

Inverse Modelling without the Tears

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With thanks to Danny Williamson, Louise Kimpton and Lauric Ferrat

Overview

- Inverse Modelling
- Bayesian Calibration
- Model discrepancy
- Kennedy & O'Hagan
- History Matching
- Why Discrepancy Matters
- Example 1 - Do present day models work in the LGM
- Example 2 - Heart Modelling

Inverse Modelling

- We have a model of some process
- Mathematically we can write this as $y=f(x)$
- We collect data on the model outputs (y) and want to make inferences on x - the model inputs
- Set up loss function (or likelihood) and optimise

$$\sum (y_i - f(x_i))^2$$

Bayesian Calibration

- A more sophisticated approach is to use Bayes theorem do the inversion

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)}$$

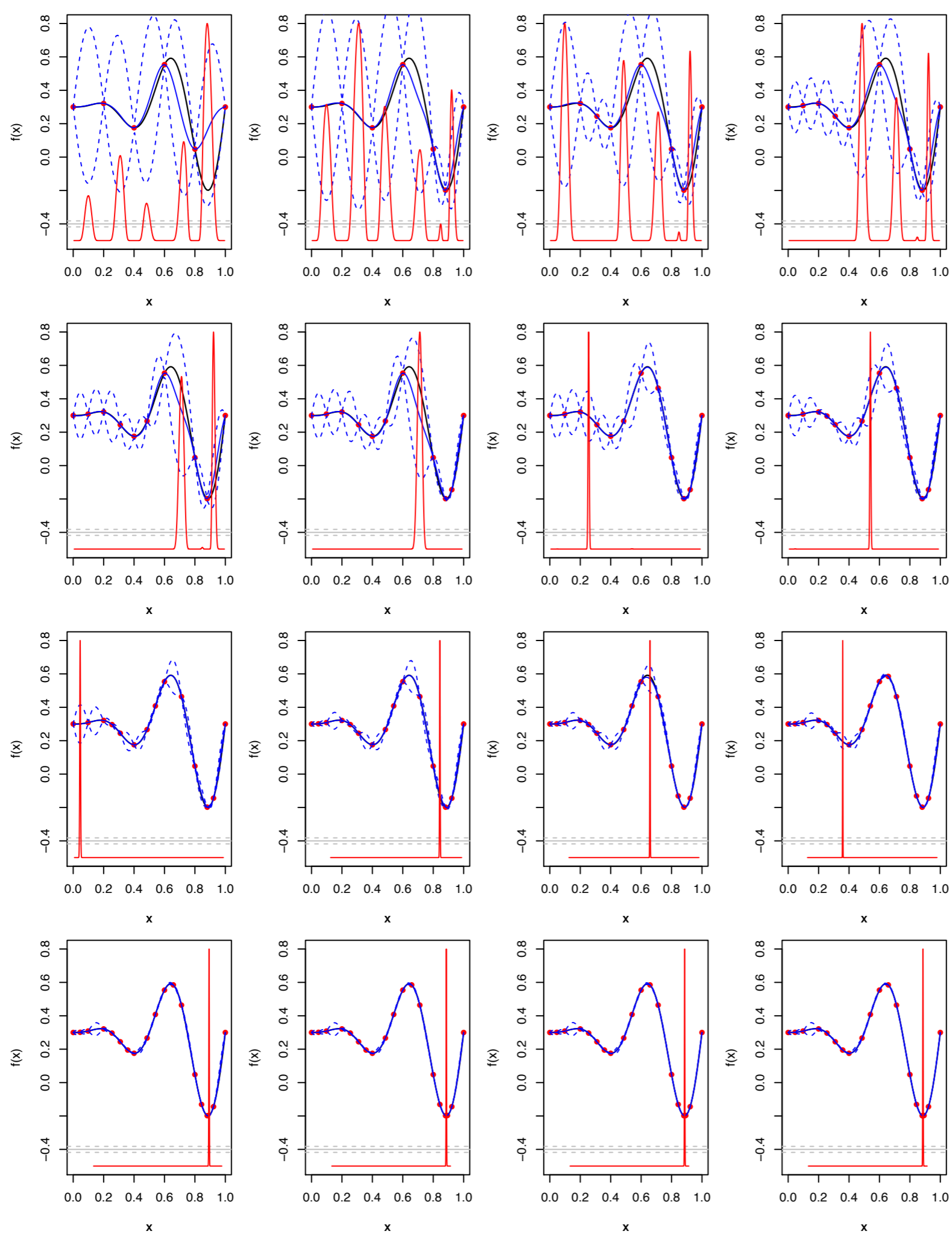
- Rather than a point estimate we now get a posterior distribution for x
- Usually done by MCMC (or similar)

The Role of an Emulator

- These are computationally expensive procedures
- Emulators are cheap alternatives to full models
- Use emulators to do the calculations

Model Discrepancy

- All models are wrong
- (All data are wrong as well)
- How wrong are we prepared to be? (Tolerance to error)
- Does model discrepancy matter?



