Bayesian Design Criterion for iterative refocussing

Victoria Volodina [1] and Daniel B. Williamson [1,2]

MASCOT NUM 2021

[1] The Alan Turing Institute

[2] University of Exeter

Overview

[1] The Alan Turing Institute

[2] University of Exeter

Uncertainty Quantification

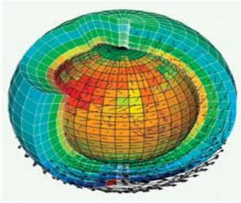
[1] The Alan Turing Institute

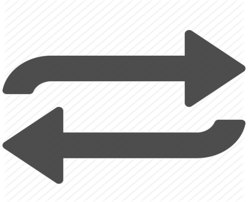
[2] University of Exeter

Uncertainty Quantification

Inferences based on complex computer models require **careful consideration and account of uncertainties**. The main sources of uncertainty are

- Parameter uncertainty
- Model error
- Code uncertainty





[1] The Alan Turing Institute

[2] University of Exeter

Complex computer models

- We represent a **complex computer model** as a **function** f that **gives a vector of outputs** $f(\mathbf{x})$ and which requires **a vector of input parameters** $\mathbf{x}$.
- Cheap surrogates (emulators) such as **neural networks, splines** and **polynomial chaos** could be used to approximate computer model behaviour across the input space, $\mathcal{X}$.
- **Gaussian Process (GP) emulators**, a non-parametric class of surrogate models, have become increasingly popular due to their flexibility as no assumptions about the form of simulator response are required.

[1]The Alan Turing Institute

[2]University of Exeter

Gaussian Process (GP) Emulation

We define a statistical model to represent $f(\mathrm{x})$

$$f(\mathrm{x}) = h(\mathrm{x})^T\beta + \epsilon(\mathrm{x}) + \nu(\mathrm{x}),$$

- **Residual term** $\epsilon(\mathrm{x}) \sim \mathrm{GP}\left(0, \sigma^2 r(\cdot, \cdot; \delta)\right)$
- **Nugget process term** $\nu(\mathrm{x}) \sim \mathrm{N}\left(0, \tau^2\right)$

[1] The Alan Turing Institute

[2] University of Exeter

Gaussian Process (GP) Emulation

The prior specification for $f(\mathbf{x})$

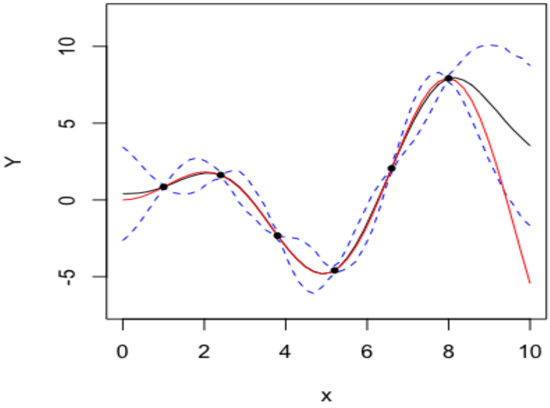
$$f(\mathbf{x})|\beta, \sigma^2, \delta, \tau^2 \sim \mathsf{GP}\Big(h(\mathbf{x})^T\beta, k(\cdot,\cdot;\sigma^2,\delta,\tau^2)\Big),$$

$$\mathsf{E}\Big[f(\mathbf{x})\Big] = h(\mathbf{x})^T\beta$$
$$\mathsf{Cov}\Big[f(\mathbf{x}), f(\mathbf{x}')\Big] = k(\mathbf{x},\mathbf{x}';\sigma^2,\delta,\tau^2) = \sigma^2 r(\mathbf{x},\mathbf{x}';\delta) + \mathbb{1}\Big\{\mathbf{x} = \mathbf{x}'\Big\}$$

We proceed to obtaining computer model runs $\mathrm{F} = \Big(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n)\Big)$ at design points $\mathrm{X} = \Big(\mathbf{x}_1, \ldots, \mathbf{x}_n\Big)$ and perform Bayesian updating for $f(\mathbf{x})$.

[1]The Alan Turing Institute

[2]University of Exeter



[1] The Alan Turing Institute

[2] University of Exeter

Inverse problem. Calibration

'Best Input Approach' to link the model $f(\mathbf{x})$ to the real system y via

$$y = f(\mathbf{x}^*) + \eta(\mathbf{x}),$$

where $\eta(\mathbf{x})$ is a **model discrepancy term** with model discrepancy error Var$[\eta(\mathbf{x})]$.
We relate the true system y to the observation z via

$$z = y + e,$$

where e is the **observation error term** with the variance of the observation error Var$[e]$.

[1] The Alan Turing Institute

[2] University of Exeter

History matching. Implausibility measure

Define an **implausibility function**:

$$\mathcal{I}(\mathbf{x}) = \frac{|z - \mathsf{E}[f(\mathbf{x})]|}{\sqrt{\mathsf{Var}[f(\mathbf{x})] + \mathsf{Var}[\eta(\mathbf{x})] + \mathsf{Var}[e]}}.$$

A threshold value a is chosen so that any value of $\mathcal{I}(\mathbf{x}) > a$ is deemed implausible.

