Bayes linear strategies for emulation and history matching for complex computer models

Michael Goldstein
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Models and physical systems: some examples

Systems biology Models of activity at the cellular level are used to make inferences about the behaviour of the biological organism.

Oil reservoirs An oil reservoir simulator is used to manage assets associated with the reservoir, in order to develop efficient production schedules, etc.

Natural Hazards Floods, volcanoes, tsunamis and so forth, are all studied by large computer simulators.

Disease modelling Agent based models are used to study interventions to control infectious diseases.

Energy planning Simulators of future energy demand and provision are key components of planning for energy investment.

Climate change Large scale climate simulators are constructed to assess likely effects of human intervention upon future climate behaviour.

Galaxy formation The study of the development of the Universe is carried out by using a Galaxy formation simulator.

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The science in each is completely different. However, the underlying methodology for handling uncertainty is the same.

Sources of Uncertainty

(i) parametric uncertainty (each model requires a, typically high dimensional, parametric specification)
(ii) condition uncertainty (uncertainty as to boundary conditions, initial conditions, and forcing functions),
(iii) functional uncertainty (model evaluations take a long time, so the function is unknown almost everywhere)
(iv) stochastic uncertainty (either the model is stochastic, or it should be),
(v) solution uncertainty (as the system equations can only be solved to some necessary level of approximation).
(vi) structural uncertainty (the model only approximates the physical system),
(vii) measurement uncertainty (as the model is calibrated against system data all of which is measured with error),
(viii) multi-model uncertainty (usually we have not one but many models related to the physical system)
(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 simulator output $f(x)$ is the assessment of the system history.

(plus other stuff which may be relevant and useful).

History matching

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More generally, the shape of the set $C(z)$ identifies the constraints on the parameter space that are imposed by the data.

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Suppose, for example, that simulator $f(.)$ takes inputs which may help control future outputs.

Evaluation of effective control over the range of inputs in $C(z)$ identifies which are the safest control strategies and whether more data is needed before controls are introduced.

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Here’s a refence to our early work.
Craig, Goldstein, Seheult, Smith (1997) Pressure matching for hydrocarbon reservoirs: a case study in the use of **Bayes linear strategies** for large computer experiments (with discussion)
In Case Studies in Bayesian Statistics, Gastonis et al New York: Springer-Verlag, III,37-93.

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This is important because the likelihood surface is complicated and multi-modal, and the Bayes answer often depends on features of the prior distribution which are hard to specify meaningfully.

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The Bayesian approach can be difficult in large problems because of the extreme level of detail which is required in the specification of beliefs.
(And the technical difficulty of the full Bayes calculations.)

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Bayes linear adjustment may be viewed as
(i) an approximation to a full Bayes analysis or
(ii) the appropriate analysis given a partial specification.
(There are rigorous foundations for this viewpoint.)

Bayesian linear adjustment

The Bayes linear adjusted expectation and variance for vector y given vector z are

$$\mathsf{E}_z[y] = \mathrm{E}(y) + \mathrm{Cov}(y,z)\mathrm{Var}(z)^{-1}(z - \mathrm{E}(z)),$$
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And the uncertainty quantification papers in this talk contain plenty of examples of Bayes linear computations.

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(ii) an assessment of the likely magnitude of the error of the approximation.

Unlike the original simulator, the emulator is fast to evaluate for any choice of inputs. This allows us to explore model behaviour for all physically meaningful input specifications.

