Efficient Computation of Rare Events: Failure Probability and Quantile

N. RAZAALY [1] D. Crommelin [2] P.M. CONGEDO [1]

[1]INRIA Saclay
[2]CWI, Amsterdam

September, 18^{th} 2019

COMMUNES Team

- DeFI Team (INRIA Saclay le-de-France, Ecole Polytechnique), CMAP Laboratory
- Scientific Computing Group at CWI

Research Program

- Development of efficient UQ-forward propagation method for scientific computing
- Data-inferred stochastic modeling when a limited amount of data is available for unsteady non-linear systems
- **Numerical simulation of fluids** (CFD) for energy application

Publications, events on the internet site !

Focus of the talk to our Joint PhD Nassim who defended July 12!

Assumptions

- $G : \mathbb{R}^d \to \mathbb{R}$, $d \sim 1 - 20$
- *Expensive* G (CFD/FEM) Limited budget ~ 500
- $\mathbf{U} \sim \mathcal{N}(0, I_d)$, $\mathbf{X} = T(\mathbf{U})$ (Rosenblatt/Nataf)

Problem

- Find α s.t. $\mathbb{P}(G(\mathbf{U}) < q) = \alpha$ Failure Probability
- Find q s.t. $\mathbb{P}(G(\mathbf{U}) < q) = \alpha$ Quantile

Challenges

Flexible method to deal with

- $\alpha \sim 10^{-2} - 10^{-9}$
- Multiple Failure Regions

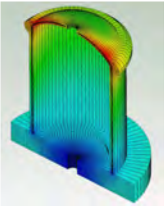
Failure Probability $\mathbb{P}(G(\mathbf{U}) < q) = ?$

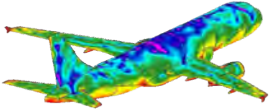
Reliability Assessment/Risk Analysis:

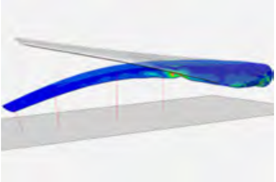
- Aeronautics/Nuclear $\implies \mathbb{P}(G(\mathbf{U}) < q) < 10^{-8}$

Reliability-Based Design Optimization:

- Min $\mathbb{E}[m(\mathbf{x}, \mathbf{u})]$ s.t. $\mathbb{P}_{\mathbf{U}}(F(\mathbf{x}, \mathbf{u}) < 25 \text{ kN}) < 10^{-7}$







Quantile $\mathbb{P}(G(\mathbf{U}) < ?) = \alpha$

- Min $q(\mathbf{x})$, with $\mathbb{P}_{\mathbf{U}}(G(\mathbf{x}, \mathbf{u}) < q(\mathbf{x})) = 10^{-7}$

Direct Methods

1. Sampling
   - Monte-Carlo (MC)
   - Importance Sampling (IS)
   - Subset Simulation (SS)
2. MPFP-based
   - FORM
   - SORM

Surrogate-Based Methods

- *AK Family*: AK-MCS[1], AK-IS, AK-SS...
- Bayesian Subset Simulation, MetaIS[2], ASVR[3]

Contributions:

- metaAL-OIS [Razaaly, JCP 2018]
- **eAK-MCS** [Razaaly, Sub. 2019]
- **QeAK-MCS** [Razaaly, Sub. 2019]

[1] R. Schobi, B. Sudret, S. Marelli. *Journal of Risk and Uncertainty in Engineering Systems*, 2016.

[2] V. Dubourg. *PhD Thesis*, 2011.

[3] J.M. Bourinet. *Habilitation Thesis*, 2018.

Contents

Section 1

Failure Probability

Failure Probability

Reference Method: Monte-Carlo (MC)

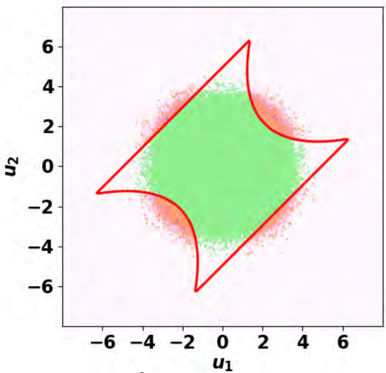
$$\alpha = \mathbb{P}(G(\mathbf{U}) < q) = \mathbb{E}[\mathbb{1}_{G<q}(\mathbf{U})]$$