The remaining parameter space is termed as **Not Ruled Out Yet (NROY)** and defined as

$$\mathcal{X}_{NROY} = \left\{\mathbf{x} \in \mathcal{X} : \mathcal{I}(\mathbf{x}) \leq a\right\}.$$

[1]The Alan Turing Institute

[2]University of Exeter

History matching. Refocussing

We choose an initial ensemble design $\mathrm{X}_{[1]} \in \mathcal{X}$, defined as

$$\mathrm{X}_{[1]} = \left(\mathbf{x}_{1,1}, \ldots, \mathbf{x}_{1,n_1}\right)^T,$$

and produce computer model runs at the intial design, $\mathrm{F}_{[1]}$

$$\mathrm{F}_{[1]} = \left(f(\mathbf{x}_{1,1}), \ldots, f(\mathbf{x}_{1,n_1})\right)^T.$$

Based on the generated ensemble, we construct an emulator and obtain

$$\mathcal{X}^1 = \left\{\mathbf{x} \in \mathcal{X} : \mathcal{I}(\mathbf{x}; \mathrm{F}_{[1]}) \leq a\right\}.$$

The whole process of deriving NROY space $\mathcal{X}^1$ is called **wave 1**.

[1]The Alan Turing Institute

[2]University of Exeter

History matching. Refocusing

To perform wave $k > 1$ of history matching

1. Generate design $\mathrm{X}_{[k]} \in \mathcal{X}^{k-1}$ and obtain computer model runs $\mathrm{F}_{[k]}$.
2. Obtain an updated distribution for $f(\mathrm{x})$

$$\pi_k\Big(f(\mathrm{x})\Big) \propto \pi_{k-1}\Big(f(\mathrm{x})\Big) \times p\Big(\mathrm{F}_{[k]} | \langle \mathrm{F} \rangle_{[k-1]}, f(\mathrm{x})\Big),$$

   where $\langle \mathrm{F} \rangle_{[k-1]} = \Big(\mathrm{F}_{[1]}, \ldots, \mathrm{F}_{[k-1]}\Big)$.

3. For $\mathrm{x} \in \mathcal{X}^{k-1}$ compute $\mathcal{I}(\mathrm{x}; \langle \mathrm{F} \rangle_{[k]}) = \frac{|z - \mathsf{E}[f(\mathrm{x}) | \langle \mathrm{F} \rangle_{[k]}]|}{\sqrt{\mathsf{Var}[f(\mathrm{x}) | \langle \mathrm{F} \rangle_{[k]}] + \mathsf{Var}[e] + \mathsf{Var}[\eta]}}$.
4. Obtain NROY space $\mathcal{X}^k = \Big\{\mathrm{x} \in \mathcal{X}^{k-1} : \mathcal{I}(\mathrm{x}; \langle \mathrm{F} \rangle_{[k]}) \leq a\Big\}$.

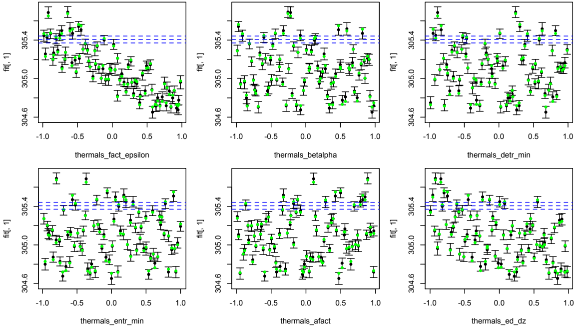
[1] The Alan Turing Institute

[2] University of Exeter

Climate model example

Introduce new
parameters to climate model.

Use statistical
tools to obtain parameter
values that matches model
output with the observation.



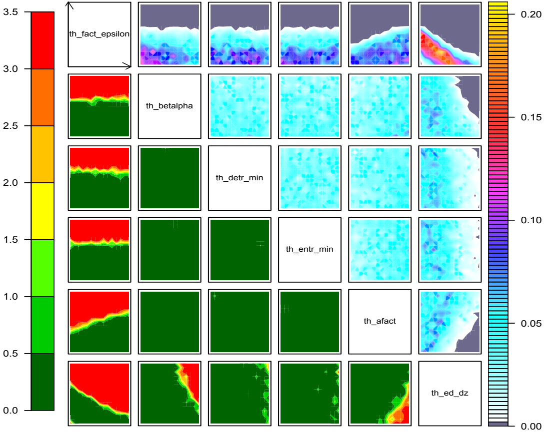


Figure: After performing wave 2 of history matching the size of NROY space, $\mathcal{X}^2$, is 4% of original input space, $\mathcal{X}$.

