    Some GASP generalizations; more work needed
  - Hierarchical models:
    \[ y_1^M, \ldots, y_k^M \text{ related} \]
    \[ b_{u1}, \ldots, b_{uk} \text{ related} \]
    * What kind or relation? how strong?
    * priors? which ones need external information?

(see also Gang Han’s talk)
• Prediction for untried (or altered) scenarios (L. Swiler)
  – scheme works well in interpolation
  – how to extrapolate bias?
  – additive vs. multiplicative bias? others?
  – hierarchical models?

• **MCMC.** Poor identifiability results in serious numerical problems. Lots of work is needed here. (D. Wilkinson talk)

• Deliverable *Software* ⇒ automatic enough ⇒ needs
  – most of the priors ⇒ ‘automatic’
  – MCMC also ‘automatic’

(L. Swiler’s talk)
• **Approximations?**

With tons and tons of (highly correlated/confounded) parameters, and little external prior information about most of them \(\sim\) full Bayes might not be feasible \(\sim\) approximations?

- Which parameters are ‘safest’ to be MLE-ed? impact?
- ‘Modular’ approaches?: learn about prior on \(y^M\) based only on \(y^M\); learn about \(u\), variances and everything else based on all data \(y^M, y^F\)

• **DAU of stochastic computer models**

- ‘emulators’ for SCM
- build stochasticity into CompMod (D. Wilkinson, M.West)
in summary ...

- huge, difficult problems
- way too little data (model runs, and/or field data) for the complexity of the models

... great challenges for working groups!

but there is only so much that we can do ;(