**Thanks to
Danny Williamson**

- Could we not add the model discrepancy to our model?
- Identifiability problems

Kennedy and O'Hagan (2001)

- To account for discrepancy KOH simultaneously fit two Gaussian processes.
 - One is an emulator for the model
 - The other models the discrepancy
- Identifiability
- Brynjarsdottir and O'Hagan (2014) - strong priors needed

An Alternative

- Don't try to find the 'best' inputs
- Find inputs (x) that are implausible given the data (y)
- This is a lot easier
- No optimisation
- No sampling posterior

History Matching

- Set up a measure of the distance between the data and the model prediction

$$Imp = \sqrt{\frac{E(y - f(x))^2}{V(y - f(x))}}$$

- If this distance is too far. That value of x is implausible

- We can expand the variance term to give

$$Imp = \sqrt{\frac{(y - E(f(x)))^2}{V_y + V_{f(x)}}$$

- Where V_y is the variance of y
- and $V_{f(x)}$ is the variance of $f(x)$
- For $Imp > 3$ we say that the inputs (x) are implausible (Pukelsheim (1994))

- Because we are using an emulator we can expand $V_{f(x)}$

$$Imp = \sqrt{\frac{y - E(f(x))^2}{V_y + V_{emul} + V_{disc}}}$$

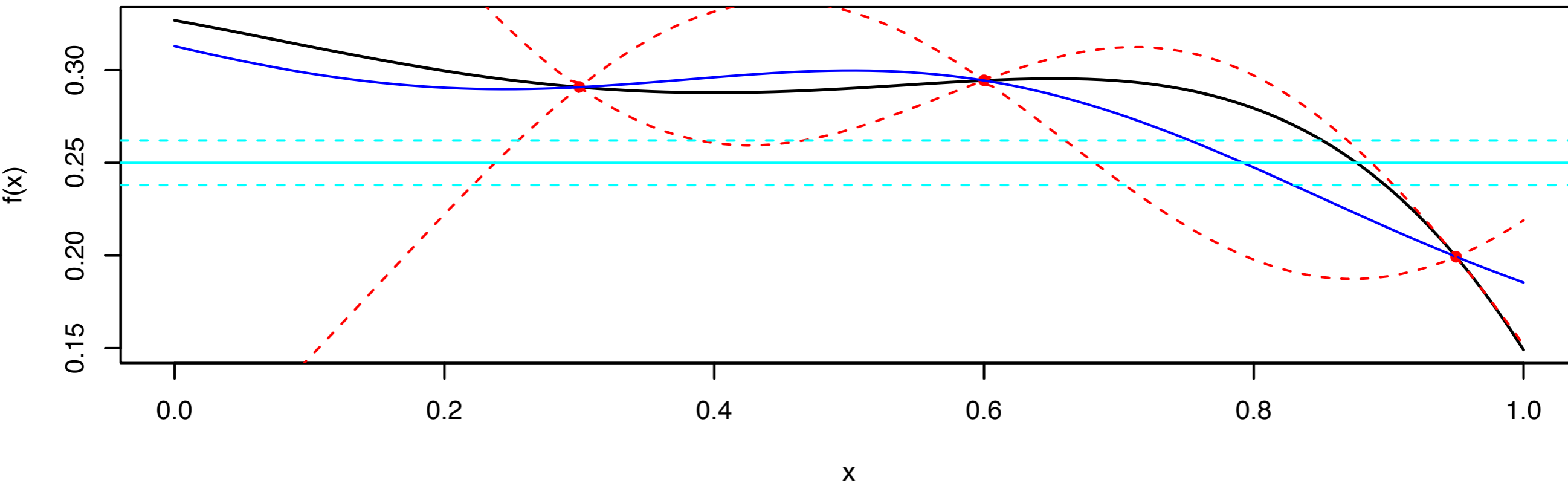
- y is the variance of the data y
- V_{emul} is the emulator variance
- V_{disc} is the model discrepancy