Form of the emulator

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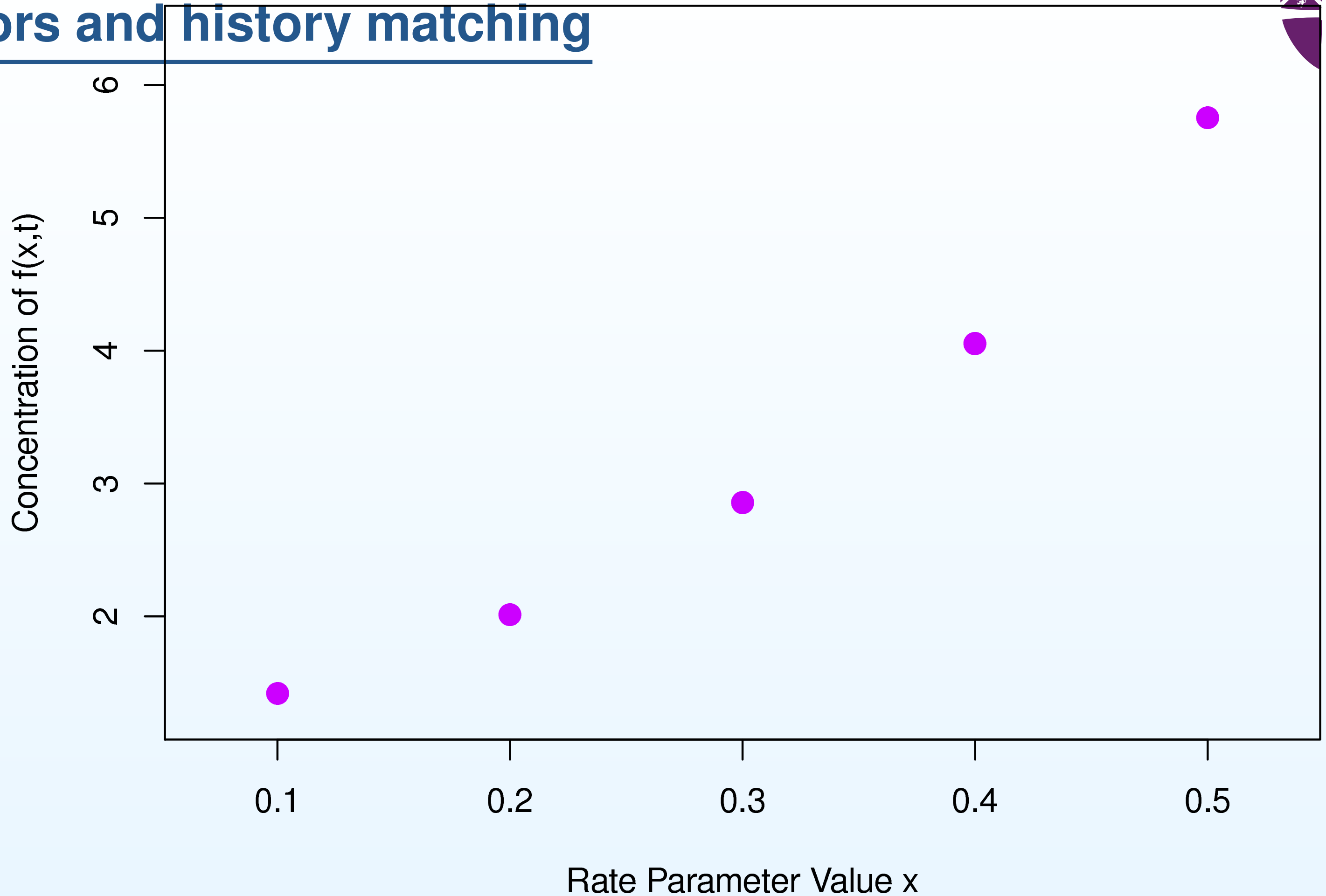
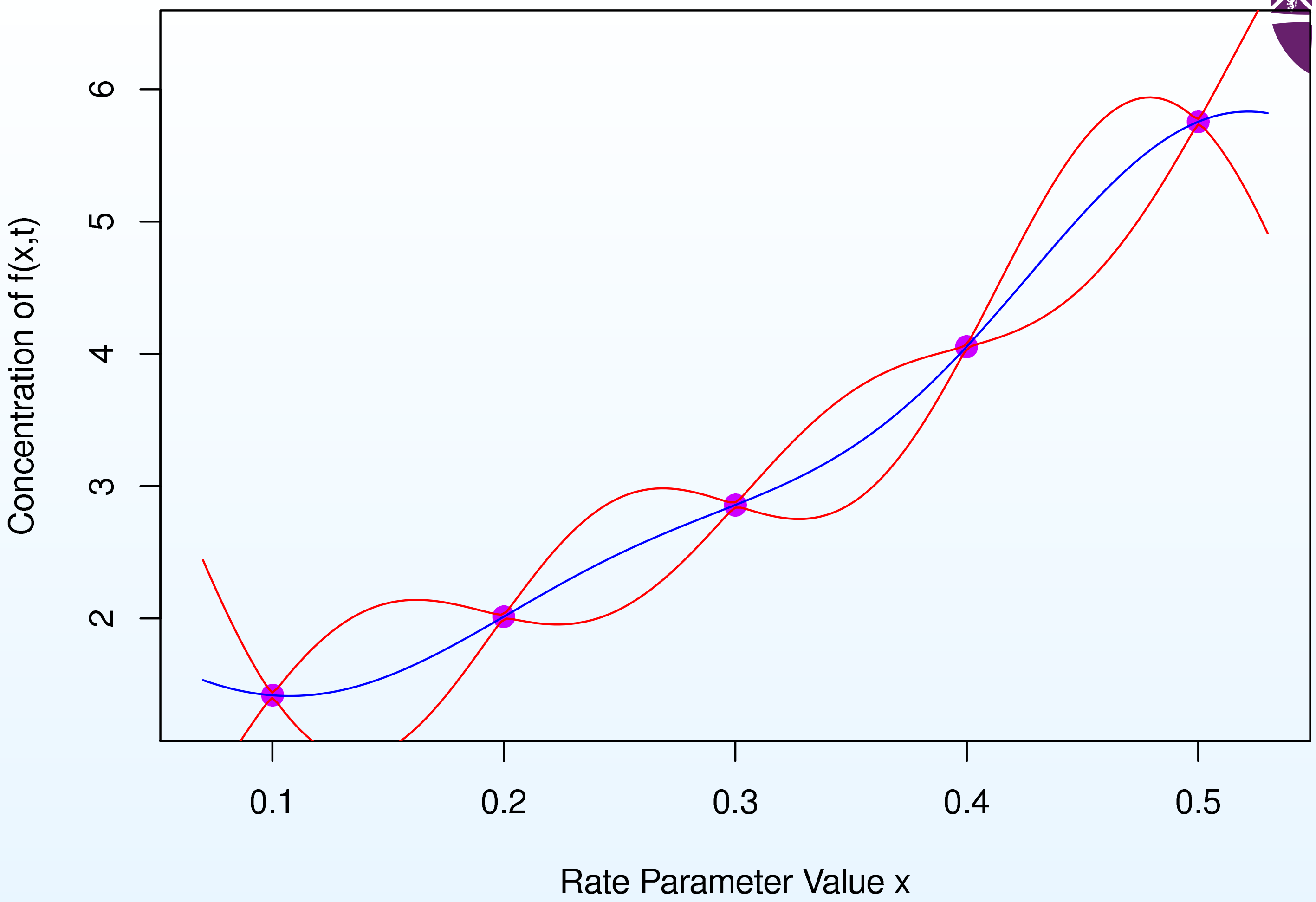
(or a more complex version of this form).

