Calibration of stochastic models using history matching and emulation.

Ioannis Andrianakis

London School of Hygiene and Tropical Medicine

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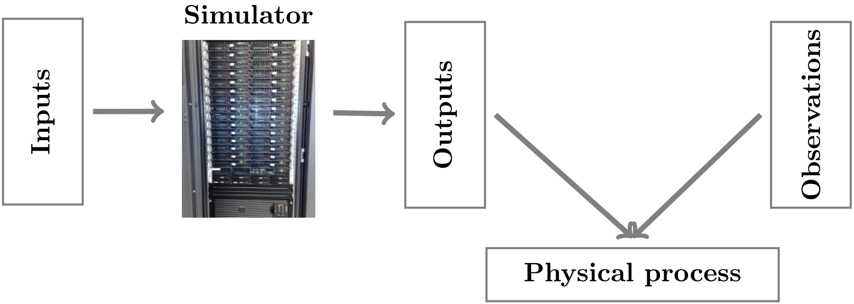
Joint work with: I.Vernon, N.McCreesh, TJ McKinley, J.Oakley, R.Nsubuga, M.Goldstein and R.White

LONDON SCHOOL of HYGIENE &TROPICAL MEDICINE

Outline

- Motivation.
- Emulation.
- History matching.
- Results.

Calibration of computer models



Calibration objective:

To find a set of input values so that the simulator represents best the physical process as this is described by observations.

The 'Mukwano' simulator

- A dynamic, stochastic, individual based model that simulates heterosexual sexual partnerships and HIV transmission.
- 22 inputs inc. contact rates, concurrency parameters, relationship duration, 2 sexual activity groups (high/low), 2 concurrency groups (high/low), 3 discrete behaviour periods.
- 18 outputs inc. population size, HIV prevalence, prevalence of men and women in long/short duration partnerships with one or more partners.
- Run time varies from 10 mins to >3 hours for 1 simulator run.
- Calibration data provided by a general population cohort in Uganda.

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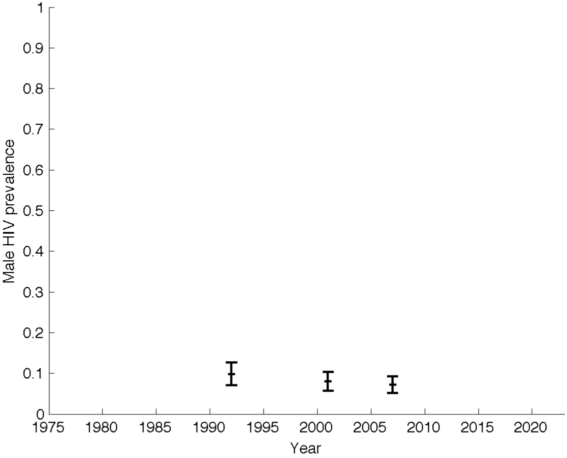
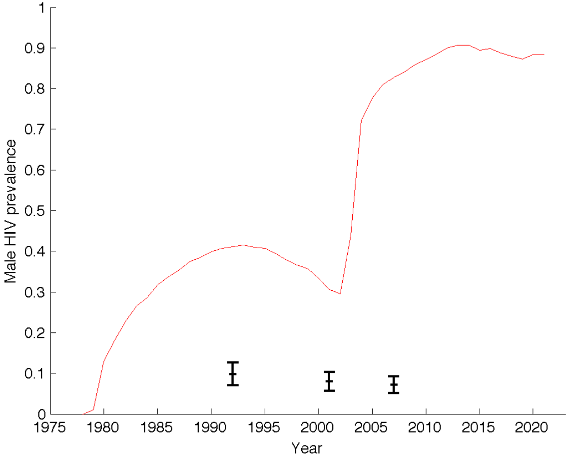
A manual approach

Suppose we want to match male HIV prevalences at 3 points in time.



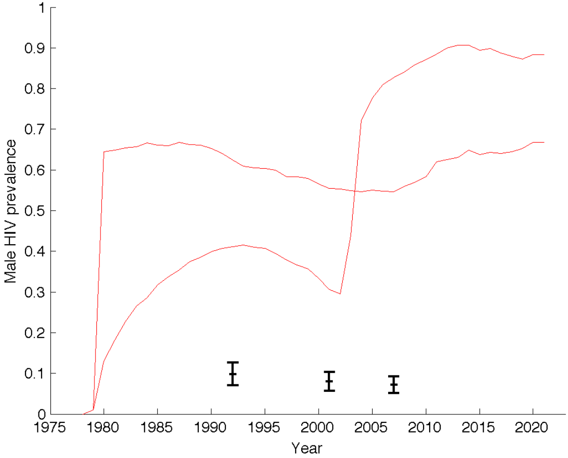
A manual approach

We choose a set of inputs run the model and...



A manual approach

...we try again...



