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An Efficient Multiple-Point Active Kriging Method for Reliability Assessment with Complex Failure Domains

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Rare failures, which occur with very small probabilities, can have a significant impact on system reliability and performance, particularly under off-design conditions. Accurately estimating such rare failure probabilities is challenging when the limit-state function is expensive to evaluate and multiple failure regions may exist. To address this challenge, we propose the Multi-Point Active-Kriging Improved-Expected-Improvement Subset-Simulation Importance-Sampling (MP-AK-IEI-SSIS) method. The method incorporates a multi-point enrichment strategy, inherited from conventional AK Monte Carlo Simulation, to enhance exploration of complex failure domains. Moreover, it leverages k-means clustering in SSIS to explore and identify multiple failure regions. Numerical results demonstrate that the method effectively identifies multiple failure regions while maintaining accurate estimation of rare failure probabilities. In addition, it has approximately a 40% faster convergence rate compared to state-of-the-art literature. Overall, the method provides an efficient tool for reliability analysis in systems governed by computationally expensive models.

Keywords: Reliability, Multiple Failure Regions, Small Failure Probability, Rare Event Estimation, Active Kriging, Subset Simulation Importance Sampling

1. Introduction

Reliability assessment of engineering systems under uncertainty is essential for ensuring system safety, reducing maintenance costs, and extending service life. This task relies on probabilistic sampling methods to accurately characterize complex failure domains. The standard sampling method is the Monte Carlo simulation (MCS), as it can naturally handle highly nonlinear limit-state functions (LSFs). However, MCS becomes computationally prohibitive when estimating low failure probabilities, which are common in engineering applications.

To mitigate this limitation, numerous surrogate-model-based reliability methods have been developed in the literature. Kriging (Gaussian process) models have been widely adopted in reliability analysis applications due to their ability to provide both mean predictions and associated uncertainty estimates of the LSF at unobserved locations. In adaptive Kriging frameworks, numerous learning functions have been employed to sequentially guide the sampling process toward the most informative regions of the input space, such as Expected Improvement (EI) Jones et al. (1998), Enhanced Expected Improvement (EEI) Huang et al. (2024), and Expected Integrated Error Reduction (EIER) Wang et al. (2024). Despite their success, improving convergence rate and learning efficiency while avoiding unnecessary model evaluations remains a significant challenge, particularly for problems involving rare events and highly nonlinear or disconnected failure regions.

In parallel, advanced Monte Carlo techniques have been proposed for rare-event estimation, including Subset Simulation (SS) Au and Beck (2001), Importance Sampling (IS) GS (1996), and hybrid approaches such as Subset Simulation Importance Sampling (SSIS) Wang et al. (2015). These methods aim to increase sampling efficiency by focusing computational effort within or near the failure domain, thereby substantially reducing the number of required model evaluations. More recently, such sampling strategies have been extensively coupled with adaptive surrogate models to further enhance efficiency, leading to methods such as AK-MCS Echard et al. (2011), AK-IS Echard et al. (2013), AK-SS Huang et al. (2016), RBIK-SS Li et al. (2023) and Meta-AL-OIS Razaaly and Congedo (2018). However, reliance on heuristic sampling strategies may limit the accurate representation of complex and irregular failure boundaries. In addition, Markov chain Monte Carlo (MCMC) methods depend on predefined probability density functions, which can require additional model evaluations to adequately characterize the target distribution, thereby increasing computational cost. Furthermore, the conditional samples generated by MCMC are generally correlated, and treating them as independent and identically distributed (i.i.d.) for statistical estimation may result in reduced efficiency Wang et al. (2015).

To address these challenges, we propose the MP-AK-IEI-SSIS method, which integrates Active Kriging (AK), an Improved Expected Improvement (IEI) learning function, and Subset Simulation Importance Sampling (SSIS). The proposed framework employs a multi-point enrichment strategy to the well-established AK-MCS Echard et al. (2011) approach, enabling the simultaneous addition of multiple informative points to the design of experiments (DoE) at each iteration. Furthermore, we incorporate a k-means clustering technique within a Gaussian mixture-based SSIS scheme to efficiently capture and sample multiple failure regions. This combined strategy aims to improve convergence speed and identify multiple failure regions in the estimation of low failure probabilities.