Emulators and history matching



We have made five evaluations of the function $f(x)$.

Suppose that we now build an emulator for $f(x)$ based on these five points.



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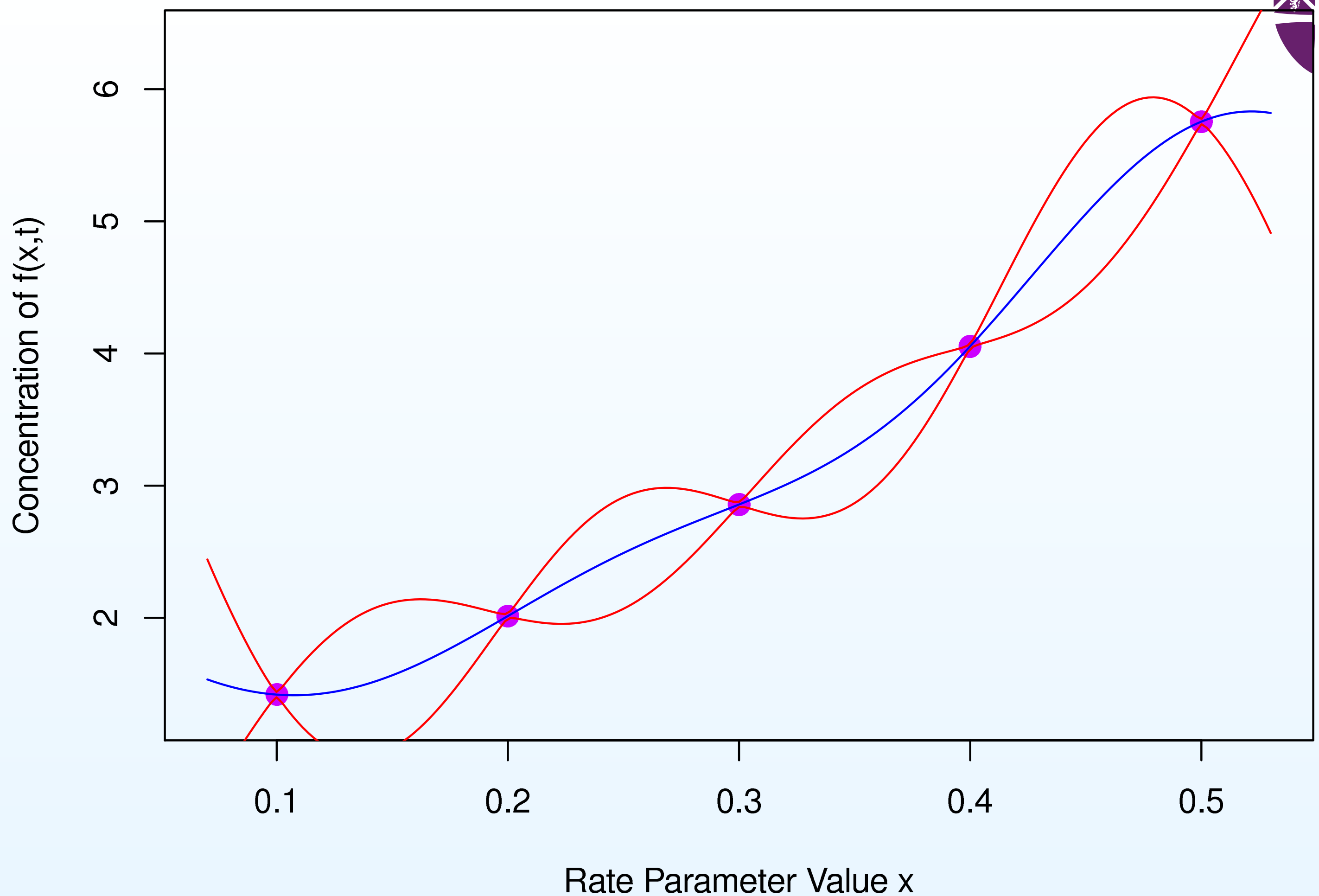
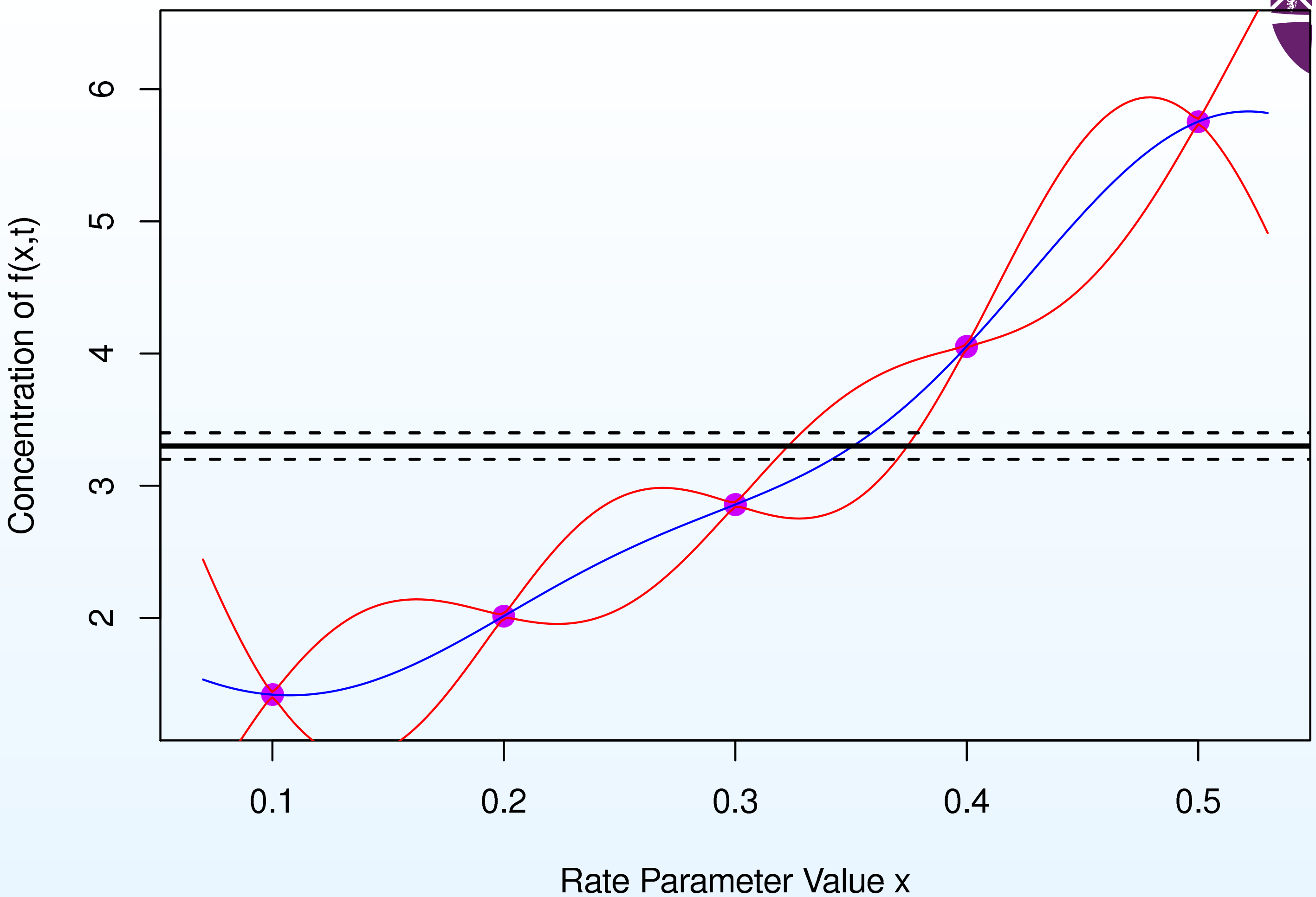


