Entropy-based adaptive design for contour finding and estimating reliability

D. Austin Cole[1,2]

Robert B. Gramacy[2], James E. Warner[3], Geoffrey F. Bomarito[3], Patrick E. Leser[3], William P. Leser[3]

DATAWorks

April 13, 2021

[1] austin.cole8@vt.edu

[2] Department of Statistics, Virginia Tech, Blacksburg, VA

[3] NASA Langley Research Center, Hampton, VA

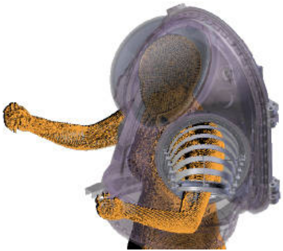
Table of contents

Table of contents

Estimating reliability of a next-generation spacesuit

- NASA needs to assess the probability of impact failure for a new spacesuit design
- There is uncertainty in the material and projectile inputs (X) of the damage simulator
- **Objective**: calculate an unbiased estimate of the probability the response is above a threshold T

$$\alpha = P(Y(x) \geq T)$$



Existing methods to assess reliability

- **Monte Carlo sampling**: draws inputs from uncertainty ($X \sim \mathbb{F}$) distribution and evaluate simulation model
- **Importance sampling (IS)**: constructs a distribution $\mathbb{F}^\star$ biased toward the failure region(s) to draw inputs

$$\hat{\alpha}_{\mathrm{IS}} = \frac{1}{M^\star} \sum_{i=1}^{M^\star} \mathbb{1}_{\{Y(\mathrm{x}_i^\star) > T\}} w(\mathrm{x}_i^\star) \quad \text{via weights} \quad w(\mathrm{x}^\star) = \frac{f(\mathrm{x}^\star)}{f_\star(\mathrm{x}^\star)}$$

- **Multifidelity importance sampling (MFIS)**: uses a surrogate model $\mathcal{S}_N$, like a Gaussian process (GP), to construct the bias distribution $\mathbb{F}^\star$
- **Adaptive designs** for contour finding: sequentially select design points to estimate failure boundary $\{x : Y(x) = T\}$

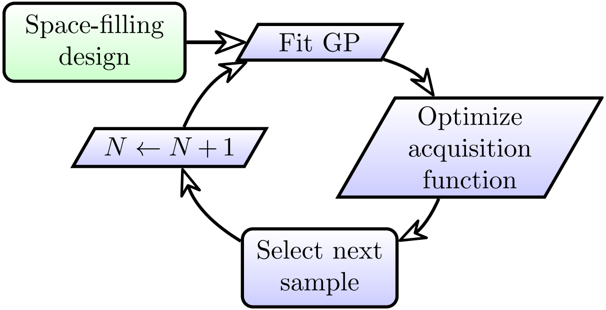
Gaussian process surrogate

- Assume the response Y_N follows a multivariate normal distribution, $Y_N \sim \mathcal{N}_N(0, \Sigma_N)$, where $\Sigma_N = \nu K_N$
- Includes hyperparameters: $\psi = \{\nu(\text{scale}), \theta(\text{lengthscale})\}$
- The correlation matrix K_N is defined as a function $k_\theta(x_i, x_j)$ of the squared Euclidean distance between inputs x_i, x_j
- Conditional predictive equations:

$$\mu_N(x|X_N, Y_N, \psi) = \Sigma(x, X_N)\Sigma_N^{-1} Y_N$$

$$\sigma_N^2(x|X_N, \psi) = \Sigma(x, x) - \Sigma(x, X_N)\Sigma_N^{-1}\Sigma(x, X_N)^\top$$

Adaptive Design for Contour Location



Existing acquisition functions based upon:

- Predictive variance (Picheny et al., 2010)
- Expected Improvement (Ranjan et al., 2008)
- Entropy (Marques et al., 2018): $-\sum_{i=1}^{k} \mathbb{P}(w_i) \log \mathbb{P}(w_i)$, with events w_i and probability mass $\mathbb{P}(w_i)$.

