Uncertainty Quantification

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What is Uncertainty Quantification?

The statistical analysis of complex numerical models

INI programme 2 years ago

In the UK ATI, Exeter, Durham, Sheffield, Southampton and UCL + others

Keen to help

No response from RAMP

(Applied Maths groups do similar, but different problems)

Uncertainty in Numerical Models

We have some model

$$y = f(x)$$

$f(x)$ may be deterministic or stochastic

We treat $f(x)$ as a 'black box'

Uncertainty can be aleatoric or epistemic

The stochastic model has aleatoric uncertainty

All our methods have stochastic versions

Epistemic uncertainty:

Unknown inputs - parameters, initial conditions, boundary conditions

Structural uncertainty -

Difference between simulator and reality

Approximations, parameterisations, numerics,. . .

Why should I care about uncertainty

Honesty

Reproducibility

Rigour

Helps us think about models

Ensembles of models

Hierarchies of models

Surrogates and Emulators

Traditional way to do UQ involves Monte Carlo, Markov Chain Monte Carlo, Quasi-Monte Carlo type methods

But what if the numerical model (simulator) is expensive to run

Use a cheap surrogate model

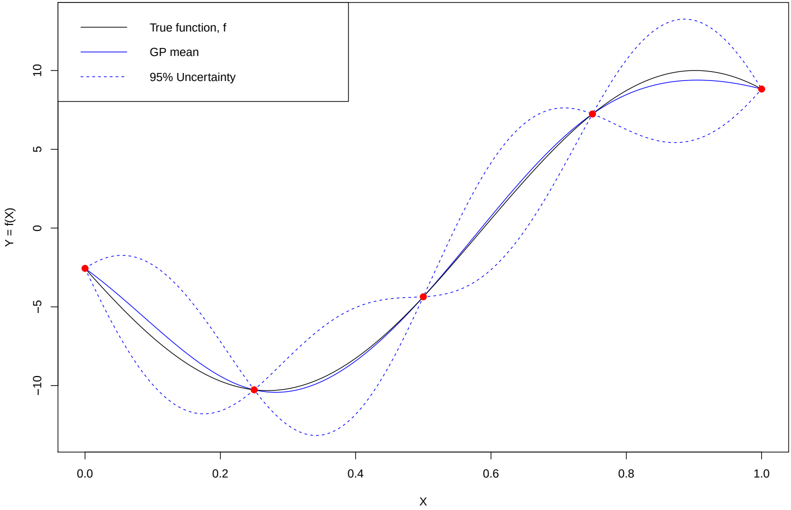
$$y \approx \tilde{f}(x)$$

Emulator = surrogate + uncertainty

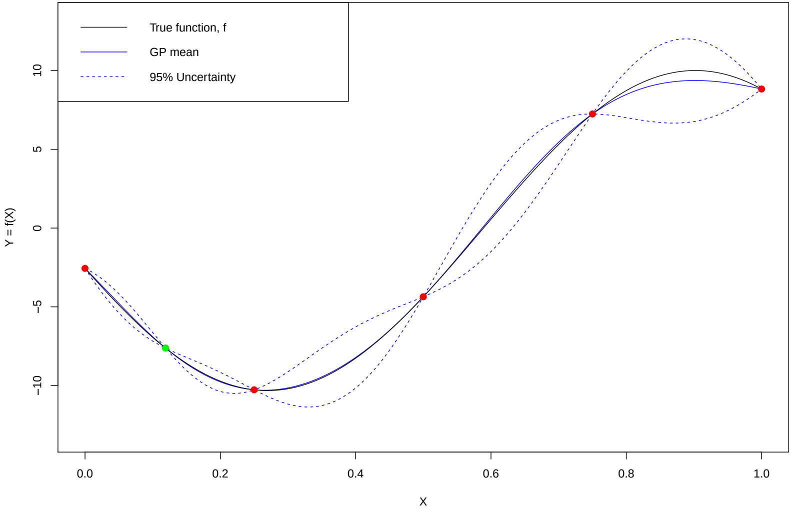
We use Gaussian Process emulators

(Does not assume the inputs or outputs have Gaussian distributions)

The Gaussian Process Emulator



The Gaussian Process Emulator - 2



Procedure

- Setup priors
- Design Experiment
- Run simulator ensemble
- Build emulator (Bayesian)
- Validate

What can I do when I have an emulator

- Prediction
- Sensitivity Analysis
- Uncertainty Analysis

Sensitivity Analysis

Which inputs are the simulator outputs sensitive to?