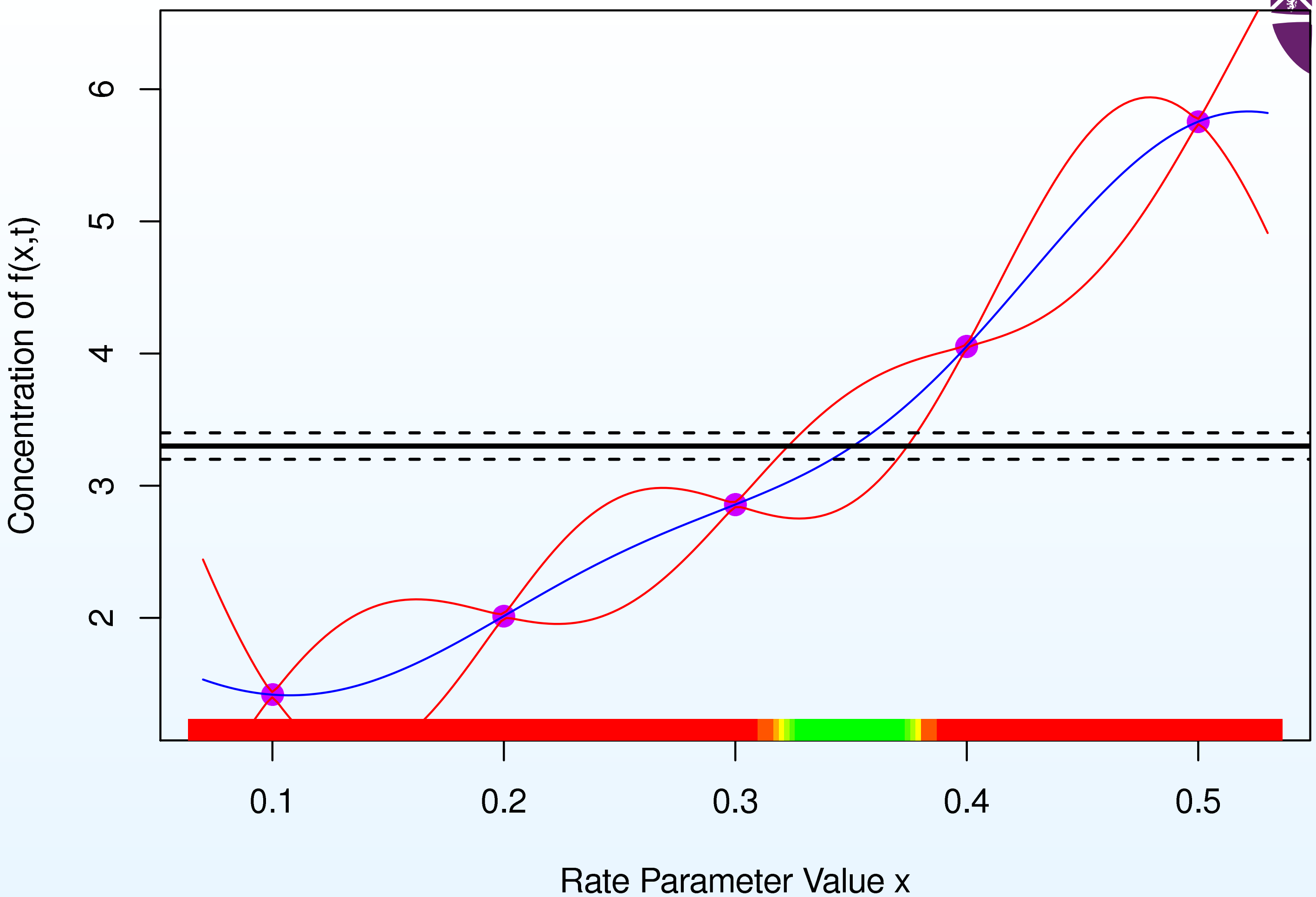
The emulator can be used to represent our beliefs about the behaviour of the model at untested values of x, and is fast to evaluate.