Adaptive Design + MFIS

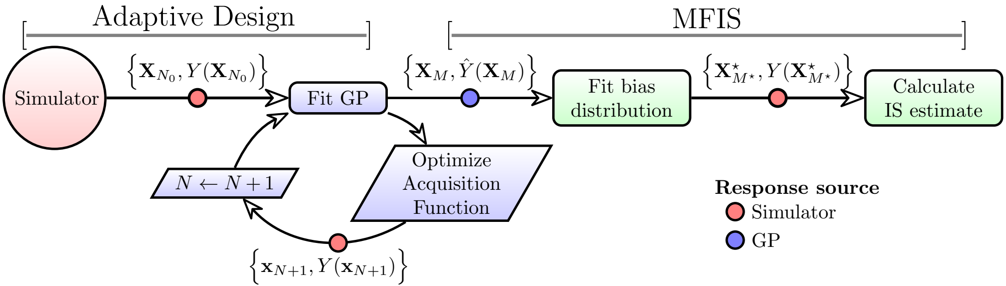


Table of contents

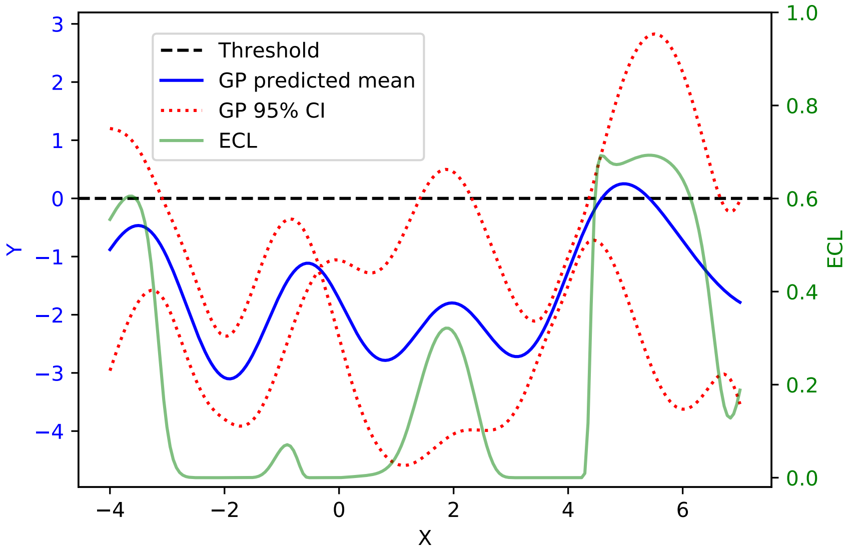
Entropy-based Contour Location

- We define the **Entropy-based Contour Locator (ECL)** using the entropy equation with
  - w_1 representing a failure (i.e. $y > T$)
  - w_2 representing a lack of failure (i.e. $y \leq T$)
- Using a GP $\mathcal{S}_N$'s predictive equations to calculate $\mathbb{P}(w_i)$,

$$\mathrm{ECL}(\mathrm{x} \mid \mathcal{S}_N, T) = -\left(1 - \Phi\left(\frac{\mu_N(\mathrm{x}) - T}{\sigma_N(\mathrm{x})}\right)\right) \log\left(1 - \Phi\left(\frac{\mu_N(\mathrm{x}) - T}{\sigma_N(\mathrm{x})}\right)\right) - \Phi\left(\frac{\mu_N(\mathrm{x}) - T}{\sigma_N(\mathrm{x})}\right) \log\left(\Phi\left(\frac{\mu_N(\mathrm{x}) - T}{\sigma_N(\mathrm{x})}\right)\right)$$

- Design can be done in batches (ECL.b) by updating $\sigma_N(x)$ with other batch design locations