[1]The Alan Turing Institute

[2]University of Exeter

Design for iterative refocussing

[1] The Alan Turing Institute

[2] University of Exeter

Current approaches

The following methods were adopted for generating design for each wave of history matching:

- **Rejection sampling** [2]: generate latin hypercubes over the full space and only keeping those points that are not ruled out by history matching.
- **Space-filling** [1]: maximin design in NROY space.
- **Implausibility Driven Evolutionary Monte Carlo algorithm** (IDEMC) to obtain a uniform design for history matching [5].
- **Subset Simulation (SuS)** technique to sample from NROY space [3, 4].

Bayesian Design Criterion. Loss function:

$$L(V_{\mathcal{X}^{k+1}}, V_{\mathcal{X}_T}; \xi) = \int_{\mathcal{X}} \Big(\mathbb{1}\{\mathbf{x} \in \mathcal{X}^{k+1}\} - \mathbb{1}\{\mathbf{x} \in \mathcal{X}_T\} \Big)^2 d\mathbf{x},$$

– the **'truth'**, volume of 'true' NROY space:

$$V_{\mathcal{X}_T} = \int_{\mathcal{X}} \mathbb{1}\{\mathbf{x} \in \mathcal{X}_T\} d\mathbf{x} = \int_{\mathcal{X}} \mathbb{1}\left\{ \frac{|z - f(\mathbf{x})|}{\sqrt{\mathsf{Var}[e] + \mathsf{Var}[\eta]}} \le a \right\} d\mathbf{x}$$

– a **decision**, a volume of NROY space at wave $k+1$

$$V_{\mathcal{X}^{k+1}} = \int_{\mathcal{X}^k} \mathbb{1}\{\mathbf{x} \in \mathcal{X}^{k+1}\} d\mathbf{x}$$

$$= \int_{\mathcal{X}^k} \mathbb{1}\left\{ \frac{|z - \mathsf{E}[f(\mathbf{x}) | \langle \mathrm{F} \rangle_{[k]}, f(\xi)]|}{\sqrt{\mathsf{Var}[f(\mathbf{x}) | \langle \mathrm{F} \rangle_{[k]}, f(\xi)] + \mathsf{Var}[\eta] + \mathsf{Var}[e]}} \le a \right\} d\mathbf{x}$$

[1]The Alan Turing Institute

[2]University of Exeter

Since we do not know the **'truth'**, we have to operate with the **expected loss**:

$$
\begin{aligned}
\Psi(\xi) &= \int\int L(V_{\mathcal{X}^{k+1}}, V_{\mathcal{X}_T}; \xi)\pi(V_{\mathcal{X}^{k+1}}, V_{\mathcal{X}_T}; \xi) dV_{\mathcal{X}^{k+1}} dV_{\mathcal{X}_T} \\
&= \int\int L(V_{\mathcal{X}^{k+1}}, V_{\mathcal{X}_T}; \xi)\pi(f(\mathrm{x})|f(\xi), \langle \mathrm{F} \rangle_{[k]})\pi(f(\xi)|\langle \mathrm{F} \rangle_{[k]}) df(\mathrm{x}) df(\xi) \\
&= \Psi_1(\xi) - 2 \times \Psi_2(\xi) + \Psi_3(\xi)
\end{aligned}
$$

Bayesian Optimal Design for wave $k+1$, ξ^*, is obtained by minimizing the expected loss function, $\Psi(\xi)$, i.e.

$$\xi^* = \arg\min \Psi(\xi).$$

[1]The Alan Turing Institute

[2]University of Exeter

Bayesian Design Criterion. $\Psi_1(\xi)$ component

The first term of the expected loss function, $\Psi_1(\xi)$, corresponds to the expected volume of NROY space at wave $k+1$.

$$\Psi_1(\xi) = \int \int_{\mathcal{X}^k} \mathbb{1}\left\{ \frac{|z - \mathsf{E}[f(\mathrm{x})|\langle \mathrm{F} \rangle_{[k]}, f(\xi)]|}{\sqrt{\mathsf{Var}[e] + \mathsf{Var}[\eta] + \mathsf{Var}[f(\mathrm{x})|\langle \mathrm{F} \rangle_{[k]}, f(\xi)]}} \leq a \right\}$$
$$\times\ \pi\Big(f(\xi)|\langle \mathrm{F} \rangle_{[k]}\Big) d\mathrm{x} df(\xi)$$

[1]The Alan Turing Institute

[2]University of Exeter

Bayesian Design Criterion. $\Psi_3(\xi)$ component

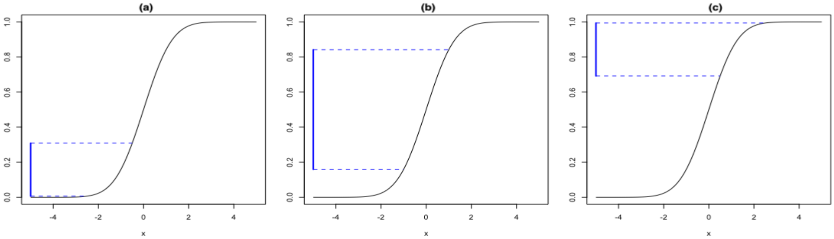
The third term of the expected loss function, $\Psi_3(\xi)$, corresponds to the expected volume of 'true' NROY space.