Estimators with $\mathbf{u}_i \overset{\text{iid}}{\sim} \mathbf{U}$

- $\hat{\alpha} = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{G<q}(\mathbf{u}_i)$
- $\hat{\delta} = \sqrt{\frac{1-\hat{\alpha}}{N\hat{\alpha}}} \implies N \sim \frac{1}{\hat{\delta}^2 \alpha}$

Slow Convergence

$\alpha \sim 10^{-6}$, $\hat{\delta}_{target} < 1\%$
$\implies$ $\mathbf{N > 10^{10}}$



10^6 points

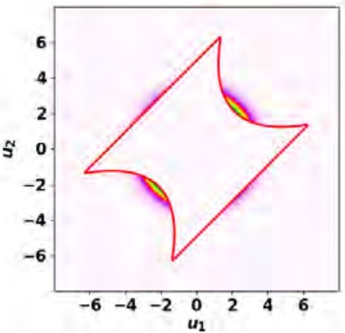
Failure Probability

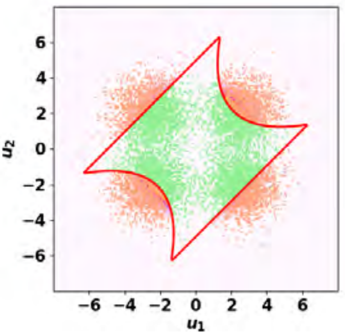
Reference Method: Importance Sampling (IS)

$$\alpha = \int \mathbb{1}_{G<q}(\mathbf{u}) \frac{f_{\mathbf{U}}(\mathbf{u})}{h(\mathbf{u})} h(\mathbf{u}) d\mathbf{u} = \mathbb{E}_h \left[\mathbb{1}_{G<q}(\mathbf{U}) \frac{f_{\mathbf{U}}(\mathbf{U})}{h(\mathbf{U})} \right]$$

$$h_{opt}(\mathbf{u}) = \frac{\mathbb{1}_{G<q}(\mathbf{u}) f_{\mathbf{u}}}{\alpha}$$

$\rightarrow$ **Careful Choice** $h \sim h_{opt}$





One Failure Region Assumption

MPFP $\mathbf{u}^*$

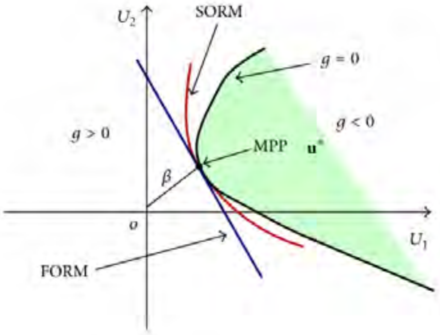
$$\mathbf{u}^* = \text{argmin}_{\mathbf{u}\ s.t.\ G(\mathbf{u})<q} |\mathbf{u}|_{L_2}$$

FORM: Linearization around $\mathbf{u}^*$

$$G(\mathbf{u}) = G(\mathbf{u}^*) + \nabla(\mathbf{u}^*)(\mathbf{u} - \mathbf{u}^*)$$
$$\hat{\alpha} = \phi(-|\mathbf{u}^*|)$$

SORM: Quadratic Form around $\mathbf{u}^*$

$$G(\mathbf{u}) = G(\mathbf{u}^*) + \nabla(\mathbf{u}^*)(\mathbf{u} - \mathbf{u}^*) + \frac{1}{2}(\mathbf{u} - \mathbf{u}^*)^T H_G(\mathbf{u}^*)(\mathbf{u} - \mathbf{u}^*)$$



Failure Probability

Reference Method: Monte-Carlo (MC) + Surrogate Model

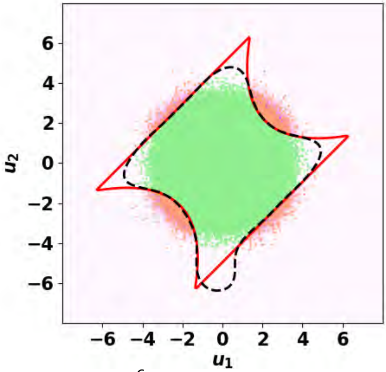
Replace G by Surrogate $\tilde{G}$

- $\mathbf{G} \to \tilde{\mathbf{G}}$
- $\tilde{\alpha} = \mathbb{P}(\tilde{G}(\mathbf{U}) < q) = \mathbb{E}[\mathbb{1}_{\tilde{G}<q}(\mathbf{U})]$
- Same MC Estimators