Procedure

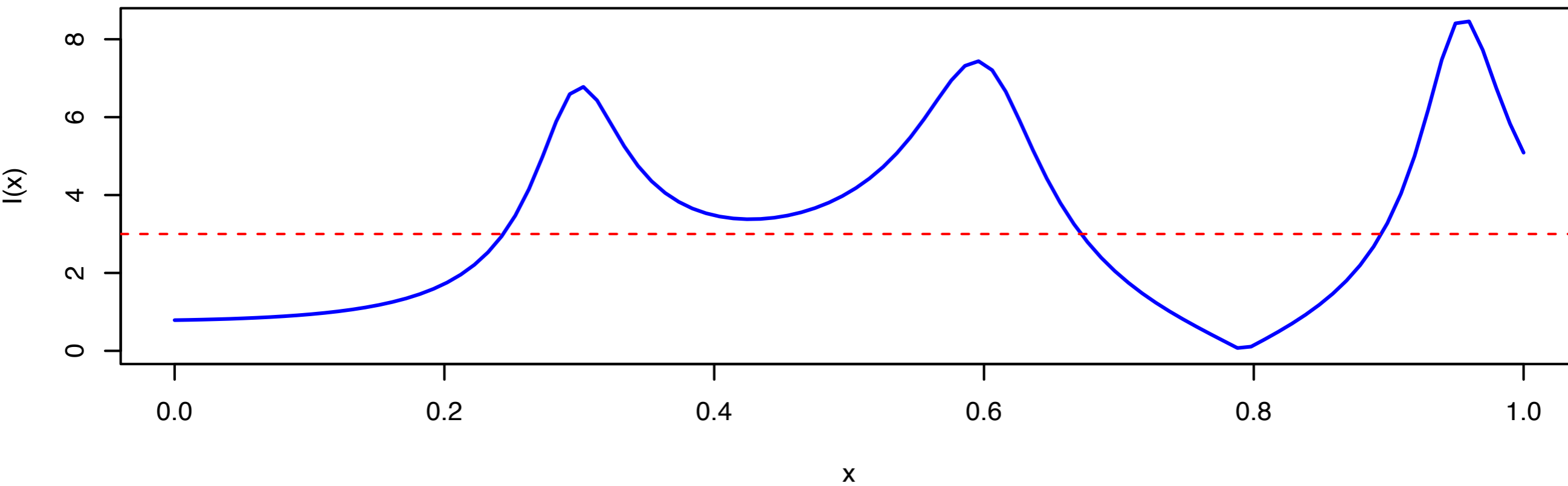
- Collect data
- Run designed experiment
- Build emulator
- Perform history matching
- All points with $\text{Imp} < 3$ deemed not implausible
- If we have many metrics take $\max(\text{Imp})$
- These constitute the Not Ruled Out Yet (NROY) space

- Design additional experiment within NROY space (wave 2)
- Rebuild emulator
- History match
- Repeat until NROY is either small enough or does not shrink
- At which point we may (i) have done enough, (ii) need to adjust our discrepancy (iii) perform a Kennedy and O'Hagan calibration on NROY or (iv) collect more data