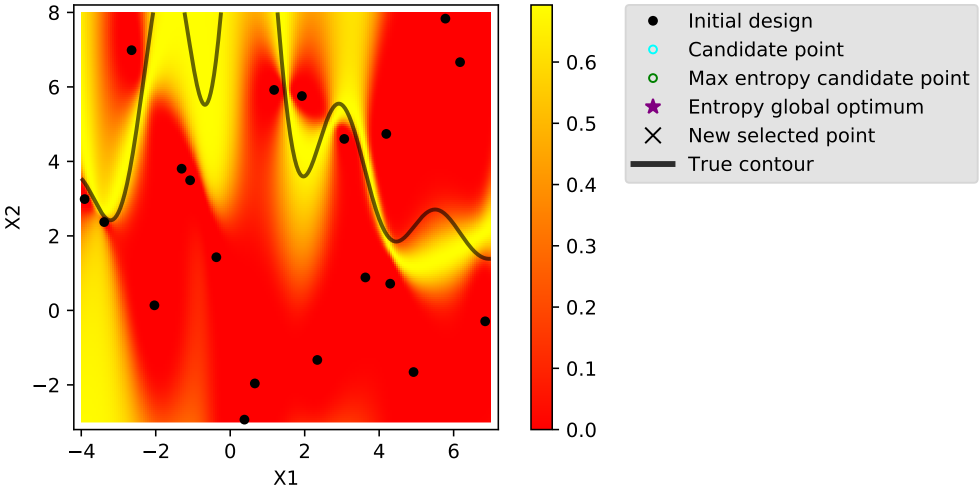
GP and ECL surfaces



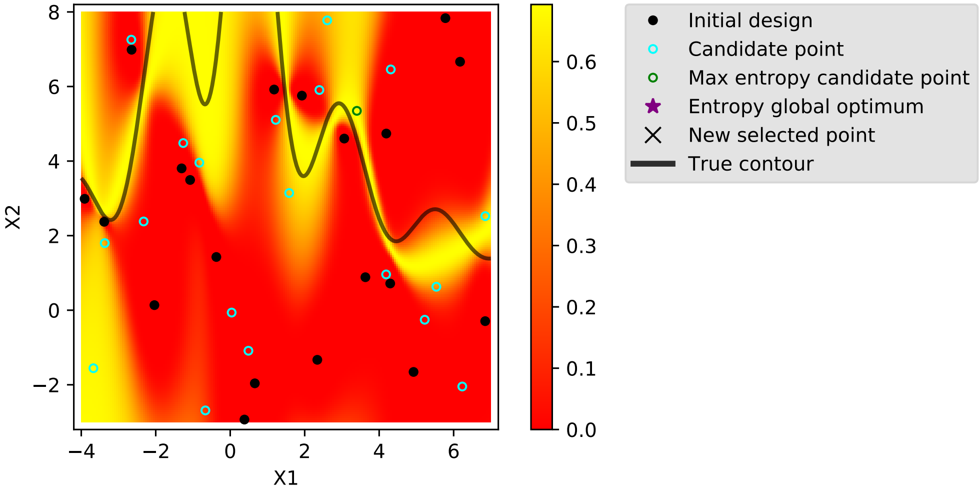
Optimization of ECL

- ECL surface contains a ridge of global maxima on the GP's predicted contour
- Other local maxima exist that are worth exploring through sample points
- **Goal**: promote exploration of global and local maxima through a small, variable set of candidate points
- **Steps**:
  1. Evaluate ECL for a candidate set of a 10*(# of dimensions) Latin hypercube sample
  2. Select the candidate point with the largest ECL
  3. Use gradient-based optimization (L-BFGS-B) to maximize ECL, with starting location from step 2