$\to$ **Need for Accurate Approximation of Limit-State Surface (LSS)** $\{G = q\}$ **by** $\{\tilde{G} = q\}$

Slow Convergence

$\tilde{\alpha} \sim 10^{-6}$, $\hat{\delta}_{target} < 1\%$
$\implies \mathbf{N} > \mathbf{10^{10}}$



10^6 points

Failure Probability

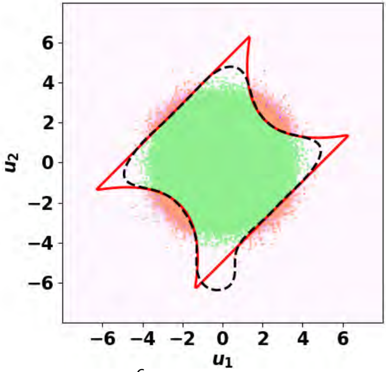
Reference Method: Monte-Carlo (MC) + Surrogate Model

Methods Investigated

- AK-MCS[1]
- **eAK-MCS**

Surrogate Modeling

- Gaussian Process based (Kriging)
- Initial DoE
- **Adaptive Sampling**

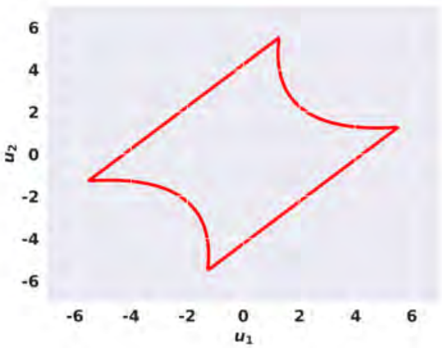


10^6 points

[1] B. Echard, N. Gayton and M. Lemaire. *Reliability Engineering and System Safety*, 2011.

[1] J. Bect, L. Li and E. Vazquez. *SIAM/ASA Journal on Uncertainty Quantification*, 2017.

$$G(\mathbf{u}) = \min \begin{cases} 3 + \frac{(u_1 - u_2)^2}{10} - \frac{u_1 + u_2}{\sqrt{2}} \\ 3 + \frac{(u_1 - u_2)^2}{10} + \frac{u_1 + u_2}{\sqrt{2}} \\ u_1 - u_2 + \frac{6}{\sqrt{2}} \\ -(u_1 - u_2) + \frac{6}{\sqrt{2}} \end{cases}$$



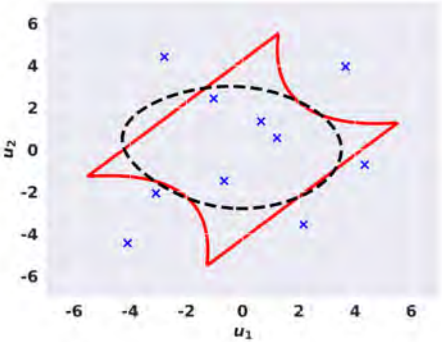
Four Failure Example

$$\alpha^{ref} = \mathbb{P}(G(\mathbf{U}) < 0) = 4.46 \times 10^{-3}$$

Build Initial GP

$$\hat{\mathbf{G}}(\mathbf{u}) \sim \mathcal{N}(\mu(\mathbf{u}), \sigma^2(\mathbf{u}))$$
$$\implies \tilde{\mathbf{G}}(\mathbf{u}) = \mu(\mathbf{u})$$