It gives both the expected value of $f(x)$ (the blue line) along with a credible interval for $f(x)$ (the red lines) representing uncertainty about the model's behaviour.

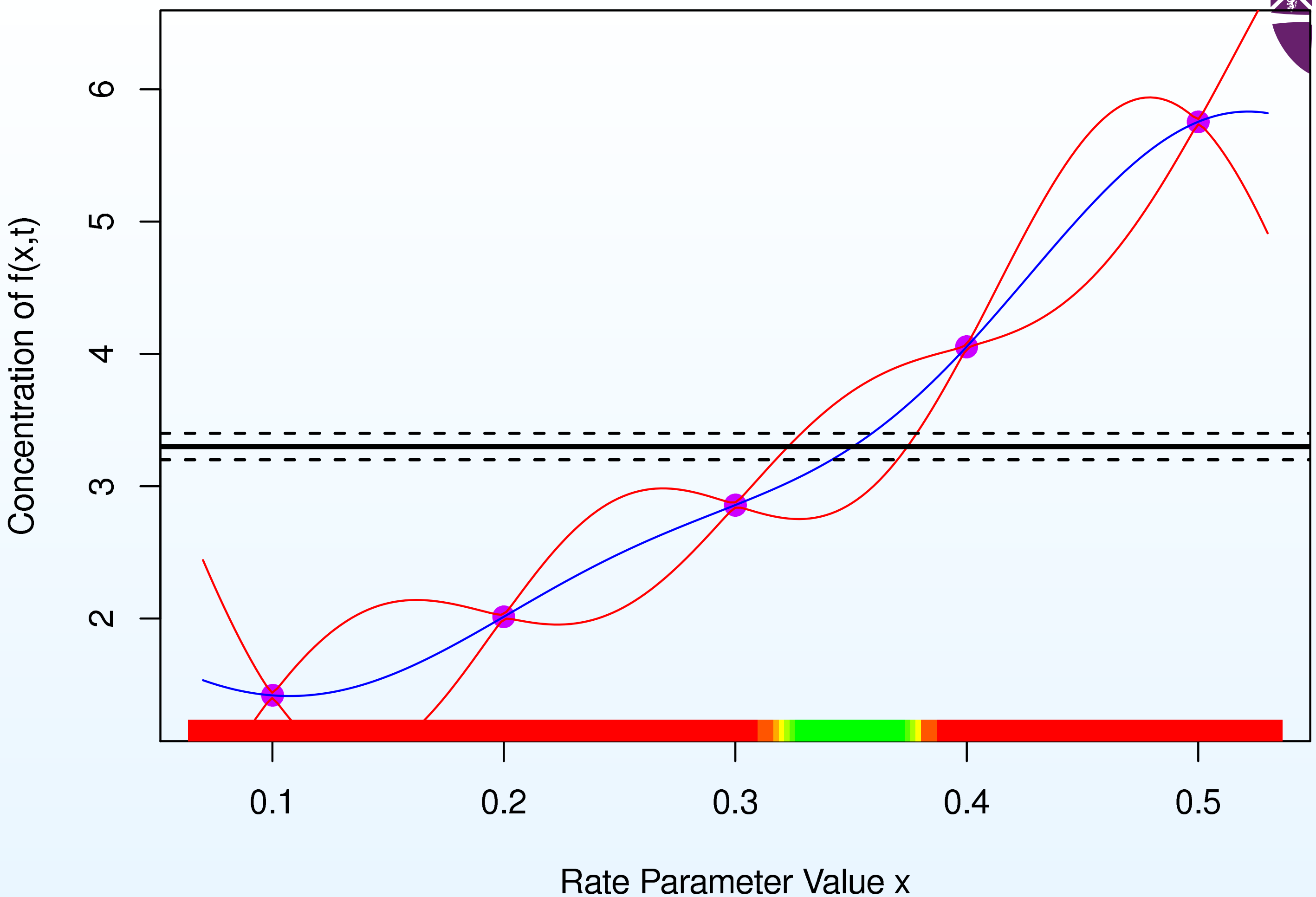


Suppose that we have an observation (represented by the black line with observational errors bounds).

Comparing the emulator to the observed measurement we can identify the set of x values which are “not inconsistent” with this data.