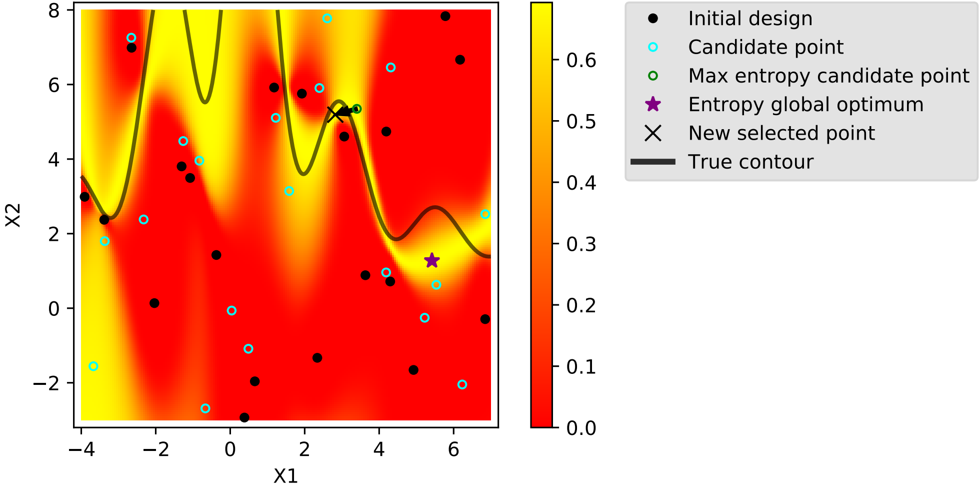
ECL 2D surface



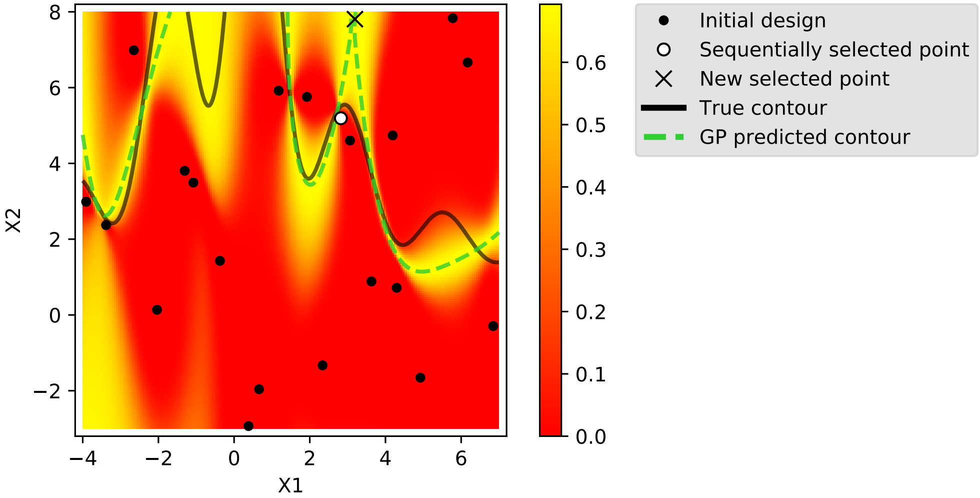
ECL 2D surface: selecting the 1st point



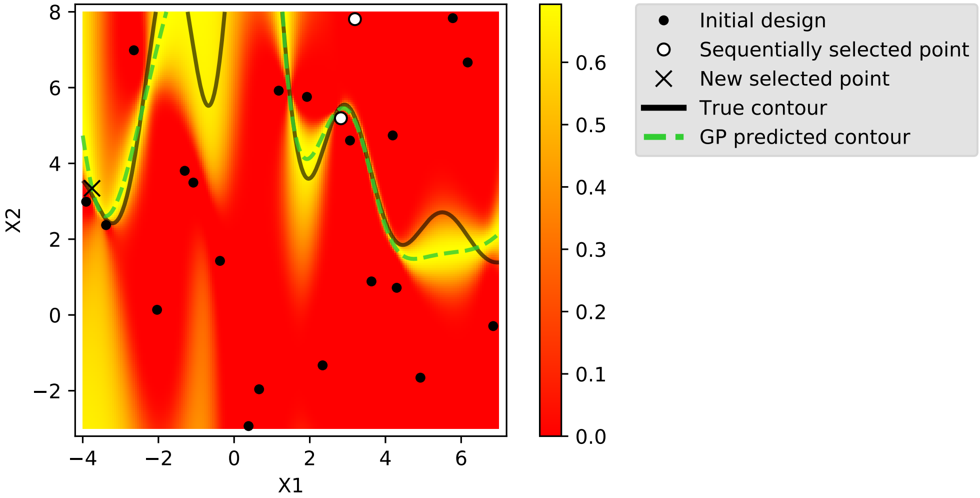
ECL 2D surface: selecting the 1st point



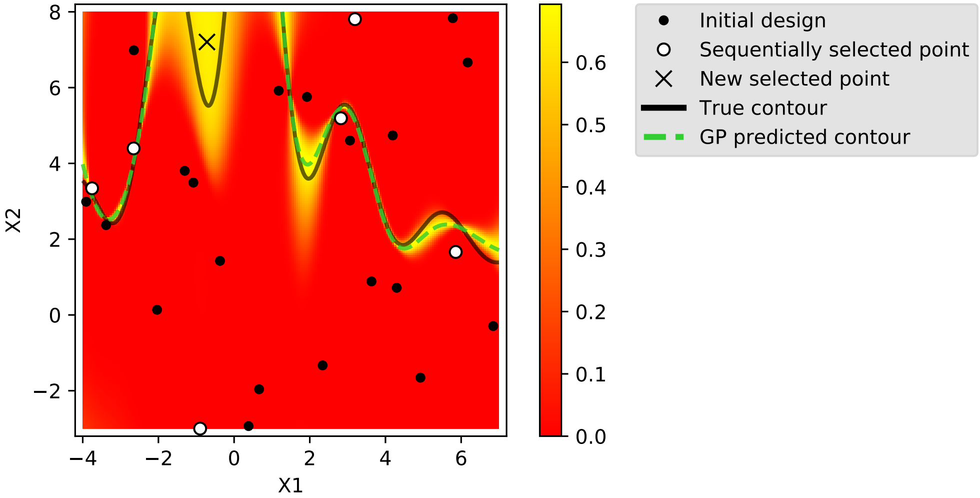