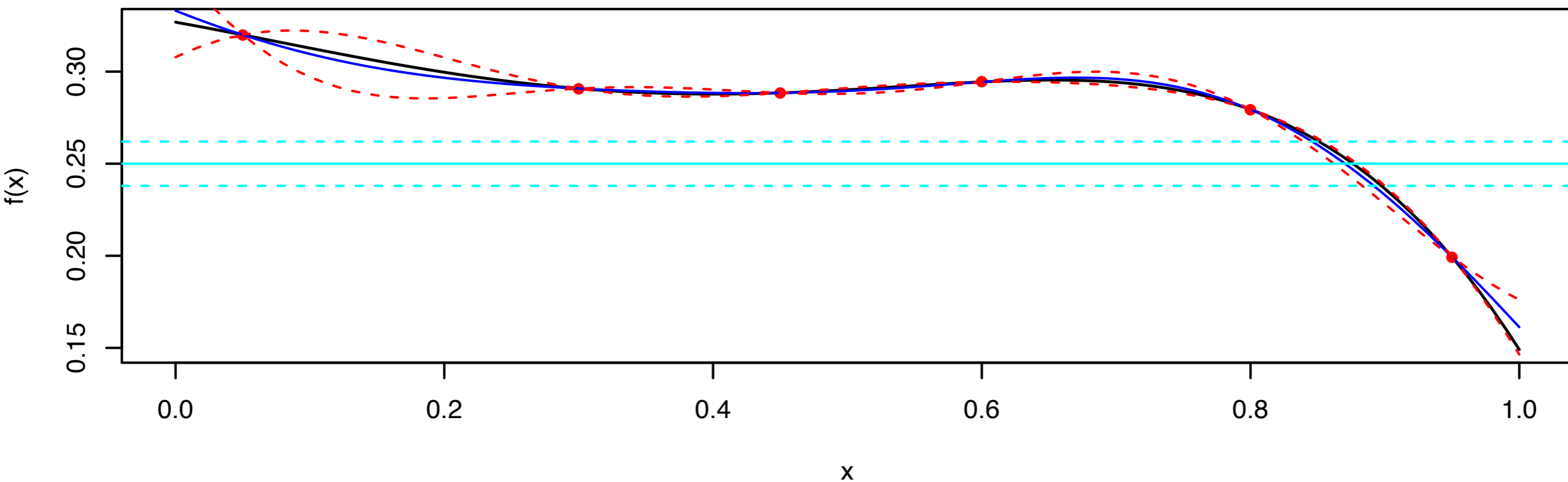
Emulator Example



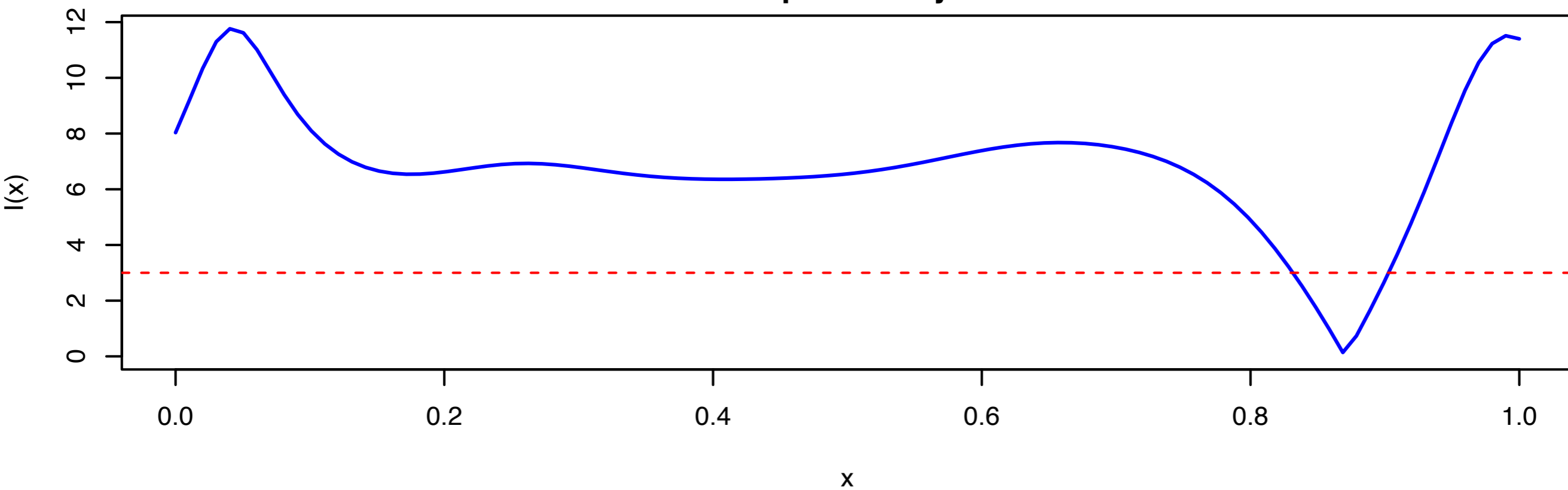
Implausibility