A manual approach

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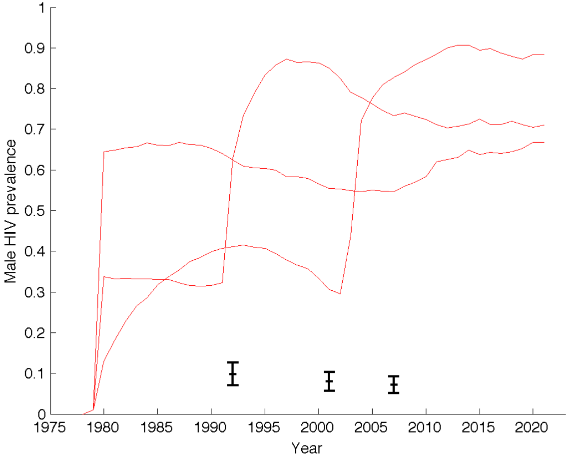
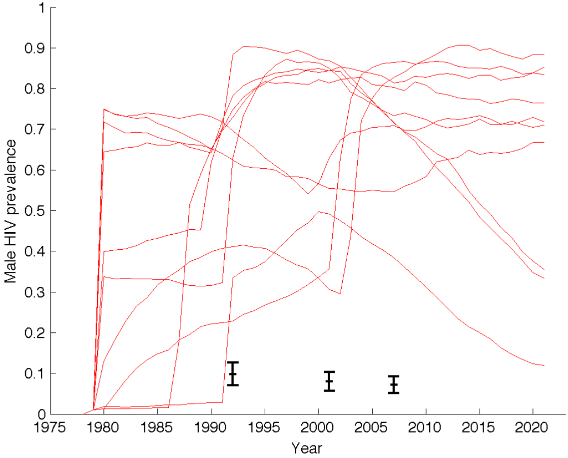


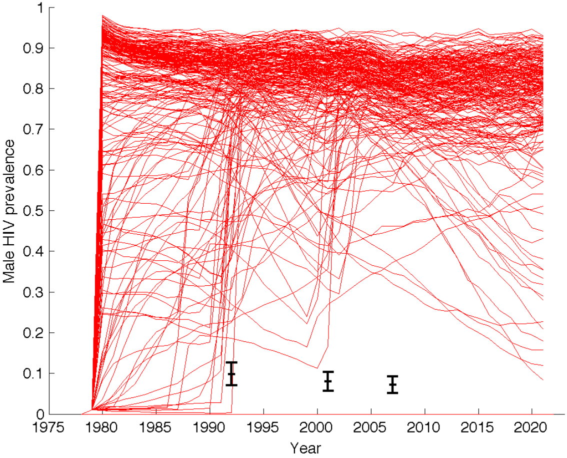
A manual approach

...after 10 runs...



A manual approach

...after 250 runs.



History matching

- Rather than looking for the best input values, history matching identifies and discards those unlikely to provide a match to the empirical data.

- The *implausible* input space is discarded in iterations known as waves.

- Not all inputs/outputs need to be considered at once.

- The simulator is often ‘better behaved’ in smaller areas of input space.

- History matching relies on *emulators* for computational efficiency.

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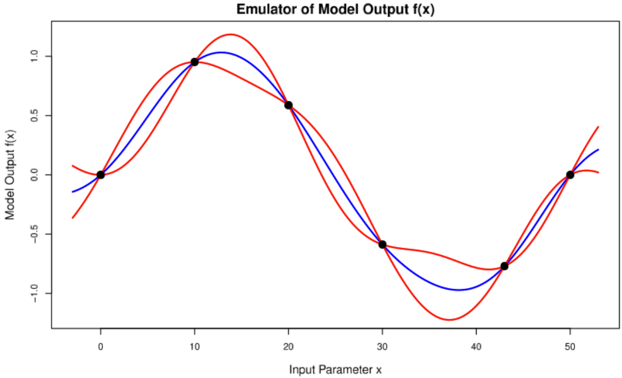
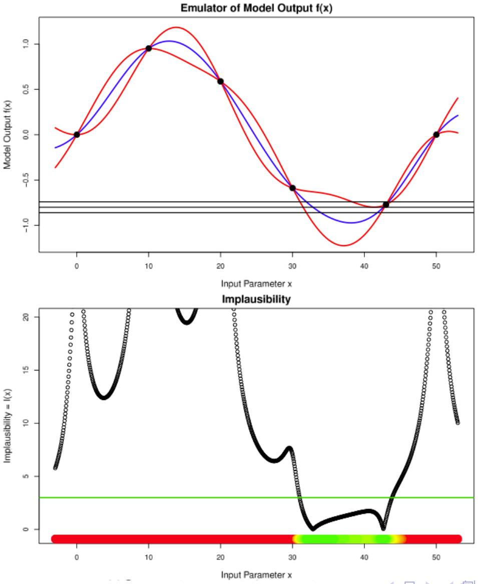
An emulator example