ECL 2D surface: selecting the 2nd point



ECL 2D surface: selecting the 3rd point



ECL 2D surface: selecting the 7th point



ECL 2D surface: selecting the 10th point

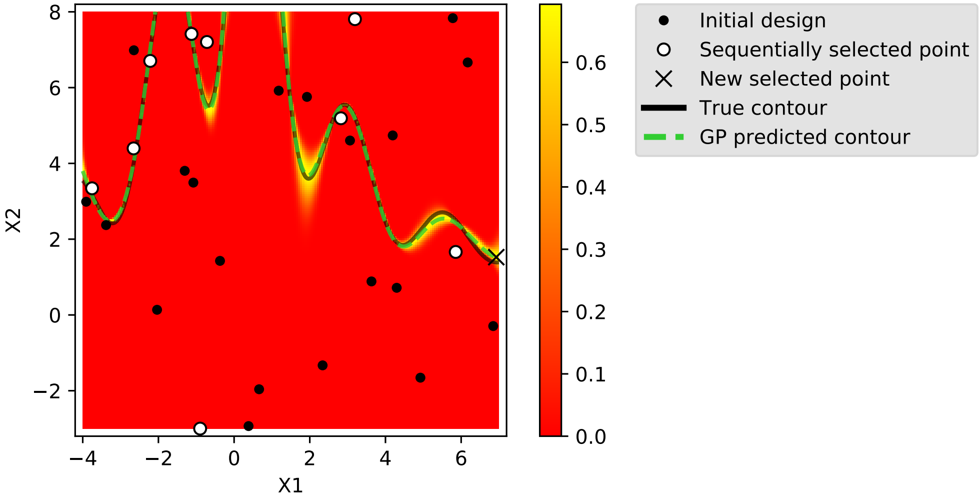
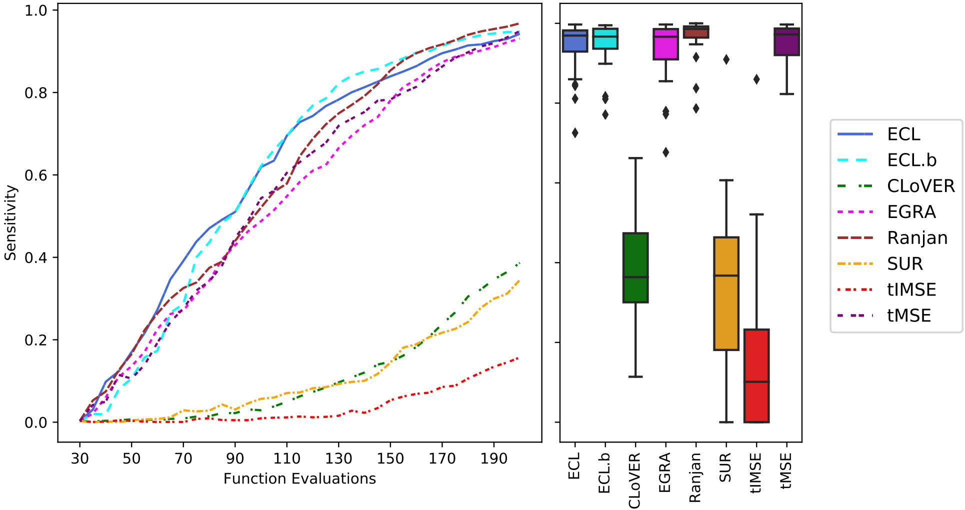