$$\Psi_3(\xi) = \int \int_{\mathcal{X}^k} \Big[\Phi(s_2) - \Phi(s_1)\Big] \pi\Big(f(\xi) | \langle \mathrm{F} \rangle_{[k]}\Big) d\mathbf{x} df(\xi)$$

with

$$s_2 = \frac{z + a\sqrt{\mathrm{Var}[e] + \mathrm{Var}[\eta]} - \mathrm{E}[f(\mathbf{x}) | \langle \mathrm{F} \rangle_{[k]}, f(\xi)]}{\sqrt{\mathrm{Var}[f(\mathbf{x}) | \langle \mathrm{F} \rangle_{[k]}, f(\xi)]}}$$

$$s_1 = \frac{z - a\sqrt{\mathrm{Var}[e] + \mathrm{Var}[\eta]} - \mathrm{E}[f(\mathbf{x}) | \langle \mathrm{F} \rangle_{[k]}, f(\xi)]}{\sqrt{\mathrm{Var}[f(\mathbf{x}) | \langle \mathrm{F} \rangle_{[k]}, f(\xi)]}}$$

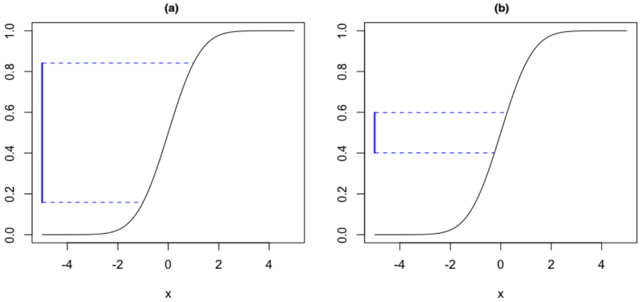


- (a): $s_1, s_2 < 0$, i.e. $\mathsf{E}[f(\mathbf{x})|\langle \mathrm{F}\rangle_{[k]}, f(\xi)] > z + a\sqrt{\mathsf{Var}[e] + \mathsf{Var}[\eta]}$
- (b): $s_2 > 0, s_1 < 0$, i.e.

$$z - a\sqrt{\mathsf{Var}[e] + \mathsf{Var}[\eta]} < \mathsf{E}[f(\mathbf{x})|\langle \mathrm{F}\rangle_{[k]}, f(\xi)] < z + a\sqrt{\mathsf{Var}[e] + \mathsf{Var}[\eta]}$$

- (c): $s_2, s_1 > 0$, i.e. $\mathsf{E}[f(\mathbf{x})|\langle \mathrm{F}\rangle_{[k]}, f(\xi)] < z - a\sqrt{\mathsf{Var}[e] + \mathsf{Var}[\eta]}$

[1] The Alan Turing Institute
[2] University of Exeter



- (a) low values of $\text{Var}[f(\mathrm{x}) | \langle \mathrm{F} \rangle_{[k]}, f(\xi)]$
- (b) large values of $\text{Var}[f(\mathrm{x}) | \langle \mathrm{F} \rangle_{[k]}, f(\xi)]$

[1]The Alan Turing Institute

[2]University of Exeter

Bayesian Design Criterion. $\Psi_2(\xi)$ component

The second term of the expected loss function, $\Psi_2(\xi)$, corresponds to the expected volume of the input region that is in both wave $k+1$ NROY space and ‘true’ NROY.

$$\Psi_2(\xi) = \int \int_{\mathcal{X}^k} \mathbb{1}\left\{ \frac{|z - \mathsf{E}[f(\mathrm{x})|\langle \mathrm{F} \rangle_{[k]}, f(\xi)]|}{\sqrt{\mathsf{Var}[e] + \mathsf{Var}[\eta] + \mathsf{Var}[f(\mathrm{x})|\langle \mathrm{F} \rangle_{[k]}, f(\xi)]}} \leq a \right\}$$

$$\times \left[\Phi(s_2) - \Phi(s_1)\right] \pi\left(f(\xi)|\langle \mathrm{F} \rangle_{[k]}\right) d\mathrm{x} df(\xi),$$

red component corresponds to the integrand function in $\Psi_1(\xi)$ and
blue component corresponds to the integrand function in $\Psi_3(\xi)$.