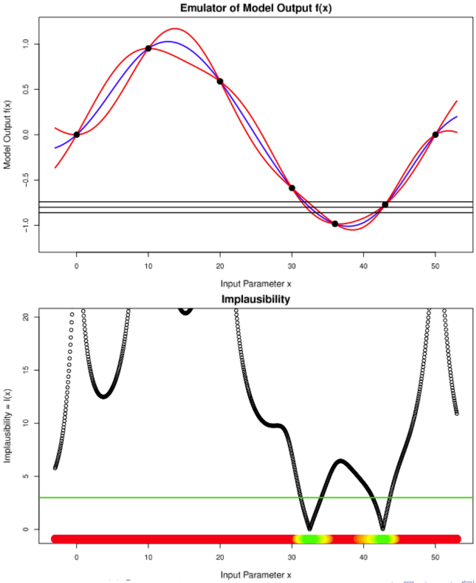
The emulator gives a posterior distribution for the model output, conditioned on the model runs we have seen so far.



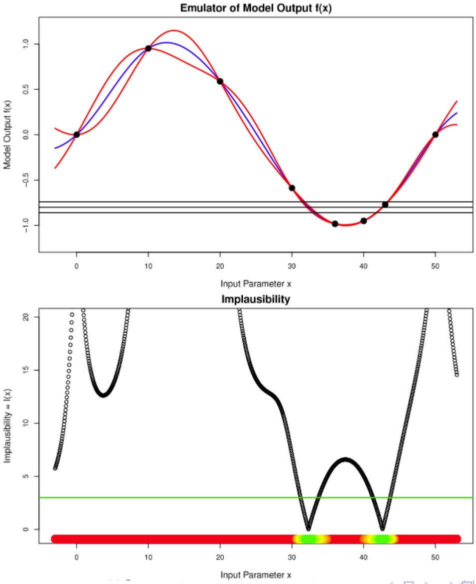
History matching - wave 1



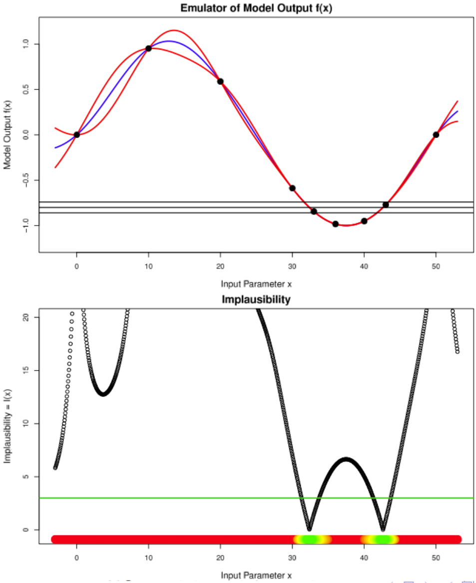
History matching - wave 2



History matching - wave 3



History matching - wave 4



Challenges

- Large number of inputs and outputs.
- Unavailable model likelihood.
- Long simulator running times.
- Stochastic model.

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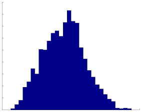
Stochastic model

For an input $\mathbf{x}$, the simulator's output is a draw from an unknown distribution, with mean $g(\mathbf{x})$ and variance $s(\mathbf{x})$.



$$g(\mathbf{x}) \equiv \mathrm{E}[f(\mathbf{x})]$$

$$s(\mathbf{x}) \equiv \mathrm{Var}[f(\mathbf{x})]$$

We can write this as:

$$f(\mathbf{x}) = g(\mathbf{x}) + \epsilon(\mathbf{x})$$

where $\epsilon(\mathbf{x})$ is a zero mean r.v. with variance $s(\mathbf{x})$.

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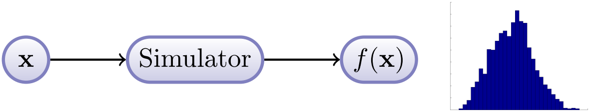

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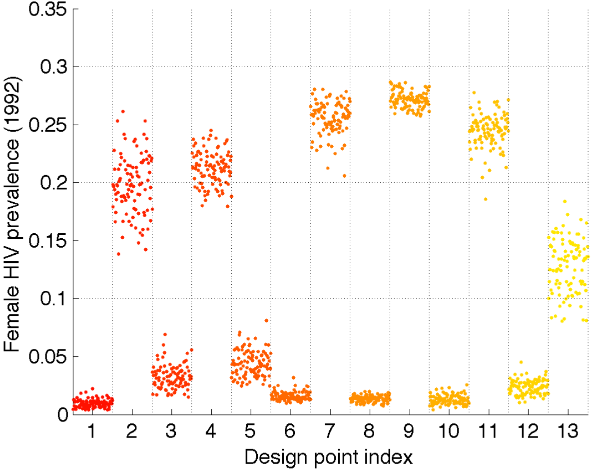
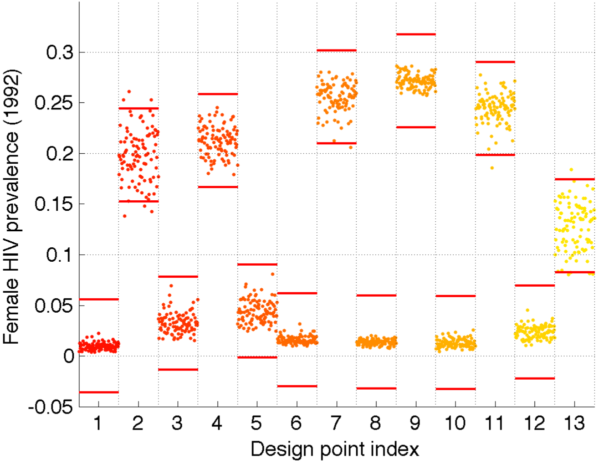
The variance $s(\mathbf{x})$