$\hat{\mathbf{G}}$ Gaussian Predictor
$\tilde{\mathbf{G}}$ Surrogate



Initial DOE

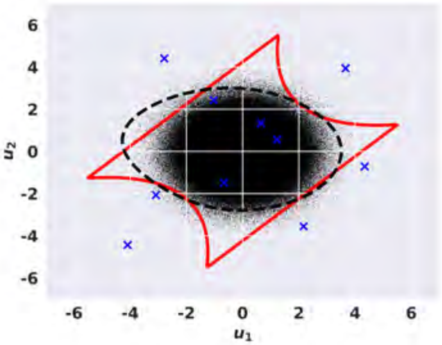
Learning Function U [Echard, 2011]

$$U(\mathbf{u}) = \frac{|\mu(\mathbf{u}) - q|}{\sigma(\mathbf{u})}$$

Probability of Misclassification

$$P_m(\mathbf{u}) = \phi(-\frac{|\mu(\mathbf{u}) - q|}{\sigma(\mathbf{u})}),$$

with ϕ cdf $\mathcal{N}(0,1)$



MC Population

Learning Function U [Echard, 2011]

$$U(\mathbf{u}) = \frac{|\mu(\mathbf{u}) - q|}{\sigma(\mathbf{u})}$$

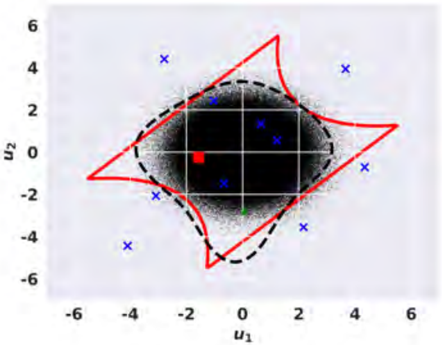
Probability of Misclassification

$$P_m(\mathbf{u}) = \phi(-\frac{|\mu(\mathbf{u}) - q|}{\sigma(\mathbf{u})}),$$

with ϕ cdf $\mathcal{N}(0,1)$

New Sample $\mathbf{u}^*$

$$\mathbf{u}^* = \text{argmin}_{\mathbf{u} \in \mathcal{X}_{MC}} U(\mathbf{u})$$
$$= \text{argmax}_{\mathbf{u} \in \mathcal{X}_{MC}} P_m(\mathbf{u})$$



Infill Selection

New Sample $\mathbf{u}^*$

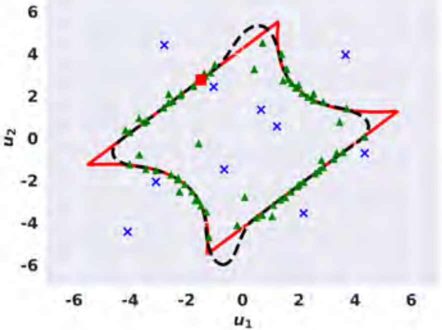
$$\mathbf{u}^* = \text{argmin}_{\mathbf{u}\in\mathcal{X}_{MC}} U(\mathbf{u})$$
$$= \text{argmax}_{\mathbf{u}\in\mathcal{X}_{MC}} P_m(\mathbf{u})$$

Stopping Criterion

$$U(\mathbf{u}^*) > 2$$
$$P_m(\mathbf{u}^*) < 2.5\%$$

α Estimation: MC

$$\hat{\alpha} = \frac{1}{N}\sum_i \mathbb{1}_{\mathbf{G}<q}(\mathbf{u}_i)$$



Refined Metamodel: $N_{calls} = 10 + 72$

Failure Probability

eAK-MCS Refinement Strategy

Based on AK-MCS[1]: $\alpha = \mathbb{P}(G(\mathbf{U}) < q)$

Refinement among $\mathcal{X} = \{\mathbf{u}_i \sim \mathcal{N}(0, \gamma^2 I_d)\}$

- 1 sample: U-criterion[2]
- K samples: weighted K-Means[1]

Estimation: Importance Sampling

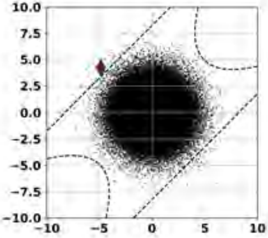
$$\alpha = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{G<\hat{q}}(\mathbf{u}_i) \frac{f_{\mathbf{U}}(\mathbf{u}_i)}{h(\mathbf{u}_i)}$$

$h \sim \mathcal{N}(0, \gamma^2 I_d)$

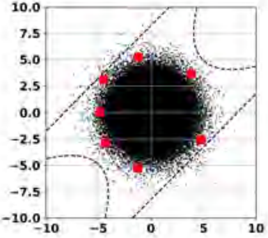
[1] R. Schobi, B. Sudret, S. Marelli. *Journal of Risk and Uncertainty in Engineering Systems*, 2016.