Implementation details

1. Estimate the GP hyperparameters θ using computer model runs, $\mathtt{F}_{[1]}$, from the initial design $\mathtt{X}_{[1]}$. Fix GP hyperparameters at MAP values θ_{MAP}, perform history matching to obtain wave 1 NROY space, $\mathcal{X}^1$.
2. At wave $k > 1$, set $\langle \mathtt{X} \rangle_{[k+1]} = (\langle \mathtt{X} \rangle_{[k]}^T, \xi^T)^T$ and obtain ξ by optimizing a design criterion with respect to the proposed additional runs. Continuous optimizations are carried out using Fedorov exchange (Fedorov, 1972).
3. Set $\mathtt{X}_{[k+1]} = \xi^*$ and collect computer model runs from $\mathtt{X}_{[k+1]}$ and re-estimate the GP hyperparametres using the entire set of runs from the augmented design $\langle \mathtt{X} \rangle_{[k+1]}$. Perform history matching to obtain wave $k+1$ NROY space, $\mathcal{X}^{k+1}$.
4. Repeat steps (2) and (3) until termination. Relevant stopping criteria include exhaustion of the experimental budget or minor (no change) in the size of NROY space.

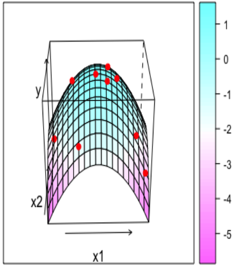
[1] The Alan Turing Institute

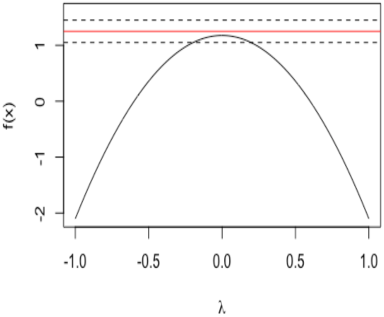
[2] University of Exeter

Toy example

[1] The Alan Turing Institute

[2] University of Exeter



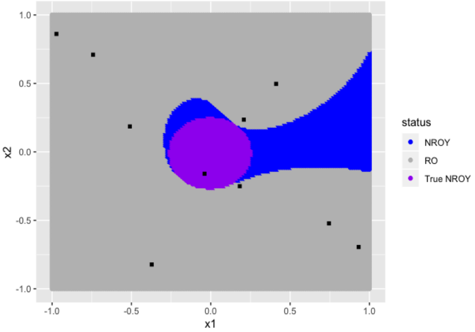


Range	z	Var$[e]$	Var$[\eta]$	Sample size (n_1)	NROY size	a
$[-2, 1]$	1.25	0.1^2	0	10	5.4%	3

Table: Toy model information for history matching.

[1] The Alan Turing Institute
[2] University of Exeter

Wave 1 History matching

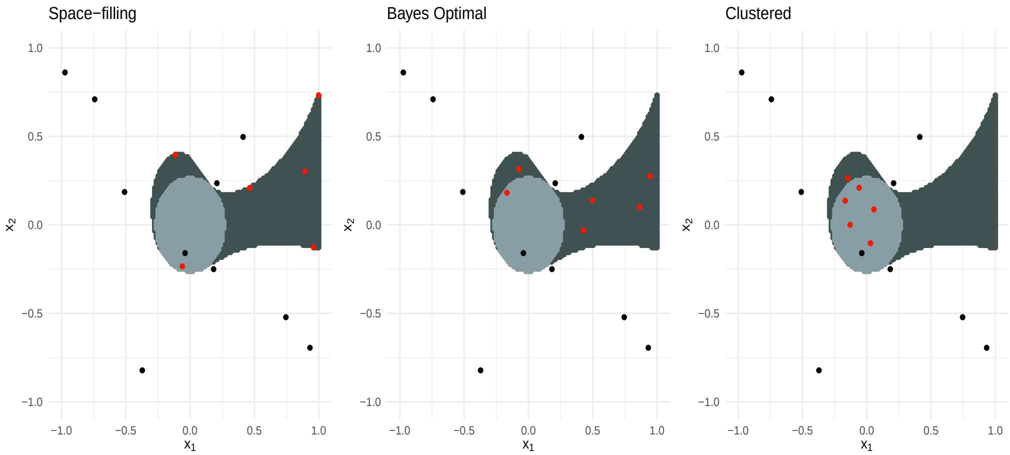


By performing Wave 1 of history matching we obtained NROY space, $\mathcal{X}^1$, of size 15.56% of original input space, $\mathcal{X}$.

[1] The Alan Turing Institute

[2] University of Exeter

Candidate designs



[1]The Alan Turing Institute

[2]University of Exeter

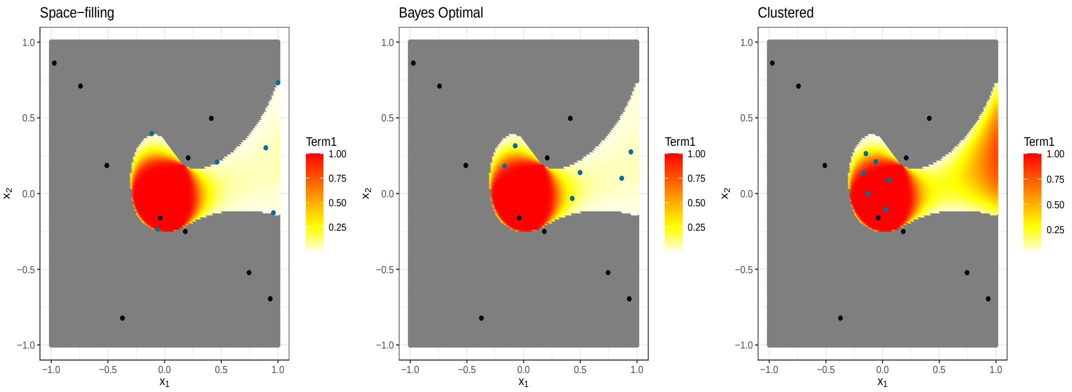
Type	Bayesian design criterion	std. error
space-filling	0.0152	9×10^{-5}
Bayes optimal	0.0093	9×10^{-5}
clustered	0.157	26×10^{-4}