The variance $s(\mathbf{x})$ is a function of $\mathbf{x}$ and this has to be taken into account in history matching.



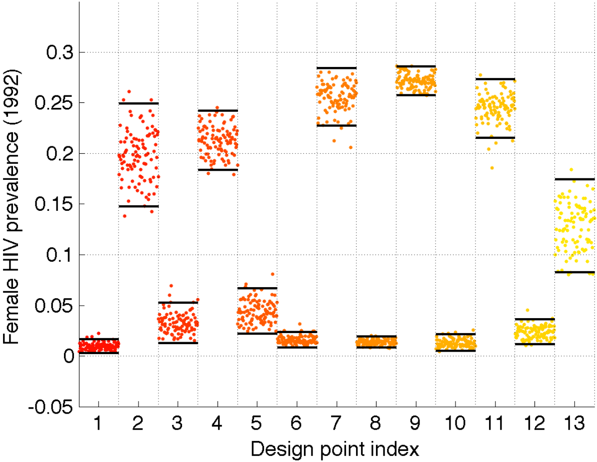
The variance $s(\mathbf{x})$

One approach is to assume a fixed variance across $\mathbf{x}$.

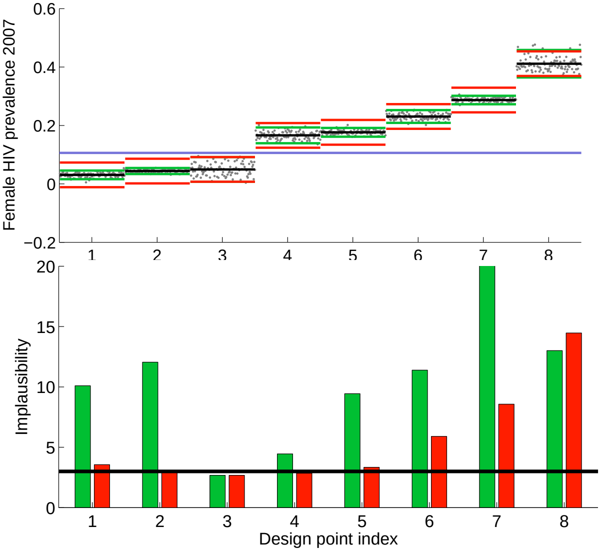


The variance $s(\mathbf{x})$

Estimating the variance can improve the results.



An example



0.6
0.4
0.2
0
−0.2
Female HIV prevalence 2007
1
2
3
4
5
6
7
8
20
15
10
5
0
Implausibility
Design point index

Emulation

- Evaluate $f(\mathbf{x})$ K times at each of N different inputs $\mathbf{x}_n$.
- Calculate means and log-variances

$$\hat{g}(\mathbf{x}_n) = \frac{1}{k}\sum_{k=1}^{K} f_k(\mathbf{x}_n), \quad \hat{\xi}(\mathbf{x}_n) = \ln\left(\frac{1}{K-1}\sum_{k=1}^{K}(f_k(\mathbf{x}_n) - \hat{g}(\mathbf{x}_n))^2\right).$$

- Gather training data $D = \{\mathbf{x}_n, \hat{g}(\mathbf{x}_n)\}$ and $D' = \{\mathbf{x}_n, \hat{\xi}(\mathbf{x}_n)\}$.
- Use a GP prior on g and ξ, i.e. $g(\mathbf{x}) \sim \mathcal{GP}(\cdot,\cdot)$, $\xi(\mathbf{x}) \sim \mathcal{GP}(\cdot,\cdot)$.
- Calculate posteriors: $\mathrm{E}^*[g(\mathbf{x})]$, $\mathrm{Var}^*[g(\mathbf{x})]$, $\mathrm{E}^*[\xi(\mathbf{x})]$ and $\mathrm{Var}^*[\xi(\mathbf{x})]$.