2. MP-AK-IEI-SSIS framework

2.1. *SSIS fundamentals*

Let $g(\mathbf{x})$ denote the limit-state function (LSF), where failure is defined as

$$\mathcal{F} = \left\{\mathbf{x} \in \mathbb{R}^d : g(\mathbf{x}) \leq 0\right\}. \qquad (1)$$

The probability of failure is given by

$$P_f = \mathbb{P}\big(g(\mathbf{x}) \leq 0\big), \qquad (2)$$

Subset Simulation with Importance Sampling (SSIS) estimates P_f by expressing the failure event as a sequence of nested intermediate events,

$$\mathcal{F}_1 \supset \mathcal{F}_2 \supset \cdots \supset \mathcal{F}_m = \mathcal{F}, \qquad (3)$$

where each subset is defined as

$$\mathcal{F}_k = \{\mathbf{x} : g(\mathbf{x}) \leq b_k\}, \qquad (4)$$

with decreasing thresholds $b_1 > b_2 > \cdots > b_m = 0$. The failure probability can then be factorized as

$$P_f = \mathbb{P}(\mathcal{F}_1) \prod_{k=2}^{m} \mathbb{P}(\mathcal{F}_k \mid \mathcal{F}_{k-1}), \qquad (5)$$

where the intermediate thresholds are chosen such that each conditional probability is approximately equal to a prescribed value p_0.

In SSIS, samples at each intermediate level are generated using importance sampling distributions constructed from the samples of the previous level. These importance distributions are designed to concentrate sampling effort in regions with a higher likelihood of satisfying the next subset condition, thereby improving estimator efficiency.

At level k, the conditional probability $\mathbb{P}(\mathcal{F}_k \mid \mathcal{F}_{k-1})$ is estimated as

$$\hat{p}_k = \frac{1}{N_k} \sum_{i=1}^{N_k} \mathbb{I}\big(g(\mathbf{x}_i^{(k)}) \leq b_k\big), \qquad (6)$$

where $\mathbf{x}_i^{(k)}$ are samples drawn from the level-$k$importance distribution and $\mathbb{I}(\cdot)$ denotes the indicator function. The final failure probability estimate is obtained as

$$\hat{P}_f = \prod_{k=1}^{m} \hat{p}_k. \qquad (7)$$

However, the failure probability can be estimated directly from the samples generated at the final level Xiao et al. (2021). Let $q_m(\mathbf{x})$ denote the importance sampling probability density function employed at the last subset level. The failure probability can then be written as

$$P_f = \mathbb{E}_{q_m}\left[\mathbb{I}\big(g(\mathbf{x}) \leq 0\big) \frac{p(\mathbf{x})}{q_m(\mathbf{x})}\right], \qquad (8)$$

where $p(\mathbf{x})$ is the joint probability density function of the original input random variables.

Accordingly, the SSIS estimator of the failure probability can be reduced to

$$\hat{P}_f = \frac{1}{N_m} \sum_{i=1}^{N_m} \mathbb{I}\big(g(\mathbf{x}_i^{(m)}) \le 0\big) \frac{p(\mathbf{x}_i^{(m)})}{q_m(\mathbf{x}_i^{(m)})}, \quad (9)$$

where $\mathbf{x}_i^{(m)}$ are samples drawn from the importance distribution at the final level.

An analytical expression for the coefficient of variation (COV) of the SSIS estimator can be derived as

$$V_m = \mathbb{E}_{q_m}\left[\mathbb{I}\big(g(\mathbf{x}) \le 0\big)\left(\frac{p(\mathbf{x})}{q_m(\mathbf{x})}\right)^2\right] \quad (10)$$

$$\mathrm{COV}\Big(\hat{P}_f\Big) = \frac{1}{\sqrt{N_m}}\left(\frac{V_m}{P_f^2} - 1\right)^{1/2}. \quad (11)$$

The COV quantifies the relative statistical uncertainty of the SSIS failure probability estimator.