Table: Bayesian design criterion for three candidate designs. The second and third columns correspond to the score and standard error on the score respectively.

Type	$\Psi_1(\xi)$	$\Psi_2(\xi)$	$\Psi_3(\xi)$
space-filling	0.419	0.408	0.413
Bayes optimal	0.417	0.411	0.413
clustered	0.560	0.407	0.412

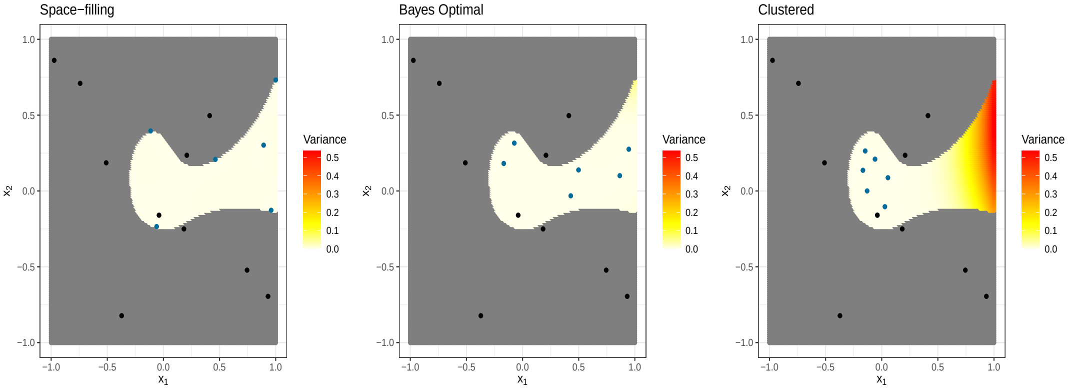
Table: Individual terms of Bayesian design criterion for three candidate designs.

Decomposition of $\Psi_1(\xi)$ component

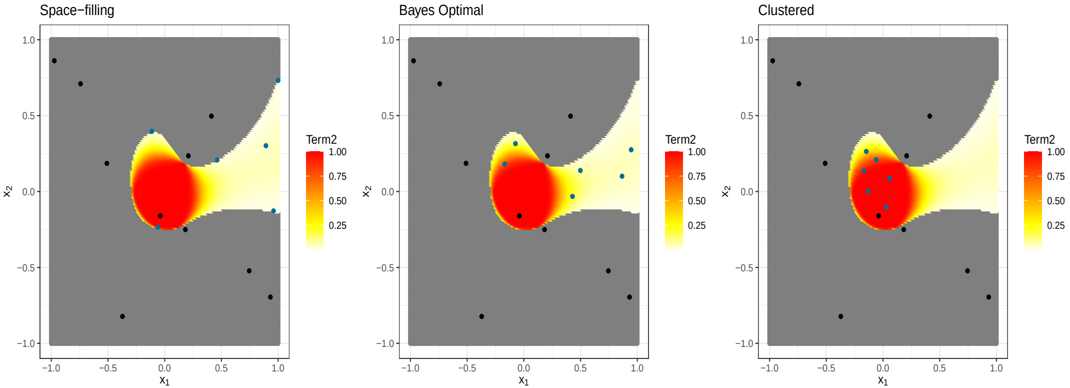


[1]The Alan Turing Institute

[2]University of Exeter


Space−filling
Bayes Optimal
Clustered
Variance
0.5
0.4
0.3
0.2
0.1
0.0
1.0
0.5
0.0
−0.5
−1.0
x_2
x_1