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Some emulator details

- $g(\mathbf{x}), \xi(\mathbf{x}) \sim \mathcal{GP}(h(\mathbf{x})\beta, \sigma^2(c(\mathbf{x}, \mathbf{x}') + \nu))$
- $h(\mathbf{x}) = 1 + \mathbf{x} + \mathbf{x}^2 + \mathbf{x}^3$.
- $c(\mathbf{x}, \mathbf{x}')$ is the Matérn 3/2 correlation function.
- β, σ^2 are marginalised with $p(\beta, \sigma^2) \propto \sigma^{-2}$.
- Correlation lengths δ and nugget ν are estimated with maximum likelihood.
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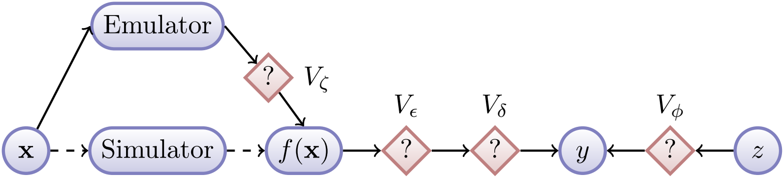
Uncertainty structure



z : Observations

y : Physical process

$f(\mathbf{x})$: Simulator's output

$\mathbf{x}$: Simulator's input

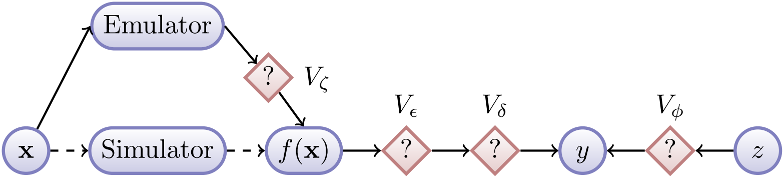
V_ζ: Code Uncertainty

V_δ: Model Discrepancy

V_ϵ: Ensemble Variability

V_ϕ: Observation Uncertainty

Uncertainty structure



- We link z with the posterior expectation of $g(\mathbf{x})$'s emulator via

$$z = \mathrm{E}^*[g(\mathbf{x})] + \zeta + \epsilon + \delta + \phi$$

where $\zeta, \epsilon, \delta, \phi$ are zero mean unimodal random variables.

- The variances V_δ, V_ϕ are provided by the model experts/data.
- $V_\zeta(\mathbf{x}) = \mathrm{Var}^*[g(\mathbf{x})]$ and $V_\epsilon(\mathbf{x}) = \exp(\mathrm{E}^*[\xi(\mathbf{x})])$.

The implausibility measure

- The link function $z = \mathrm{E}^*[g(\mathbf{x})] + \zeta + \epsilon + \delta + \phi$ allows us to write the implausibility measure as:

$$I(\mathbf{x}) = \frac{|z - \mathrm{E}^*[g(\mathbf{x})])|}{(V_\zeta(\mathbf{x}) + V_\epsilon(\mathbf{x}) + V_\delta + V_\phi)^{1/2}}$$

- A large value of $I(\mathbf{x})$, indicates that $\mathbf{x}$ is unlikely to result in a good match between the model and the data.
- A small value of $\mathbf{x}$ does not imply that $\mathbf{x}$ is good! We do not know yet.
- The magnitude of $I(\mathbf{x})$ is often judged based on Pukelsheim's 3σ rule.
- The use of emulators allows to evaluate the implausibility almost instantaneously.

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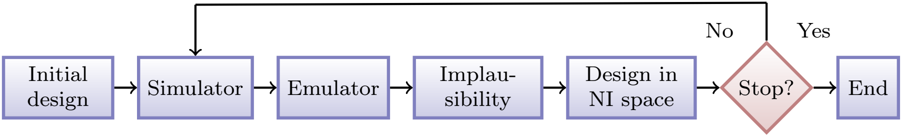
- The use of emulators allows to evaluate the implausibility almost instantaneously.

History matching procedure



Outline

- Motivation.
- Emulation.
- History matching.
- Results.