Emulator Example



Implausibility



An Example

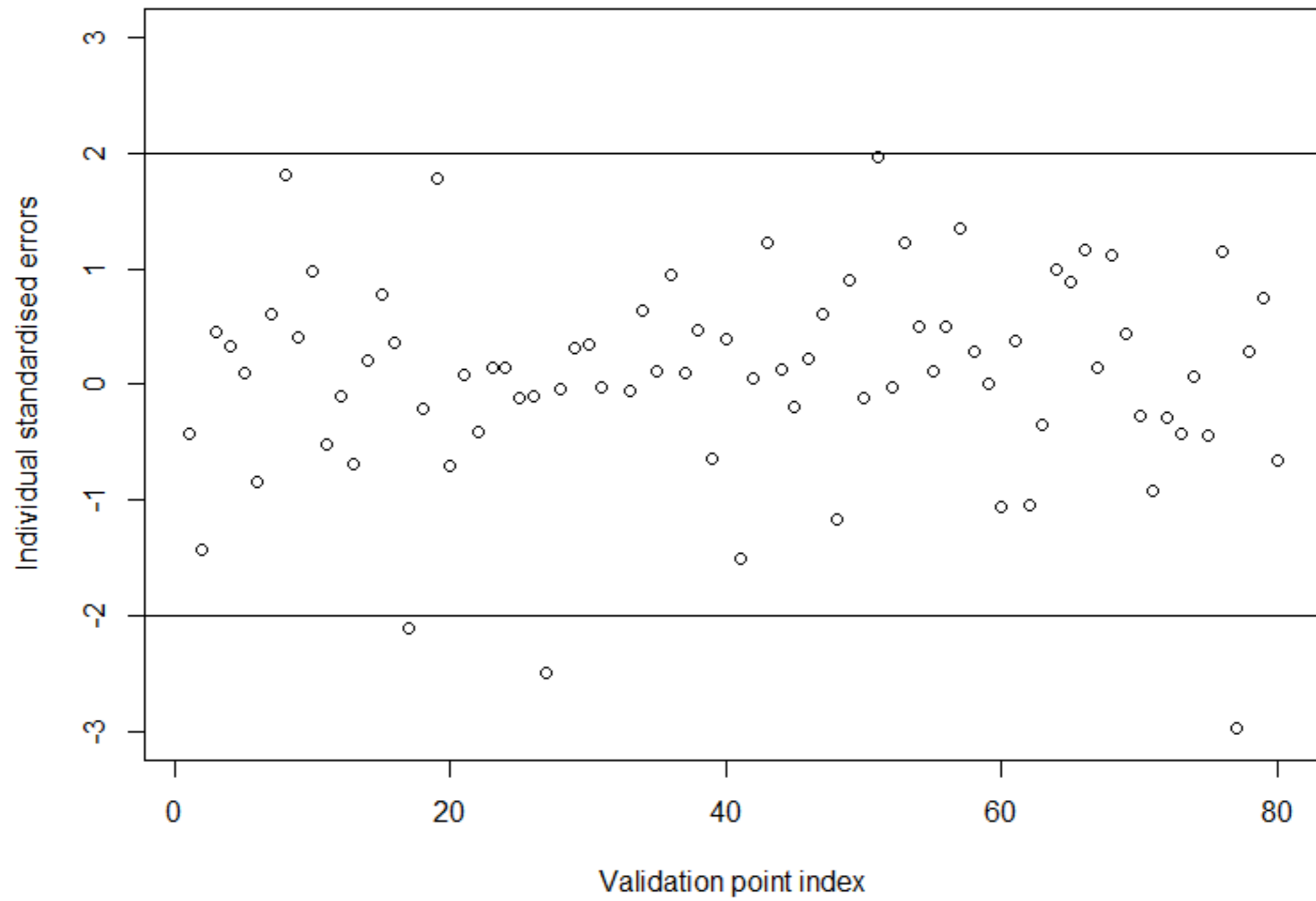
(Louise Kimpton's MMath project)