Table of contents

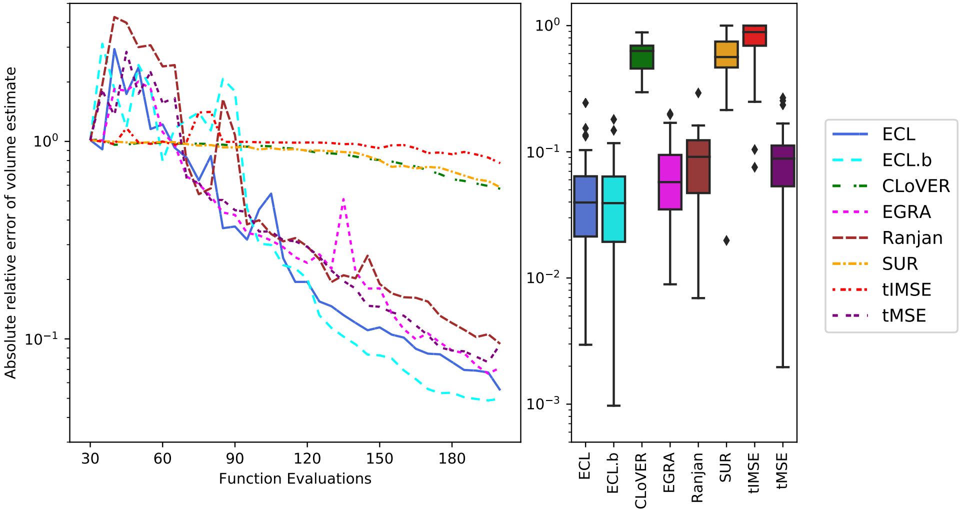
Synthetic Function Experiments

	Ishigami	Hartmann-6
Number of dimensions	3	6
Failure threshold (T)	10.244	2.63
Number of failure regions	6	2
Quantile	0.9999	0.9989
Initial design size	30	60
Number of sequential points	170	440
Failure probability (α)	1.9×10^{-4}	1×10^{-5}
Number of MFIS samples	800	500