One at a time (main effects)?

Variance based sensitivity analysis (main effects + interactions)

Uncertainty Analysis

Put a joint pdf (prior) on the inputs

What is the statistical distribution of the outputs?

Monte Carlo with an emulator (balance of uncertainty)

In some special cases this can be done analytically

Calibration (tuning, estimation, inverse modelling)

Given some data what can we say about the simulator inputs (parameters)

Traditionally done by least squares, MLE, Bayes,. . .

But

Model Discrepancy

Our simulators are not the same as reality

(our data are not the same as reality either)

Fitting to the data without including a discrepancy terms leads to overfitting

Kennedy and O'Hagan

Kennedy and O'Hagan use two Gaussian processes: one is an emulator for the simulator the second fits the discrepancy

Good for prediction

Identifiability problems

History Matching

As an alternative to trying to find the best set of model inputs is to find all implausible sets of inputs

Set up an implausibility measure

$$I_{mp}(\theta) = \sqrt{\frac{(y_{obs} - E[\tilde{f}(x)])^2}{\sigma^2_{emul}(x) + \sigma^2_{obs} + \sigma^2_{discrep}}}$$

History Matching - 2

1 Run our simulator in a designed experiment

2 Build and validate a GP emulator

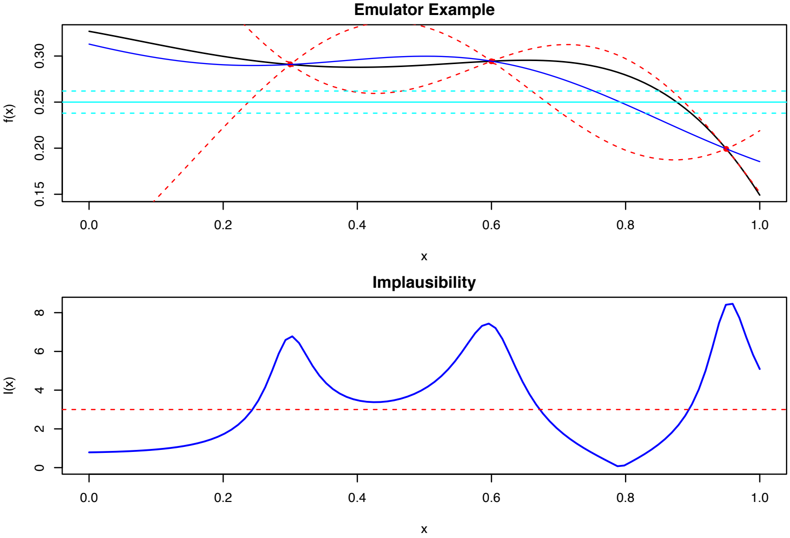
3 Calculate the implausibility

4 All points with implausibility > 3 are ruled implausible (Pukelsheim (1994))

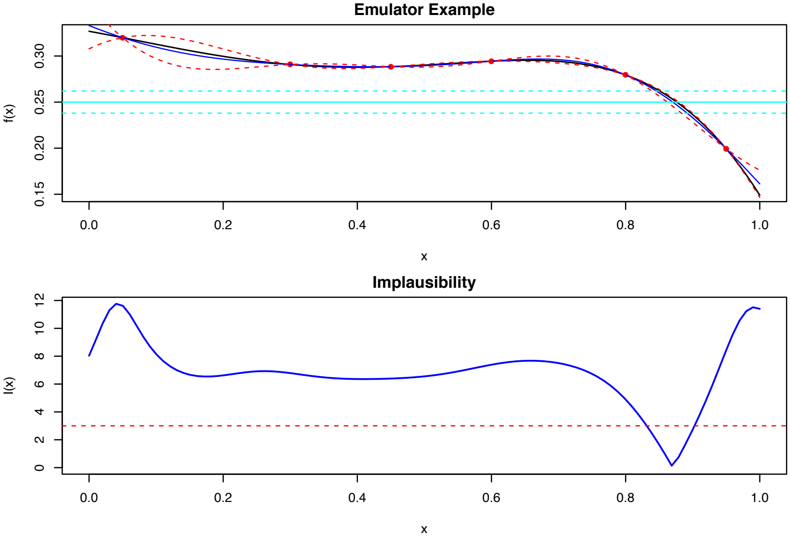
5 What remains is termed Not Ruled Out Yet (NROY) space