- Biogeochemistry models used in palaeoclimate are tuned (calibrated) to present data data
- Can such a model reproduce conditions at the Last Glacial Maximum?
- (Biology unlike physics changes with time)

- History match the model to current data (total amount of carbon)
- Is data from the LGM in implausible region?

Experiment

- Met O ran HADOCC in a 80 member Latin Hypercube (8 uncertain parameters)
- Model has internal variability so model mean + variance (over last 50 years of the run)



Results

- The LGM data is not at all implausible given this calibration (within 3)
- In fact the present data is 'less plausible'
- Only one wave possible

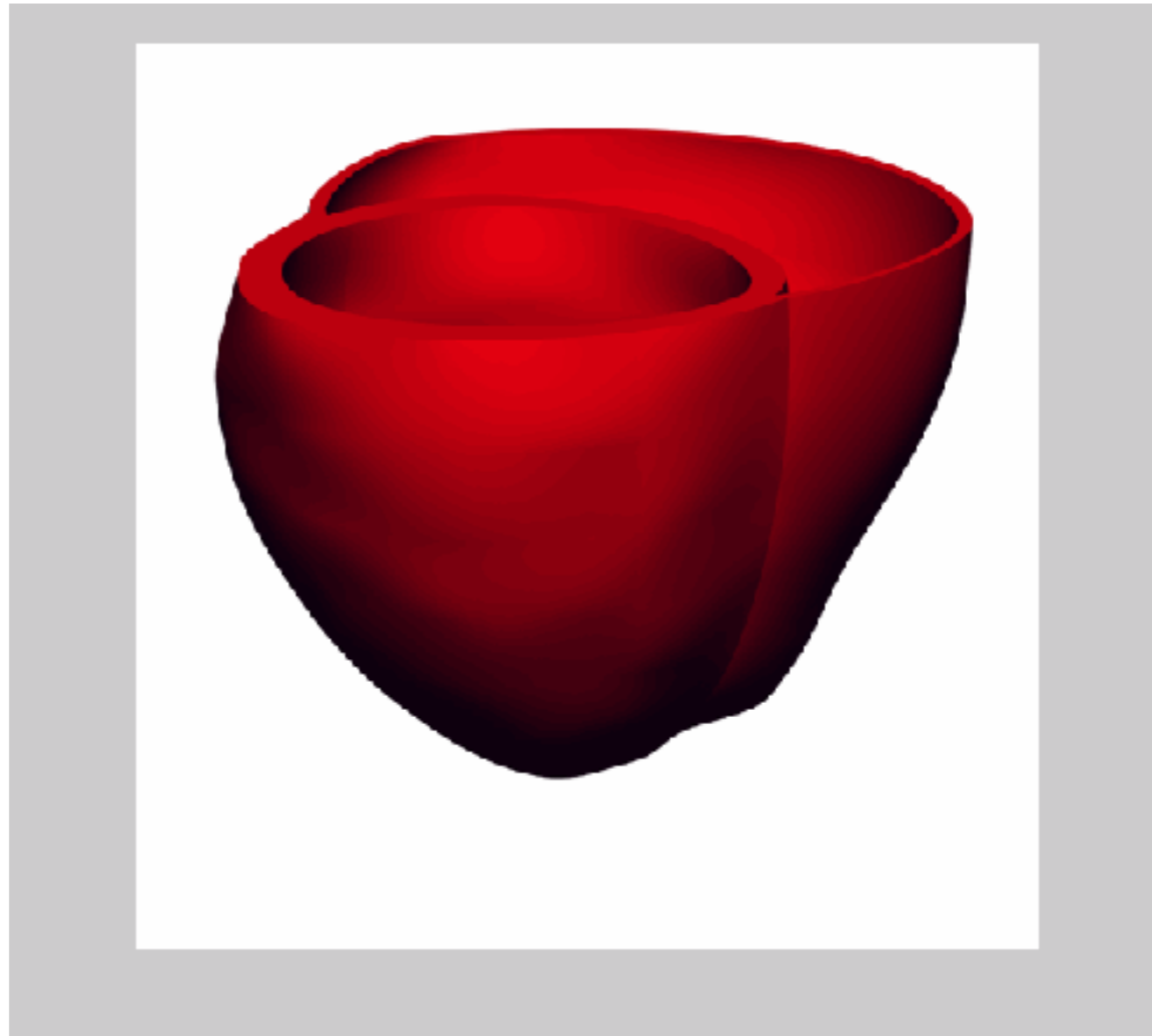
Second Example

Heart Disease

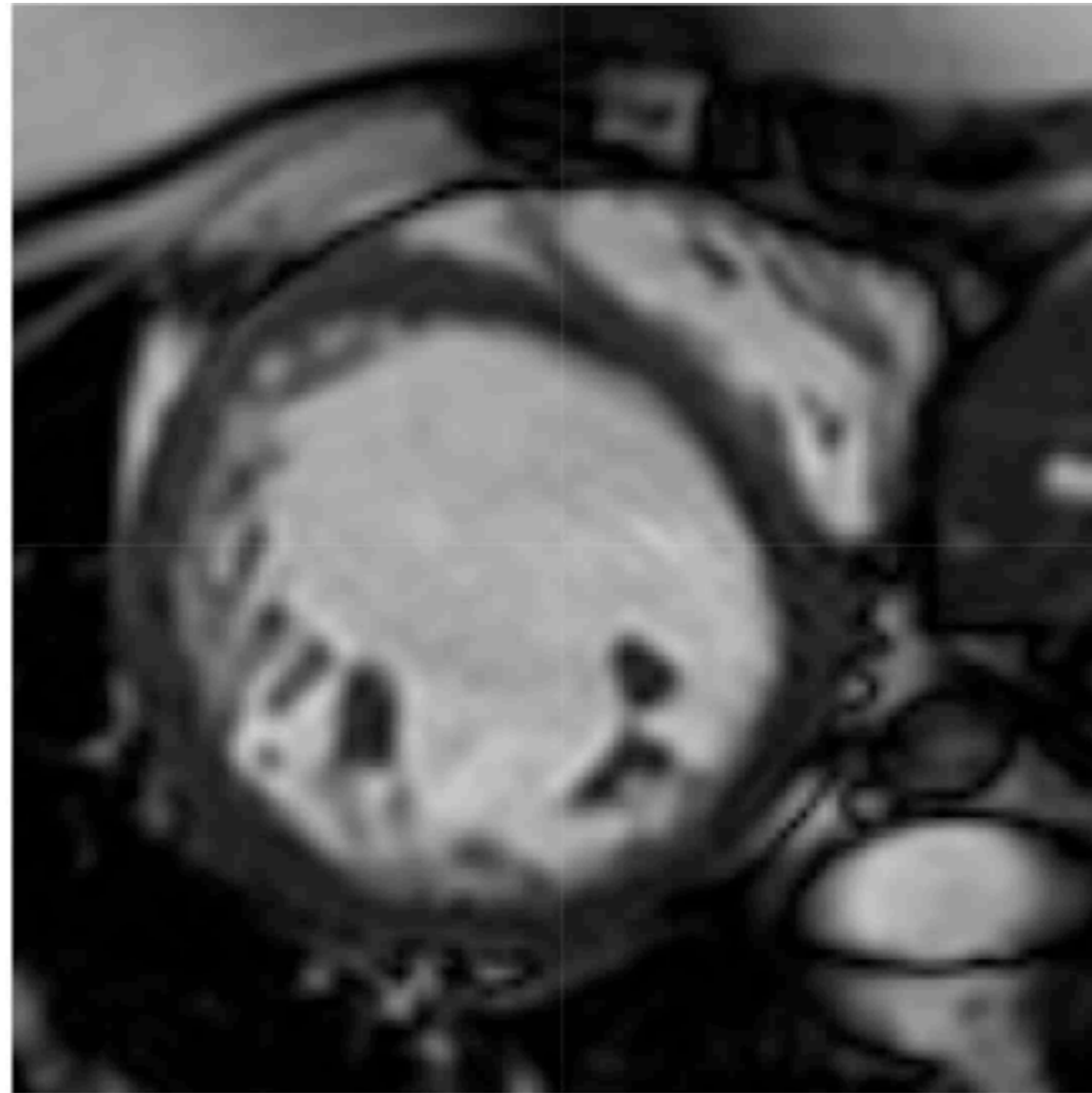
- About 900,000 people in the UK suffer from heart failure
- Diastolic dysfunction (Heart failure with preserved ejection fraction) patients have high hospital re-admission (29% in 60-90 days) and mortality rates (68% 4 year survival)
- There is no treatment despite many drug trials
- Could it be more than one condition?
- Can we use models to diagnose disease and possibly varieties?