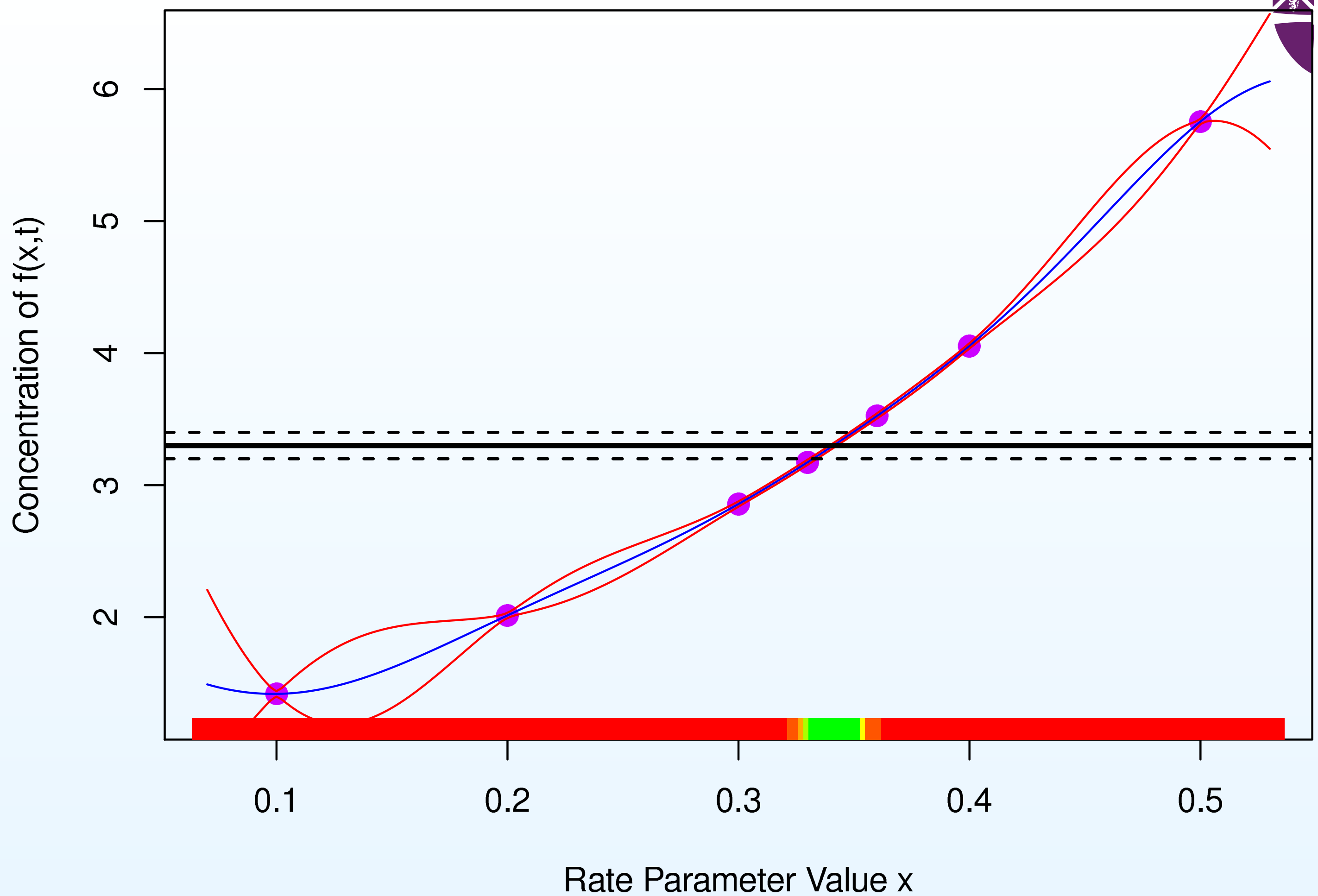


Comparing the emulator to the observed measurement we have identified the set of x values (the green values) which “match” the observed history, when we take into account all of the uncertainties (here, measurement and emulator error).



We now remove all of the implausible x values (the red values) and resample and re-emulate within the green region.

We perform a 2nd iteration or wave of runs to improve emulator accuracy. The runs are located only at non-implausible (green/yellow) points.



Now the emulator is more accurate than the observation, and we can identify the set of all x values of interest.

Emulation for history matching

History matching is an iterative procedure.

At each wave,
[1] we take a sample in the current green space,
[2] refit our emulator(s)
[3] eliminate as much of the green space as we can.

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We only need accurate emulation of the simulator in the region close to the output match.