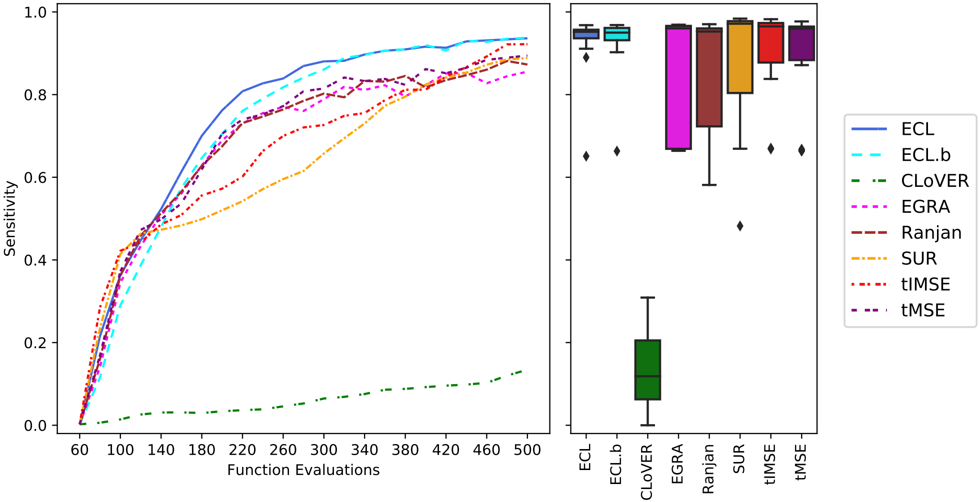
Ishigami sensitivity



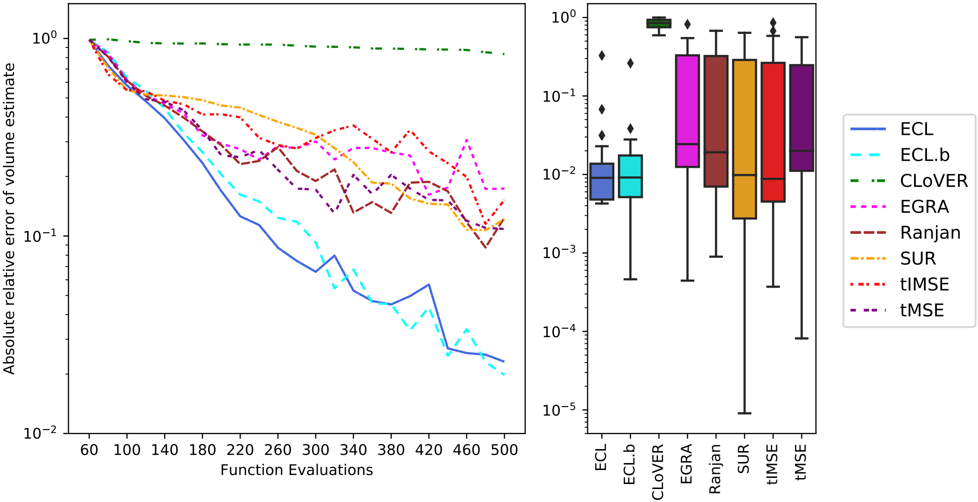
Ishigami volume estimate error



Hartmann-6 sensitivity



Hartmann-6 volume estimate error

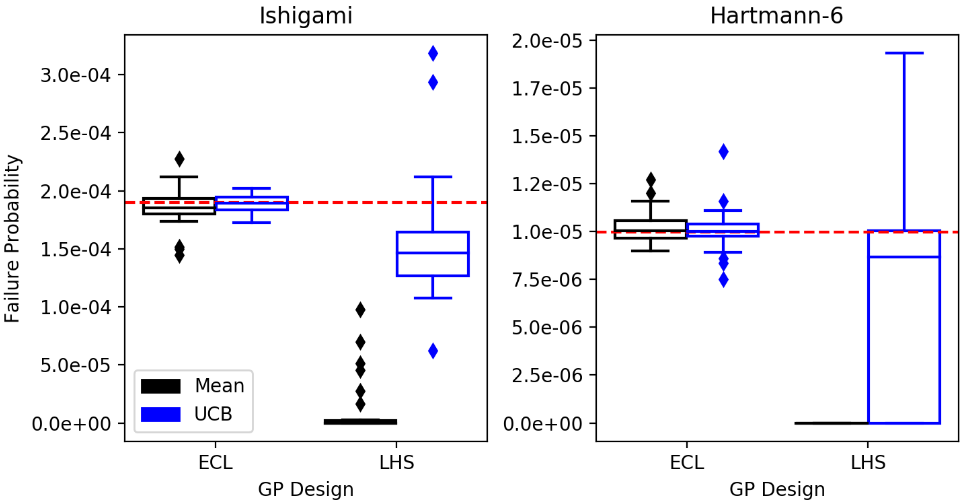


Computation Time

Method	Ishigami	Hartmann-6
ECL	**0.10**	**4.40**
ECL.b	**0.08**	**0.78**
CLoVER	17.8	428.4
EGRA	3.9	66.0
Ranjan	4.5	59.2
SUR	3.5	109.1
tIMSE	3.4	11.7
tMSE	3.9	59.5

Table 1: Average computation times (minutes) to select points across 30 Monte Carlo repetitions.