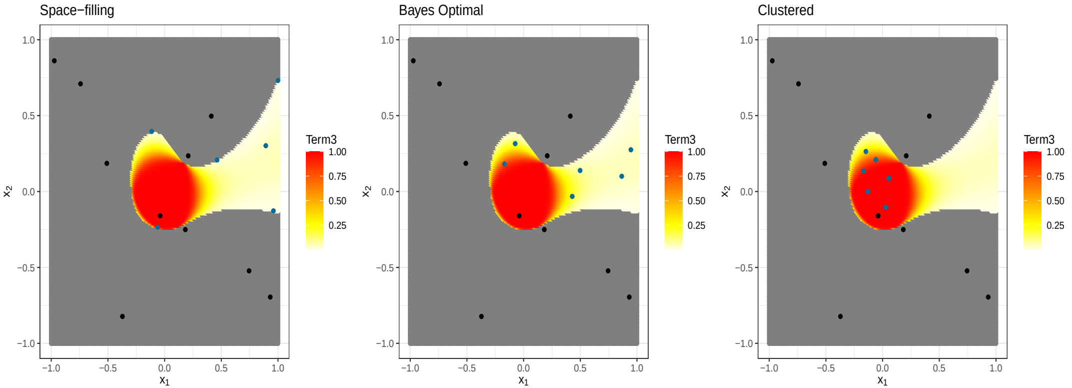
Decomposition of $\Psi_2(\xi)$



[1] The Alan Turing Institute

[2] University of Exeter

Decomposition of $\Psi_3(\xi)$



[1]The Alan Turing Institute

[2]University of Exeter

Wave 2 history matching

Nothing impressive...

Type	NROY size
space-filling	5.23%
Bayes optimal	5.27%
clustered	5.28%

Table: Summary of history matching results after Wave 2 with candidate designs.

[1] The Alan Turing Institute

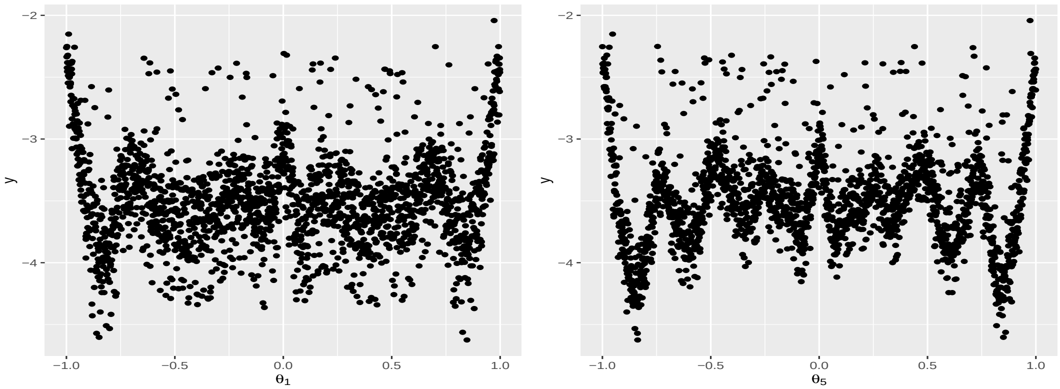
[2] University of Exeter

Beam displacement example

[1] The Alan Turing Institute

[2] University of Exeter

Figure: Mean displacement value plotted against θ_1 and θ_5.

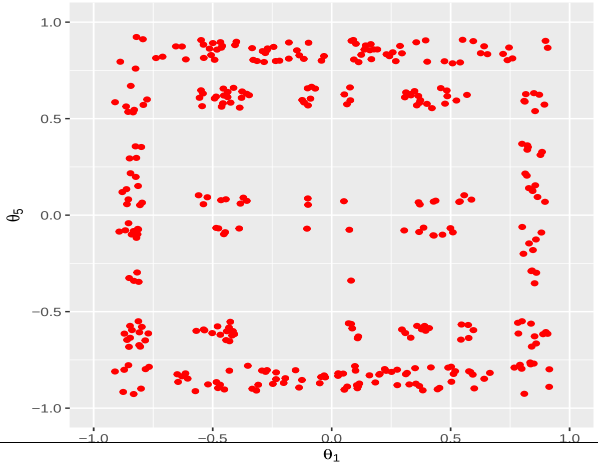


Specify $z = -4$, Var$[\eta] = 0$ and Var$[e] = 0.005$. Set threshold value a at 3.

[1] The Alan Turing Institute

[2] University of Exeter

Figure: Representation of "true" NROY space. Red points correspond to input values at which computer model output is close to observation z based on the implausibility function.



[1]The Alan Turing Institute

[2]University of Exeter

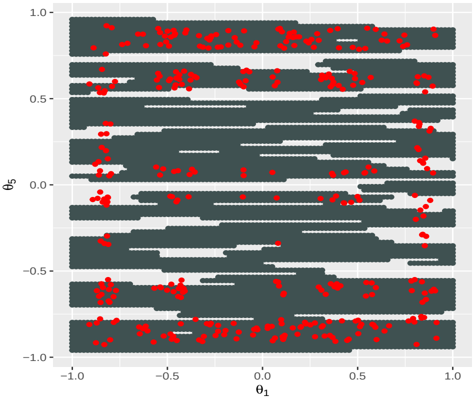


Figure: Grey points correspond to those points classified as being in NROY space after one wave. Points in red correspond to the "true" NROY space. The wave 1 NROY space $\mathcal{X}^1$ consists of 68.65% of the full space $\mathcal{X}$.