Further, if we are matching many outputs, then at each wave of history matching we only need to emulate those outputs which are relatively straightforward to emulate at that stage.

(As the green space shrinks, the behaviour of complex functions often simplifies.)

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Identify a key collection of outputs to construct emulators for.

For each of the chosen outputs, $f_i(x)$ say, identify a collection of 'active' inputs, $x_{A(i)}$ say, which are most important in driving variation in that output.
Fit the emulator

$$f_i(x) = \sum_j \beta_{ij} g_{ij}(x_{A(i)}) + u_i(x)$$

and decompose the local residual $u_i(x)$ as the sum of one term involving $x_{A(i)}$, and one term involving all of the other inputs (possibly just a nugget).

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If the model is stochastic, then we also emulate the variance, for example using Bayes linear estimation for the variance of each $f(x)$ given evaluation of some repetitions at chosen design runs.

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We don't judge the simulator to be a perfect representation of reality, so we introduce a structural discrepancy for example viewing the relation between y and $f(x)$ at an acceptable choice of x as $y = f(x) + \epsilon$ with variance σ_ϵ^2.

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We use an 'implausibility measure' $I(x)$ based on a probabilistic metric such as

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The package is customised for epidemic models, but the underlying methodology is fully general.

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105 countries were successfully matched (i.e. producing many parameter choices which match history)

The remaining 9 countries revealed evidence of model or data misspecification.

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Use the collections β_i^*, u_i^* as priors for our judgements for the elements of the emulator for the slow simulator

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J. Cumming, M. Goldstein Bayes Linear Uncertainty Analysis for Oil Reservoirs Based on Multiscale Computer Experiments (2009), in the Handbook of Applied Bayesian Analysis,eds A. O'Hagan, M. West, OUP

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In such cases, when using an emulator of form $f_i(x) = \sum_j \beta_{ij} g_{ij}(x_{A(i)}) + u_i(x)$, it is the global part of the emulator $\sum_j \beta_{ij} g_{ij}(x_{A(i)})$ which dominates the emulator prediction.

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So this form needs to be chosen carefully for scientific plausibility and needs to be subjected to careful diagnostic testing.

Varying coefficient emulators

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For how these are fitted and used for computer design problems, see **Wilson, Amy L., Goldstein, Michael & Dent, Chris J.** (2022). Varying Coefficient Models and Design Choice for Bayes Linear Emulation of Complex Computer Models with Limited Model Evaluations. SIAM/ASA Journal on Uncertainty Quantification 10(1): 350-378.

Limitations of physical models

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Neither of these approximations invalidates the modelling process.

Problems only arise when we forget these simplifications and confuse the analysis of the model with the corresponding analysis for the physical system itself.

Structural discrepancy

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(ii) **External discrepancy**

This arises from the inherent limitations of the modelling process embodied in the simulator.

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Sometimes, this is called **reification**,
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This analysis is tractable even for large systems. Careful discrepancy assessment will

(i) correct our overconfidence in our projections
(by adding appropriate levels of additional uncertainty)

(ii) increase our forecast accuracy
(by correcting for systematic biases in our simulator).

Forecasting

Suppose that we want to predict some future outcome y_p, given observed historical data on earlier values z_h. The Bayes linear update of y_p given z_h requires the joint variance structure of y_p, z_h.

This can be derived directly from the decomposition

$$y = f(x^*) + \epsilon^*, \; z_h = y_h + e$$

This analysis is tractable even for large systems. Careful discrepancy assessment will

(i) correct our overconfidence in our projections
(by adding appropriate levels of additional uncertainty)

(ii) increase our forecast accuracy
(by correcting for systematic biases in our simulator).

Goldstein, M. and Rougier, J. C. (2006) 'Bayes linear calibrated prediction for complex systems.', Journal of the American Statistical Association.

Optimisation via history matching

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Du, Hailiang, Sun, Wei, Goldstein, Michael & Harrison, Gareth (2021). Optimization via Statistical Emulation and Uncertainty Quantification: Hosting Capacity Analysis of Distribution Networks. IEEE Access 9: 118472-118483.

Systems integration

Much systems work involves individual systems talking to each other. So, for example, we might have system one, $f_1(x)$, whose output y forms an input to system two , $f_2(y, w)$. The way to assess uncertainty for the combined system, over the whole range of input choices, is

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Oughton, R, Goldstein, M. & Hemmings, J. (2022). Intermediate Variable Emulation: using internal processes in simulators to build more informative emulators. SIAM/ASA Journal on Uncertainty Quantification: 268-293.

Concluding comments

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Reminder: here's the HMER project web-page

https://hmer-package.github.io/website/