Results

- We compare results of the fixed variance and emulated variance approaches.
- At the end of both history matches, the non-implausible samples had a 70% probability to match all outputs.
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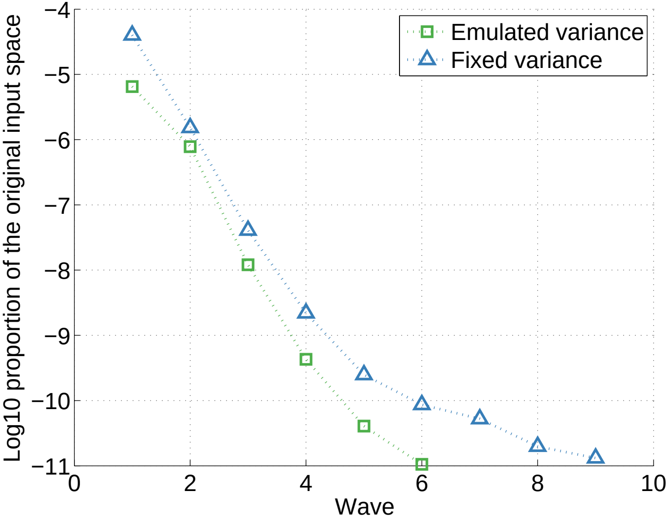
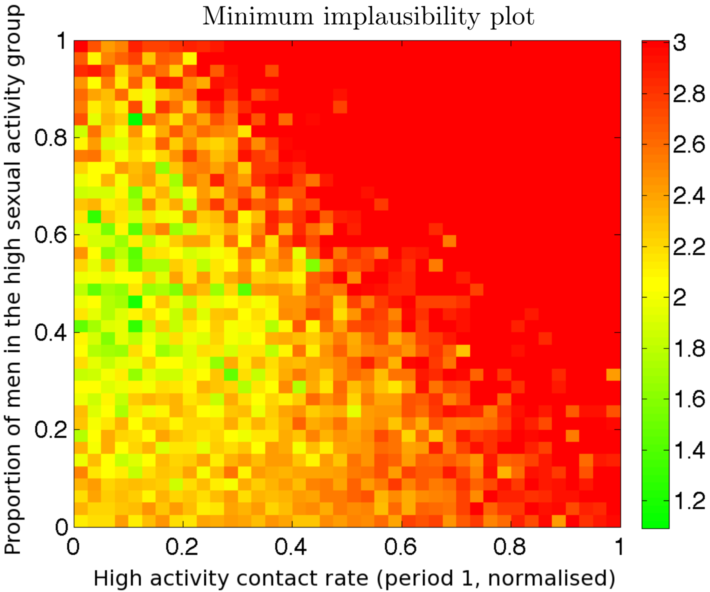
Rejection rates



Visualising the implausible space

The implausible space can be visualised with minimum implausibility and optical depth plots.

Visualising the implausible space



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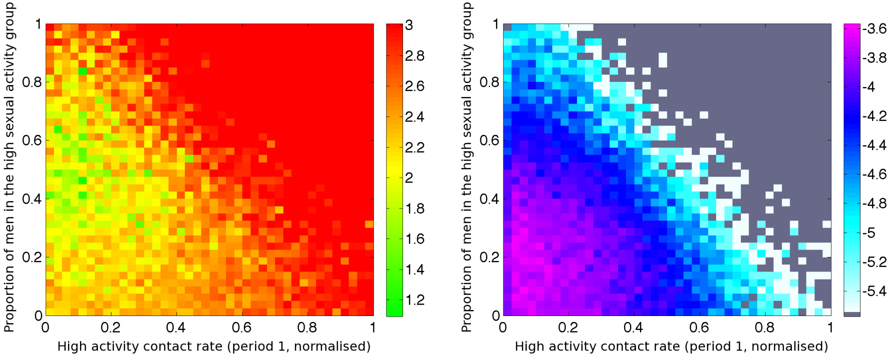
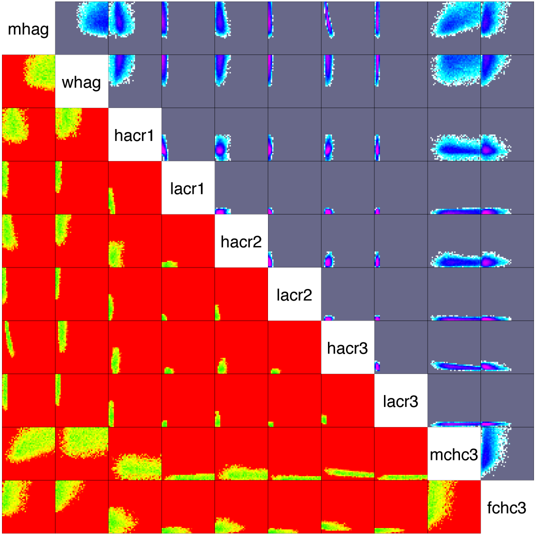
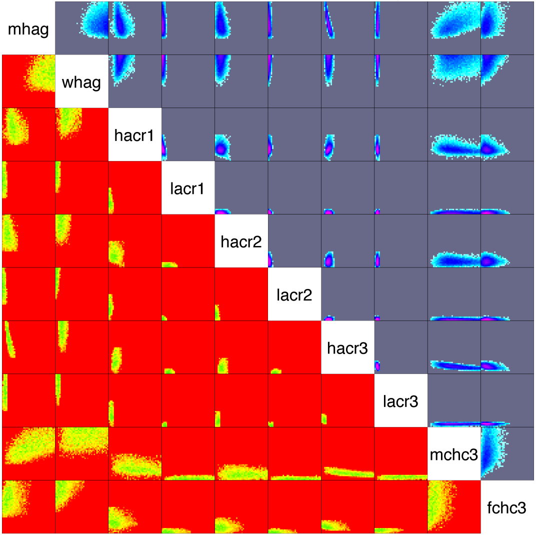
Optical depth plot