[1]The Alan Turing Institute

[2]University of Exeter

Design for subsequent waves

For later waves, new design of 100 runs are sampled from the current NROY space. We use our proposed Bayesian design criterion to rank three different design options. At each wave, we have 3 potential candidates:

1. Space-filling design [1]
2. Random design: choose 100 design points from the previous wave NROY space
3. Maximum variance design: choose 100 design points from the previous wave NROY space with high variance (sampling along the ridges)

[1] The Alan Turing Institute

[2] University of Exeter

Design for subsequent waves

Type	Wave 2	Wave 3	Wave 4
space-filling	0.265 (3×10^{-4})	0.521 (2×10^{-4})	0.254 (2×10^{-4})
random	0.339 (3×10^{-4})	0.552 (2×10^{-4})	0.349 (2×10^{-4})
max variance	0.576 (2×10^{-4})	0.561 (2×10^{-4})	0.303 (2×10^{-4})

Table: Bayesian design criterion for three candidate designs with standard error in brackets.

[1] The Alan Turing Institute

[2] University of Exeter

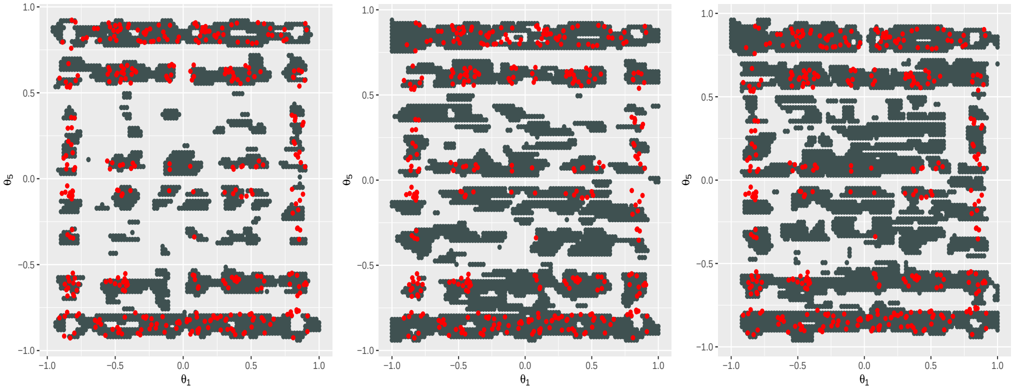


Figure: Grey points correspond to those points classified as being in NROY space after four waves of history matching. Points in red correspond to the "true" NROY space.

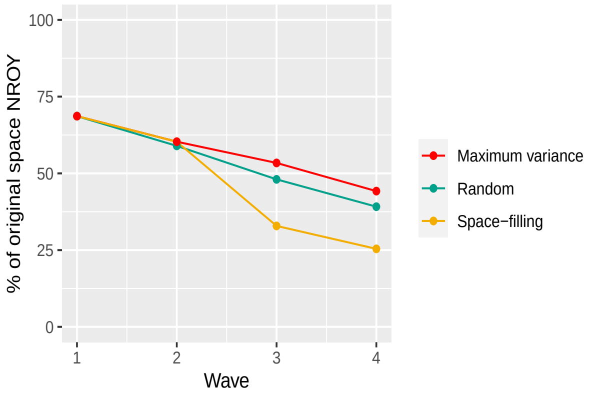


Figure: The progression of the sizes of NROY space.

[1]The Alan Turing Institute

[2]University of Exeter

Final remarks

[1] The Alan Turing Institute

[2] University of Exeter

Final remarks

1. A new approach for obtaining a design for the next wave (iteration) of history matching. Our proposed design criterion is easily decomposed into three meaningful and interpretable terms.
2. It is computationally expensive to obtain ξ^* (multi-dimensional optimization problem), we demonstrate we can use our criterion for ranking.
3. Specification of the number of design points to perform k waves of history matching, as well as the division of runs across waves.
4. Extension to a multi-dimensional Bayesian design criterion.

[1] The Alan Turing Institute

[2] University of Exeter

References I

- Ioannis Andrianakis, Nicky McCreesh, Ian Vernon, Trevelyan J McKinley, Jeremy E Oakley, Rebecca N Nsubuga, Michael Goldstein, and Richard G White.
  Efficient history matching of a high dimensional individual-based hiv transmission model.
  SIAM/ASA Journal on Uncertainty Quantification, 5(1):694–719, 2017.

- Richard G Bower, Michael Goldstein, and Ian Vernon.
  Galaxy formation: a bayesian uncertainty analysis.
  Bayesian analysis, 5(4):619–669, 2010.

References II

ZT Gong, FA DiazDelaO, and M Beer.
Bayesian model calibration using subset simulation.
2017.

ZT Gong, FA DiazDelaO, Peter O Hristov, and M Beer.
History matching with subset simulation.
International Journal for Uncertainty Quantification, 11(5), 2021.

Daniel Williamson and Ian Vernon.
Efficient uniform designs for multi-wave computer experiments.
arXiv preprint arXiv:1309.3520, 2013.

[1] The Alan Turing Institute

[2] University of Exeter