- Use model from KCL (6 hour run)
- + data from an MRI scan
- Reduce MRI data using principal components from model ensemble (with James Salter's extension to include the data)
- + data on the pressure at the top of the heart

The Model



The Data



Multidimensional History Matching

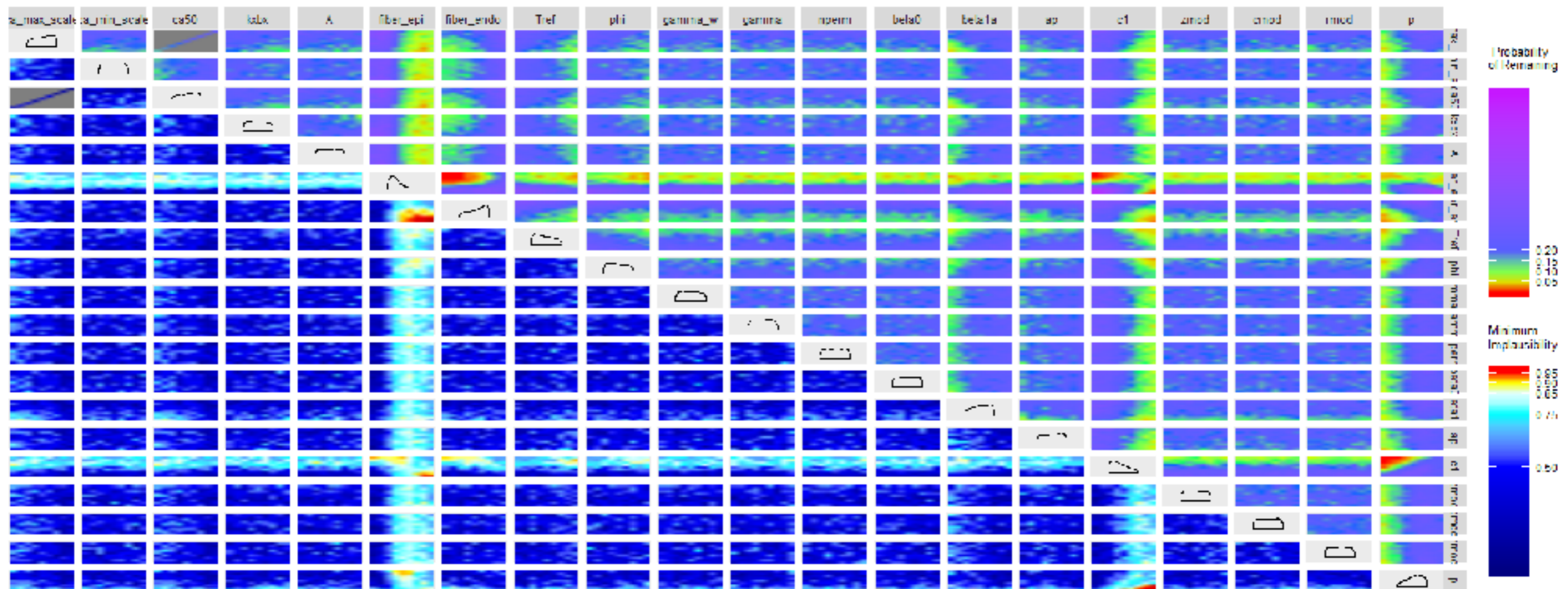
$$(y - E(y_{emul}))^T (\Sigma_y + \Sigma_{emul} + \Sigma_{disc})^{-1} (y - E(y_{emul}))$$

- Fully non-dimensional version
- Work with each variable separately
- Univariate emulators
- If one is implausible then x is implausible