[2] B. Echard, N. Gayton and M. Lemaire. *Reliability Engineering and System Safety*, 2011.

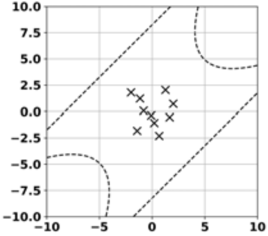
eAK-MCS Refinement (1)



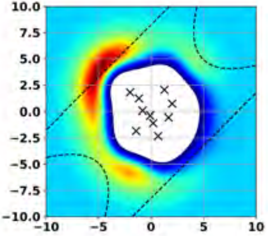
1 Sample



K Samples

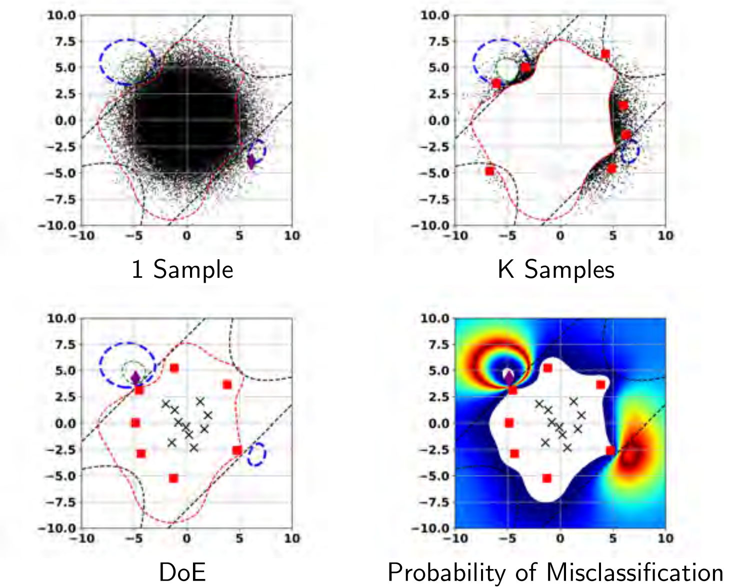


DoE

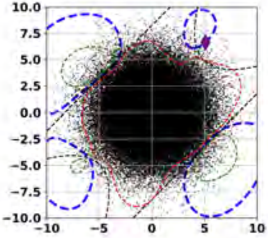


Probability of Misclassification

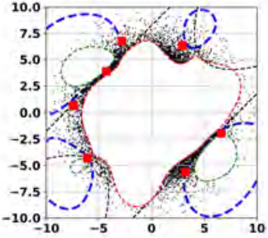
eAK-MCS Refinement (2)



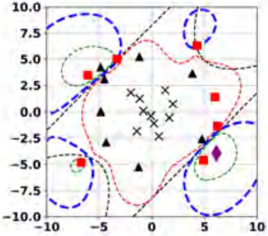
eAK-MCS Refinement (3)