6 Repeat steps 1-5 in waves until we reach a stopping rule

History Matching - 3



History Matching - 4



Cardiac Model Example

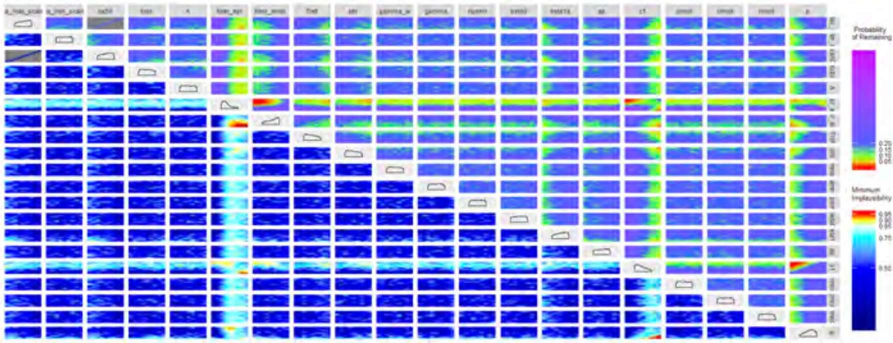
Model of the human heart

6 hour run time

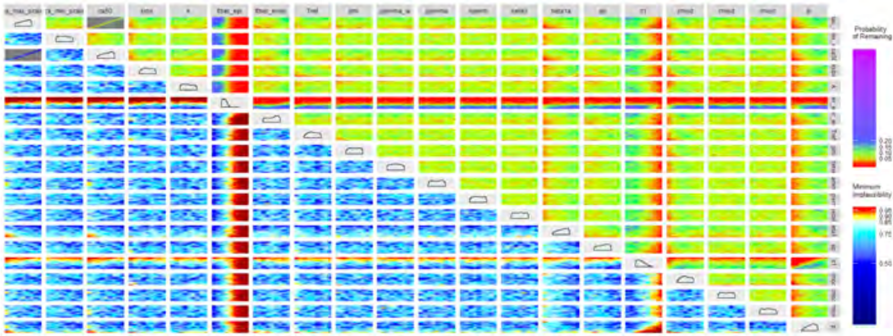
Preprocessing to reduce dimensionality

Initally $\sigma^2_{discrep} = 0$ NROY empty after first wave.

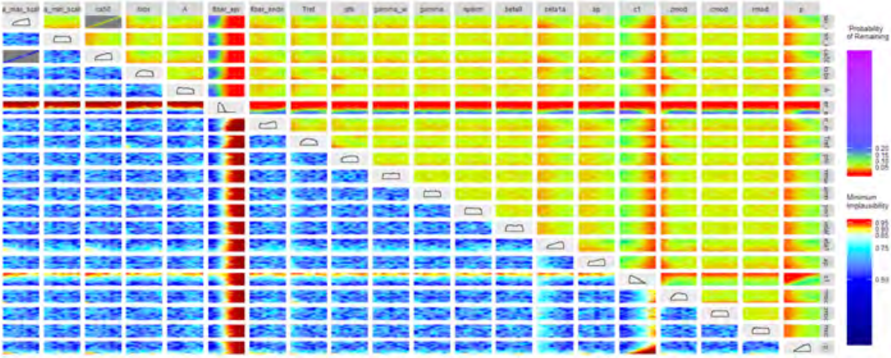
Wave 1 25% of space remains



Wave 2 6% of space remains



Wave 3 55% of space remains



Stopping Rules

NROY shrinks to some prespecified value and we do a K&OH calibration in this reduced space

NROY becomes so small we can effectively use it as a point estimate

NROY disappears completely. The simulator and the data are not compatible

NROY disappears

If the simulator and the data are incompatible NROY will go to zero (all points are implausible)

If you do classical calibration this will not be apparent. You will get the set of inputs closest to the data (even if they are a long way away) and this estimator will appear to get less and less uncertain even though the simulator and data are incompatible

The discrepancy between the simulator and the reality, $\sigma^2_{discrep}$, is too small. By increasing this term we can make NROY finite again.

This gives us a 'tolerance to error' to discuss with the modeller/decision maker.

Things I don't have time to talk about

Stochastic models

Agent based models

Estimating the discrepancy

Hierarchies of models (simple to complex)

Multiple models

Value of information

Data assimilation

Happy to Help

The UK statistical UQ community wants to help

In Exeter we are starting to work with Leon Danon's MetaWards model

Anyone else need help with UQ?