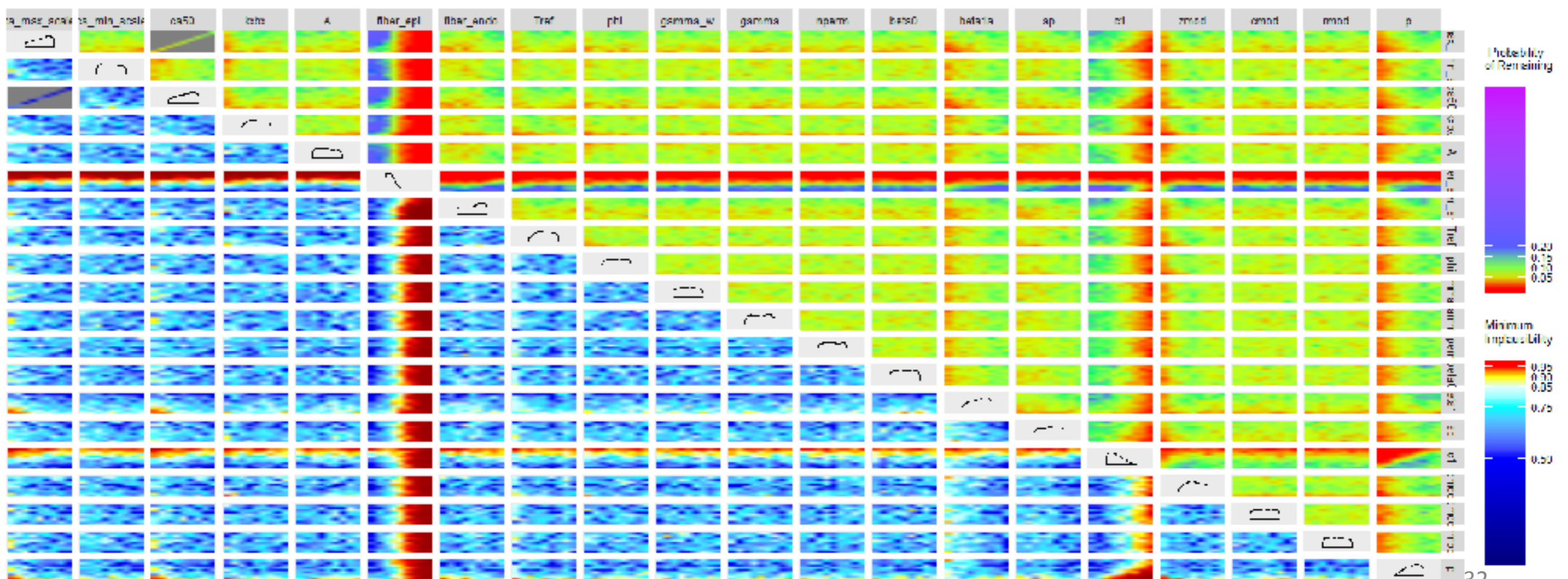
Healthy Patient

- Discrepancy elicited from experts
- No discrepancy - all of space is ruled out
- Discrepancy as tolerance to error

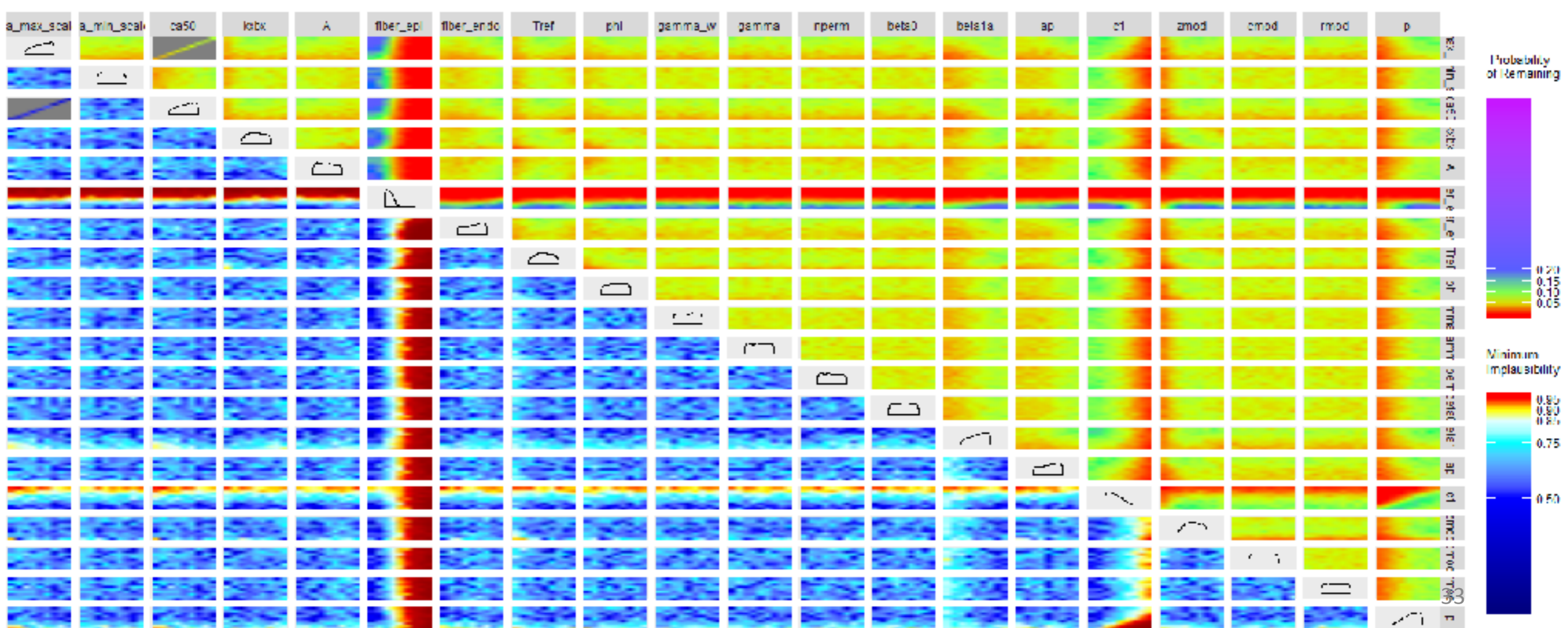
Wave 1: 25% of the parameter space remains



Wave 2: 6% of the parameter space remains



Wave 3: 5% of the parameter space remains



- More waves are unlikely to reduce space
- Could now do a calibration in the reduced space
- But for our purposes having a 'small' region not ruled out is OK
- Repeat procedure with unhealthy heart
- Similar results
- Depending on discrepancy (tolerance to error) the two regions overlap or are disjoint.

Conclusions

(Points for Discussion)

- History matching quick and easy way to calibrate models
- ‘Bayesian calibration’ - discrepancy
- K&OH - identifiability problems
- Discrepancy important - tolerance to error
- Other issues
 - Model failures
 - Principal components