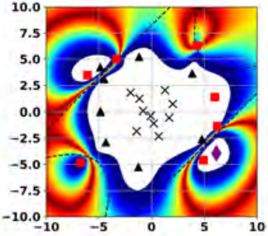
1 Sample



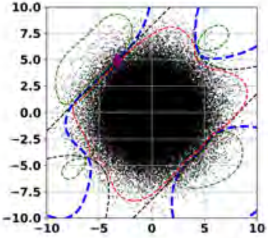
K Samples



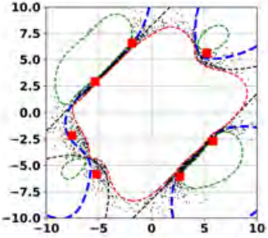
DoE



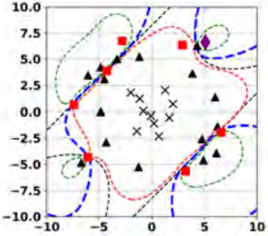
Probability of Misclassification



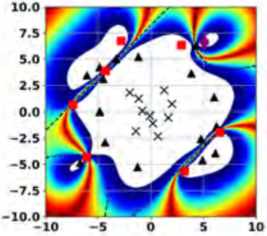
1 Sample



K Samples

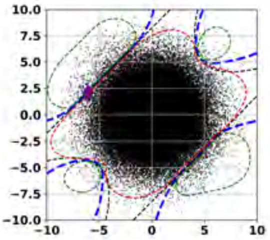


DoE

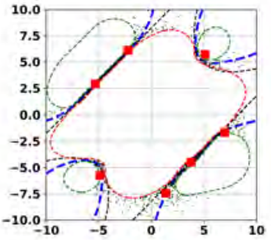


Probability of Misclassification

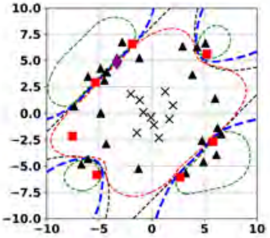
eAK-MCS Refinement (5)



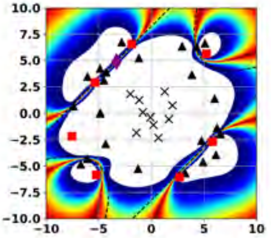
1 Sample



K Samples



DoE



Probability of Misclassification

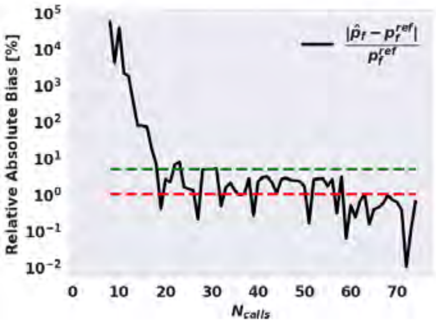
Application

8D: Borehole[1]

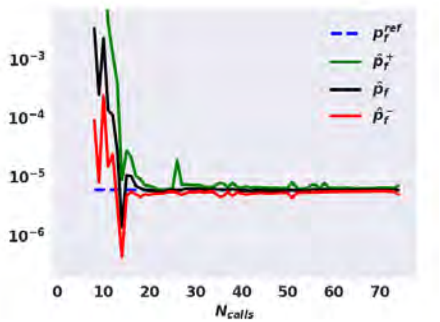
$$v(\mathbf{x}) = \frac{2\pi T_u(H_u - H_l)}{\ln(\frac{r}{r_w})(1 + \frac{T_u}{T_l} + \frac{2LT_u}{\ln(\frac{r}{r_w})r_w^2 K_w})}, \quad \mathbf{x} = (r_w, r, T_u, H_u, T_l, H_l, L, K_w)$$

$\mathbf{X}_i$: Uniform or LogNormal

$\mathbb{P}(v(\mathbf{X}) > 280) = 5.77 \times 10^{-6}$



Relative Absolute Bias



$\hat{\alpha}^{\pm}$ Monitoring

Section 2

Quantile Estimation

Extreme Quantile

Formulation

Assumptions

- $G\ :\ \mathbb{R}^d \to \mathbb{R}$, $d \sim 1 - 20$
- *Expensive* G (CFD/FEM) Limited budget ~ 500
- $\mathbf{U} \sim \mathcal{N}(0, I_d)$, $\mathbf{X} = T(\mathbf{U})$ (Rosenblatt/Nataf)

Problem

- Find q s.t. $\mathbb{P}(G(\mathbf{U}) < q) = \alpha$

Challenges

Flexible method to deal with

- $\alpha \sim 10^{-2} - 10^{-9}$
- Multiple Failure Regions

Literature:

- AK-MCS [Schobi, 2016] $\to \alpha > 10^{-4}$

Strategy:

1. Initial Surrogate $\tilde{G}$
2. Adaptive Sampling
   a. (Surrogate) Quantile Estimator $\hat{q}$
   b. New DoE $\{\mathbf{u}_i\}_i$: $\mathbb{P}(\tilde{G}(\mathbf{U}) < \hat{q})$ $\rightarrow$ **Failure Probability Algorithm**
   c. Update Surrogate $\tilde{G}$

(2a) IS Quantile Estimator $\hat{q}$

$$\alpha = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{G<\hat{q}}(\mathbf{u}_i) \frac{f_{\mathbf{U}}(\mathbf{u}_i)}{h(\mathbf{u}_i)}$$

with $\mathbf{u}_i \overset{\text{iid}}{\sim} h = f_{\mathcal{N}(0,\gamma^2 I_d)}$