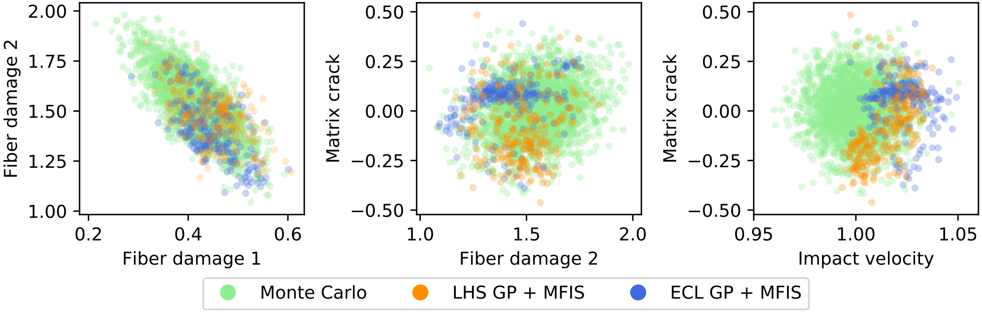
MFIS estimates for Ishigami and Hartmann-6



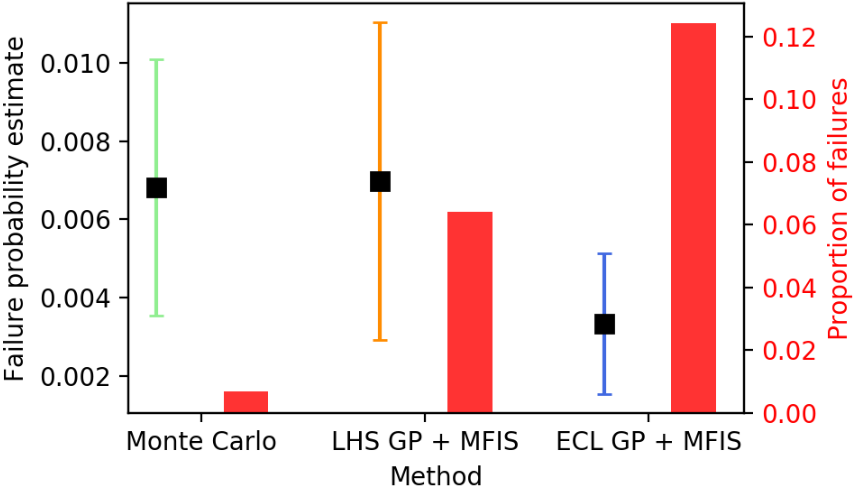
Spacesuit Simulator: samples for estimation

- MFIS estimates: 200 sample design used to train GP + 250 samples from bias distribution
- Monte Carlo: 2500 samples from input distribution

Samples used to estimate failure probability:



Spacesuit Simulator: failure probability estimates



Summary

- Using a GP surrogate with MFIS provides a cheaper approach to failure probability estimation for expensive simulators
- Pairing an adaptively designed GP improves MFIS estimation by producing a more accurate bias distribution
- Using ECL with a simple optimization strategy balances exploration (somewhat randomly) with exploitation to drive down contour uncertainty
- ECL adaptive design can be 20-100 times faster than existing adaptive designs
- ECL with batch selection is faster than ECL, without sacrificing accuracy

Bibliography I

Marques, A., Lam, R., and Willcox, K. (2018). "Contour location via entropy reduction leveraging multiple information sources." In *Advances in neural information processing systems*, 5217–5227.

Picheny, V., Ginsbourger, D., Roustant, O., Haftka, R. T., and Kim, N.-H. (2010). "Adaptive designs of experiments for accurate approximation of a target region." *Journal of Mechanical Design*, 132, 7.

Ranjan, P., Bingham, D., and Michailidis, G. (2008). "Sequential experiment design for contour estimation from complex computer codes." *Technometrics*, 50, 4, 527–541.