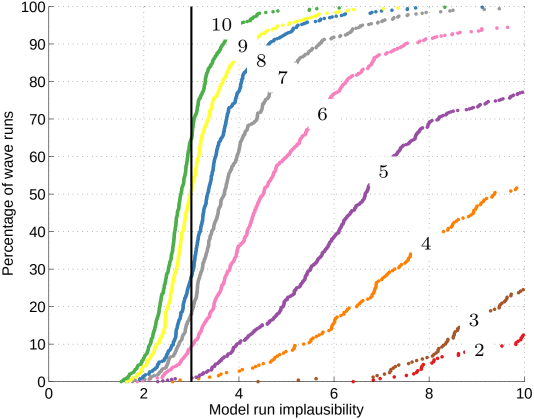
Implausibility plots wave 9 (fixed variance)



Implausibility plots wave 6



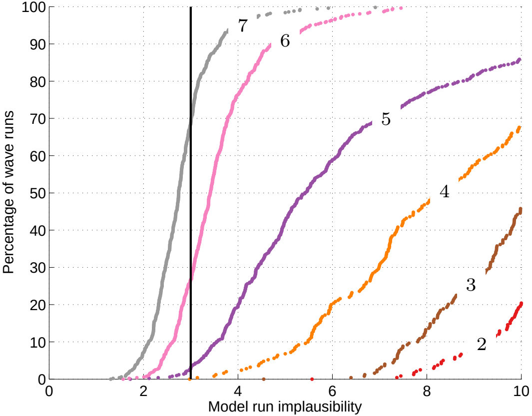
Implausibility of model runs (fixed variance)



Implausibility of the *actual* simulator runs (no emulation involved)

$$I(\mathbf{x}) = \frac{|z - \hat{g}(\mathbf{x})|}{(\hat{s}(\mathbf{x}) + V_\delta + V_\phi)^{1/2}}$$

Implausibility of model runs



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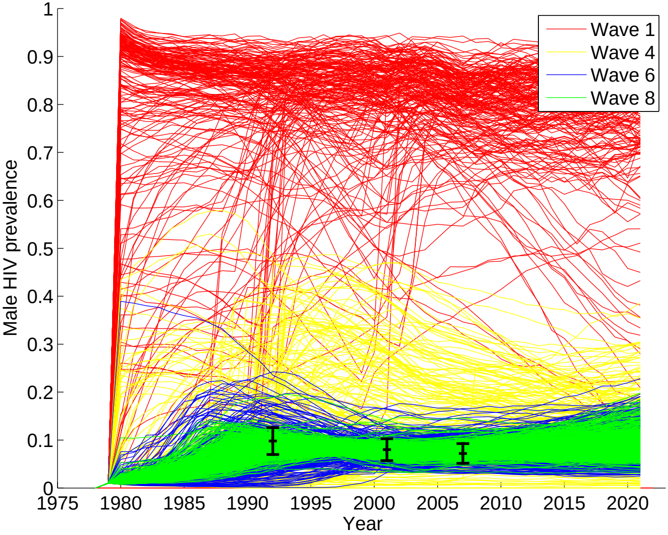

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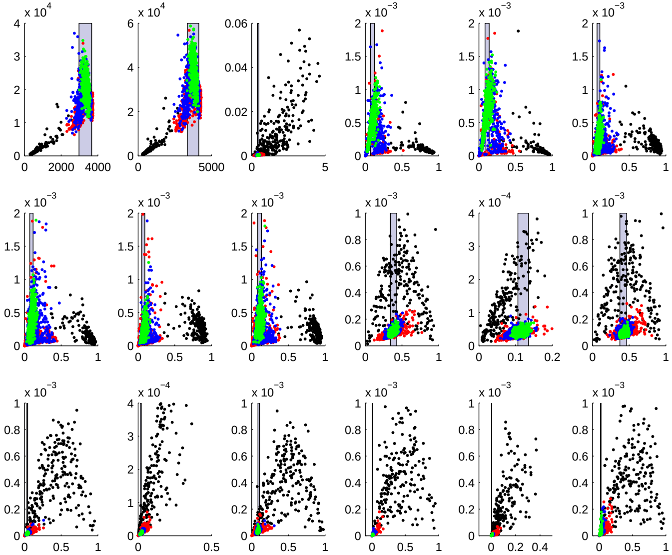

Conclusion

- We extended history matching so that it can efficiently handle stochastic models.
- The mean and variance of the simulator's output were both emulated using a Gaussian process.
- The simulator was calibrated in 6 waves instead of 9, requiring ~ 2000 simulator evaluations instead of ~ 3500.
- Linear regression models can be used for the variance instead of full GP ones (Boukouvalas 2014).
- Variance emulation can inform the number of replications needed at each design point.