(2b) Failure Probability Algorithm

eAK-MCS: K_p samples for $\mathbb{P}(\tilde{G}(\mathbf{U}) < \hat{q})$

Strategy:

1. Initial Surrogate $\tilde{G}$
2. Adaptive Sampling
   - (Surrogate) Quantile Estimator $\hat{q}$
     New DoE $\{\mathbf{u}_i^{(1)}\}_i$: $\mathbb{P}(\tilde{G}(\mathbf{U}) < \hat{q}_1)$
     ...
     New DoE $\{\mathbf{u}_i^{(K_q)}\}_i$: $\mathbb{P}(\tilde{G}(\mathbf{U}) < \hat{q}_{K_q})$
   - Update Surrogate $\tilde{G}$

Increase parallelization: Multiple Quantile Selection

- Bounds $\hat{q}^-$, $\hat{q}^+$ s.t. $\alpha = \mathbb{P}(\mu(\mathbf{U}) \pm k\sigma(\mathbf{U}) < \hat{q}^{\mp})$
- K_q quantiles selected in $[\hat{q}^-, \hat{q}^+]$: $\hat{q}_1, ..., \hat{q}_{K_q}$

At each step, $K_q K_p$ samples to refine $\tilde{G}$.

Extreme Quantile

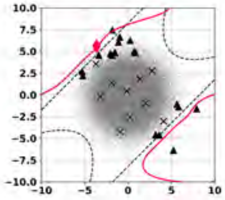
Refinement Illustration: $K_q = 3,\ K_p = 8$

Quantiles Estimates

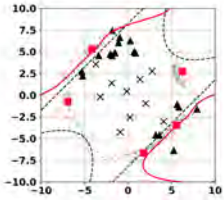
- $\hat{\mathbf{q}}_1 = \hat{\mathbf{q}}^-$
- $\hat{q}_2 = \hat{q}$
- $\hat{q}_3 = \hat{q}^+$

Refinement

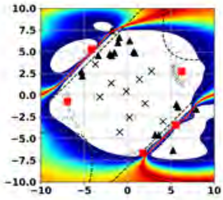
- DoE $\{\mathbf{u}_i\}_i$: $\mathbb{P}(\tilde{G}(\mathbf{U}) < \hat{q}_1)$
- $K_p = 8$ New Samples proposed



Single Selection



Parallel Selection



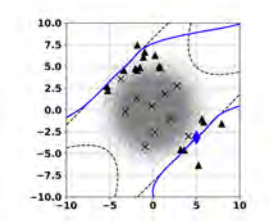
Proba Misclassification

Quantiles Estimates

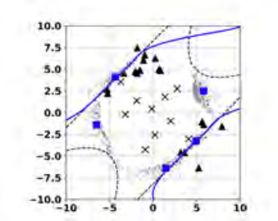
- $\hat{q}_1 = \hat{q}^-$
- $\hat{\mathbf{q}}_2 = \hat{\mathbf{q}}$
- $\hat{q}_3 = \hat{q}^+$

Refinement

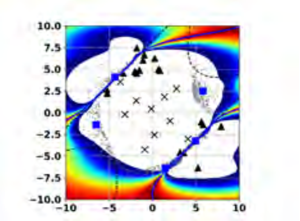
- DoE $\{\mathbf{u}_i\}_i$: $\mathbb{P}(\tilde{G}(\mathbf{U}) < \hat{q}_1)$
- $K_p = 8$ New Samples proposed



Single Selection



Parallel Selection



Proba Misclassification

Extreme Quantile

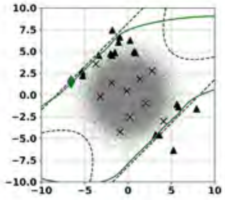
Refinement Illustration: $K_q = 3,\ K_p = 8$

Quantiles Estimates

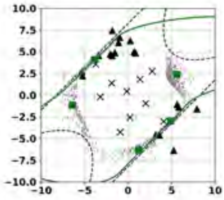
- $\hat{q}_1 = \hat{q}^-$
- $\hat{q}_2 = \hat{q}$
- $\hat{\mathbf{q}}_3 = \hat{\mathbf{q}}^+$

Refinement

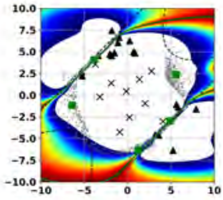
- DoE $\{\mathbf{u}_i\}_i$: $\mathbb{P}(\tilde{G}(\mathbf{U}) < \hat{q}_1)$
- $K_p = 8$ New Samples proposed



