Entropy-based adaptive design for contour finding and estimating reliability

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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 \( \mathbb{F}^* \) biased toward the failure region(s) to draw inputs

\[
\hat{\alpha}_{\text{IS}} = \frac{1}{M^*} \sum_{i=1}^{M^*} \mathbb{I}_{\{Y(x_i^*) > T\}} w(x_i^*) \quad \text{via weights} \quad w(x^*) = \frac{f(x^*)}{f_*(x^*)}
\]

- **Multifidelity importance sampling (MFIS)**: uses a surrogate model \( S_N \), like a Gaussian process (GP), to construct the bias distribution \( \mathbb{F}^* \)

- **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:
  \[
  \mu_N(x|X_N, Y_N, \psi) = \Sigma(x, X_N)\Sigma_N^{-1} Y_N \\
  \sigma^2_N(x|X_N, \psi) = \Sigma(x, x) - \Sigma(x, X_N)\Sigma_N^{-1}\Sigma(x, X_N)^\top
  \]
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 $\mathbb{P}(w_i)$. 

![Diagram of Adaptive Design for Contour Location](diagram.png)
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Adaptive Design + MFIS

Simulator

{X_{N_0}, Y(X_{N_0})} → Fit GP

{X_{N}, \hat{Y}(X_{M})} → Fit bias distribution

{X_{M^{\star}}, \hat{Y}(X_{M^{\star}})} → Calculate IS estimate

N ← N + 1

Optimize Acquisition Function

{x_{N+1}, Y(x_{N+1})}

Response source

- Simulator
- GP
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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 \( S_N \)'s predictive equations to calculate \( \mathbb{P}(w_i) \),

\[
ECL(x \mid S_N, T) = -\left(1 - \Phi\left(\frac{\mu_N(x) - T}{\sigma_N(x)}\right)\right) \log \left(1 - \Phi\left(\frac{\mu_N(x) - T}{\sigma_N(x)}\right)\right) \\
- \Phi\left(\frac{\mu_N(x) - T}{\sigma_N(x)}\right) \log \left(\Phi\left(\frac{\mu_N(x) - T}{\sigma_N(x)}\right)\right)
\]

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

Threshold
GP predicted mean
GP 95% CI
ECL

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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

- Initial design
- Candidate point
- Max entropy candidate point
- Entropy global optimum
- New selected point
- True contour
**ECL 2D surface: selecting the 1st point**

- **Initial design**
- **Candidate point**
- **Max entropy candidate point**
- **Entropy global optimum**
- **New selected point**
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ECL 2D surface: selecting the 1st point

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ECL 2D surface: selecting the 2nd point

- **Initial design**
- **Sequentially selected point**
- **New selected point**
- **True contour**
- **GP predicted contour**
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ECL 2D surface: selecting the 3rd point

Multimodal function's Entropy surface

seq point #3

Initial design

Sequentially selected point

New selected point

True contour

GP predicted contour
ECL 2D surface: selecting the 7th point

- Initial design
- Sequentially selected point
- New selected point
- True contour
- GP predicted contour
ECL 2D surface: selecting the 10th point

- Initial design
- Sequentially selected point
- New selected point
- True contour
- GP predicted contour
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## Synthetic Function Experiments

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<thead>
<tr>
<th></th>
<th>Ishigami</th>
<th>Hartmann-6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of dimensions</td>
<td>3</td>
<td>6</td>
</tr>
<tr>
<td>Failure threshold ( T )</td>
<td>10.244</td>
<td>2.63</td>
</tr>
<tr>
<td>Number of failure regions</td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>Quantile</td>
<td>0.9999</td>
<td>0.9989</td>
</tr>
<tr>
<td>Initial design size</td>
<td>30</td>
<td>60</td>
</tr>
<tr>
<td>Number of sequential points</td>
<td>170</td>
<td>440</td>
</tr>
<tr>
<td>Failure probability ( \alpha )</td>
<td>(1.9 \times 10^{-4})</td>
<td>(1 \times 10^{-5})</td>
</tr>
<tr>
<td>Number of MFIS samples</td>
<td>800</td>
<td>500</td>
</tr>
</tbody>
</table>
Ishigami sensitivity

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Ishigami predicted failure volume over 30 samples

Function Evaluations

Sensitivity

ECL
ECL.b
CLoVER
EGRA
Ranjan
SUR
tIMSE
tMSE

Relative error

Function Evaluations

ECL
ECL.b
CLoVER
EGRA
Ranjan
SUR
tIMSE
tMSE
Ishigami volume estimate error

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Hartmann-6 sensitivity

![Hartmann-6 sensitivity graph]

- Sensitivity vs Function Evaluations
- Comparison of methods: ECL, ECL.b, CLoVER, EGRA, Ranjan, SUR, tIMSE, tMSE

Relative error
Ishigami predicted failure volume over 30 samples

- Comparison of methods: ECL, ECL.b, CLoVER, EGRA, Ranjan, SUR, tIMSE, tMSE
Hartmann-6 volume estimate error

![Graph showing absolute relative error of volume estimate against function evaluations.](Graph.png)

**Background**
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**Results**

- **Ishigami predicted failure volume** over 30 samples

**References**
## Computation Time

<table>
<thead>
<tr>
<th>Method</th>
<th>Ishigami</th>
<th>Hartmann-6</th>
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</thead>
<tbody>
<tr>
<td>ECL</td>
<td>0.10</td>
<td>4.40</td>
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<tr>
<td>ECL.b</td>
<td>0.08</td>
<td>0.78</td>
</tr>
<tr>
<td>CLoVER</td>
<td>17.8</td>
<td>428.4</td>
</tr>
<tr>
<td>EGRA</td>
<td>3.9</td>
<td>66.0</td>
</tr>
<tr>
<td>Ranjan</td>
<td>4.5</td>
<td>59.2</td>
</tr>
<tr>
<td>SUR</td>
<td>3.5</td>
<td>109.1</td>
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<tr>
<td>tIMSE</td>
<td>3.4</td>
<td>11.7</td>
</tr>
<tr>
<td>tMSE</td>
<td>3.9</td>
<td>59.5</td>
</tr>
</tbody>
</table>

Table 1: Average computation times (minutes) to select points across 30 Monte Carlo repetitions.
MFIS estimates for Ishigami and Hartmann-6

Ishigami

- Mean
- UCB

Hartmann-6

- Mean
- UCB

GP Design

ECL

LHS
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

![Bar chart showing failure probability estimates for Monte Carlo, LHS GP + MFIS, and ECL GP + MFIS methods.](chart.png)
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