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Mukwano 2.0

- Our epidemiologists came up with a larger version of Mukwano.(96 inputs, 50 outputs)
- Simulates HIV transmission under various ART treatment strategies.
- Predicts the effects of ART on mortality and transmission over the next 15-20 years.
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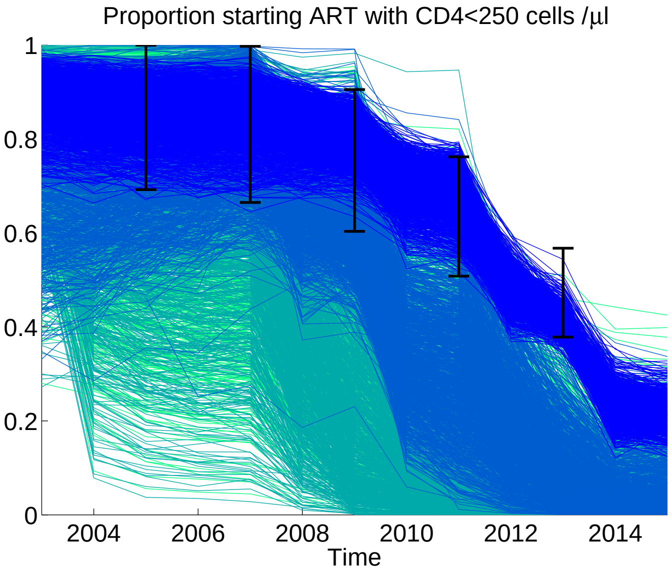

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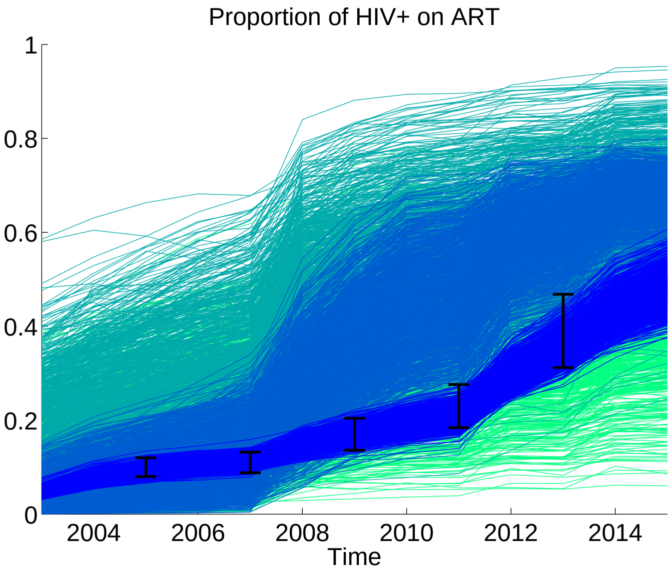

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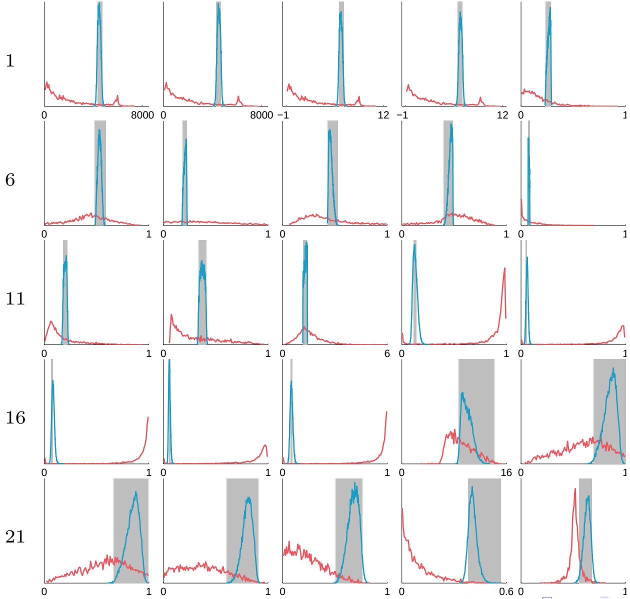

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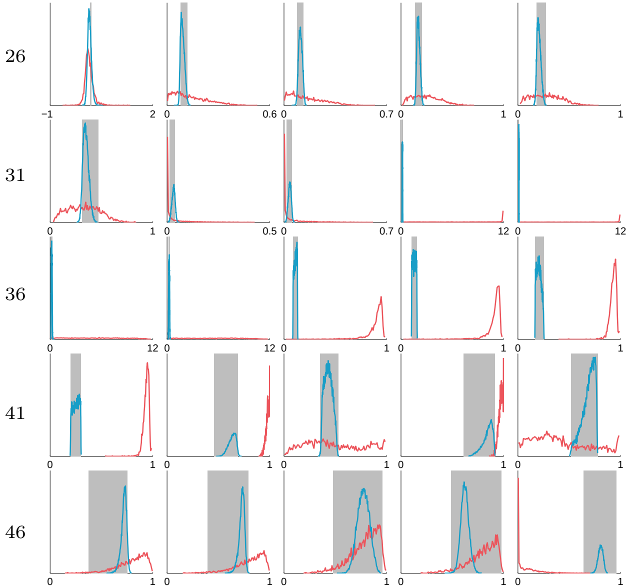

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- History matching provided hundreds of input points that match all the outputs simultaneously.
- These inputs are used to run the simulator into the future and predict the effect of different ART interventions to mortality, HIV prevalence etc.
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