Single Selection



Parallel Selection

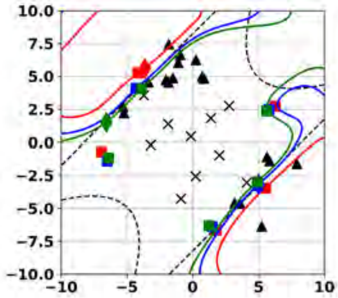


Proba Misclassification

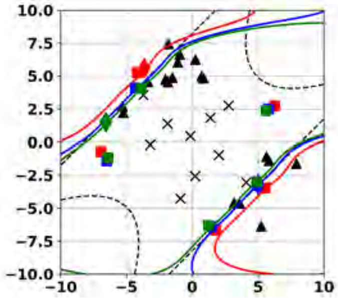
Extreme Quantile

Refinement Illustration: $K_q = 3$, $K_p = 8$

$K_q K_p = 24$ Samples after 1 iteration.



Batch Selection



Updated Surrogate

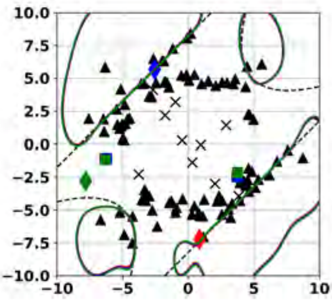
$\rightarrow$ Levels $\tilde{G} = \hat{q}_i$ closer to $G = q$.

Quantile Estimation

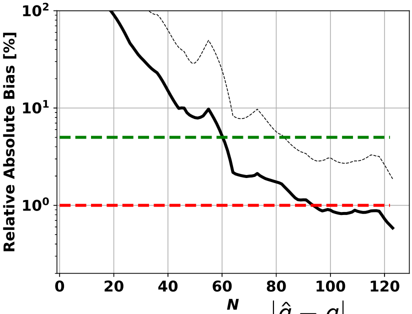
$$\text{Find } q \text{ s.t. } \mathbb{P}(G(\mathbf{U}) < q) = 5.59 \times 10^{-9}$$

Reference Value: $q = -4$ $\mathbb{E}[N_{calls}] = 98.4$

(based on 50 independent runs.)



Surrogate

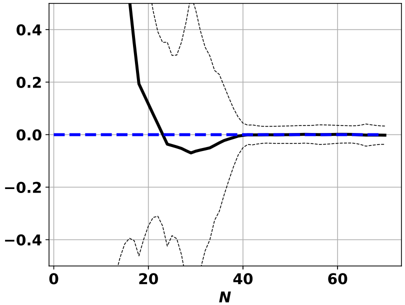


Error History: $\frac{|\hat{q} - q|}{q_{ref}}$

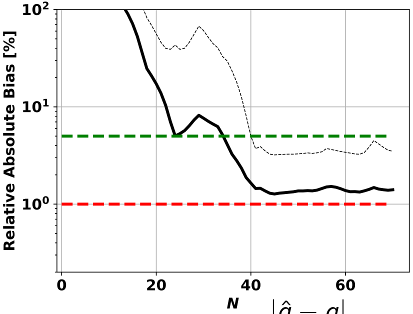
Quantile Estimation (based on 50 independent runs)

$$\text{Find } q \text{ s.t. } \mathbb{P}(v(\mathbf{X}) > q) = 8.7 \times 10^{-9}$$

Reference Value: $q = 300$ $\mathbb{E}[N_{calls}] = 34.9$



Normalized $\hat{q}$ Monitoring



Error History: $\frac{|\hat{q} - q|}{q_{ref}}$

Section 3

Conclusion

Conclusion

Achievements

- GP-based Rare Event Estimation
- Versatile: Multiple Failures, small probabilities
- N_{calls} Low
- Parallel Strategy
- Original Extreme Quantile Estimation

Limits

- $\mathbf{U} \sim \mathcal{N}(0, I_d)$, $\mathbf{X} = T^{-1}(\mathbf{U})$ (Rosenblatt/Nataf)
- GP ability to fit G
- Low Input Dimension
- Limited IS-based quantile accuracy in high dimensions.