2.2. *Active Kriging with improved expected improvement*

Adaptive Kriging-based reliability methods iteratively refine the surrogate model by selectively enriching the training set with informative samples. This process is guided by a learning function designed to identify candidate points that improve surrogate accuracy in regions critical to failure probability estimation.

Given a Kriging surrogate $\hat{g}(\mathbf{x})$, the limit-state function is approximated as a Gaussian random field of the form

$$\hat{g}(\mathbf{x}) = \mu(\mathbf{x}) + \sigma(\mathbf{x})\, Z, \quad (12)$$

where $\mu(\mathbf{x})$ and $\sigma(\mathbf{x})$ denote the Kriging predictive mean and standard deviation, respectively, and Z is a standard normal random variable representing the random prediction error due to model uncertainty. The associated predictive distribution quantifies both the estimated response and the local epistemic uncertainty induced by limited training data.

Moreover, the Improved Expected Improvement (IEI) learning function, developed by Liu et al. (2026), is employed to balance exploration and exploitation near the intermediate failure boundary $g(\mathbf{x}) = b_k$. The IEI criterion is defined as

$$\begin{aligned}\mathrm{IEI}(\mathbf{x}) = (b_k - \mu(\mathbf{x}))\, \Phi\left(\frac{b_k - \mu(\mathbf{x})}{\sigma(\mathbf{x})}\right) \\ + \sigma(\mathbf{x})\, \phi\left(\frac{b_k - \mu(\mathbf{x})}{\sigma(\mathbf{x})}\right).\end{aligned} \quad (13)$$

where $\Phi(\cdot)$ and $\phi(\cdot)$ denote the cumulative distribution function and probability density function of the standard normal distribution, respectively.

The IEI function assigns high values to points that either: (i) lie close to the estimated limit-state boundary ($\mu(\mathbf{x}) \approx b_k$), or (ii) exhibit large predictive uncertainty ($\sigma(\mathbf{x})$ large). This dual behavior enables efficient identification of samples that contribute most to improving boundary resolution. In addition, this active learning strategy enables accurate approximation of highly irregular failure boundaries arising from stochastic bubble dynamics and phase-change interactions while significantly reducing the number of expensive LSF evaluations required.

2.3. *SSIS with k-means clustering*

The combination of conventional SSIS methods with surrogate models is generally limited to problems with a single failure mode. This limitation arises because surrogate models can only indicate whether a sample fails but cannot identify the specific failure mode it belongs to. In SSIS, the sample with the highest probability density within the failure region is selected as the sample center, which means that only one center can be identified for each level.

For problems involving multiple failure modes, multiple sample centers are required. The k-means clustering algorithm offers an effective way to group failure samples according to their corresponding failure modes. The cluster centers obtained from k-means can then serve as sample centers for generating conditional samples specific to each failure mode. Moreover, empirical cluster variances and weights are obtained through k-means and employed to construct Gaussian mixture-based importance sampling density distribution.

Formally, given h failure samples $\{\mathbf{x}_i\}_{i=1}^{h}$ at a certain SSIS level, the goal of k-means clustering is to partition these samples into z clusters $\{S_i\}_{i=1}^{z}$ by minimizing the following objective function:

$$C = \arg\min \sum_{i=1}^{z} \sum_{\mathbf{x} \in S_i} \|\mathbf{x} - \boldsymbol{\eta}_i\|^2, \qquad (14)$$

where $\boldsymbol{\eta}_i$ denotes the center of cluster S_i, and z corresponds to the number of distinct failure modes. Once the cluster centers are determined, each failure sample is assigned to the nearest cluster center based on Euclidean distance.

2.4. *Multi-point enrichment algorithm*

The multipoint enrichment algorithm extends the classical AK-MCS method by allowing multiple points to be added to the design of experiments (DoE) at each iteration, providing a more efficient estimation of failure probability exploiting the uncertainty estimation of Gaussian Kriging surrogate model predictions Razaaly and Congedo (2020). This approach is particularly advantageous when parallel computing is available, as several samples can be evaluated simultaneously.

The algorithm operates as follows:

(1) **Selection of the first sample.** A single sample $\mathbf{y}_0^*$ is chosen according to the AK-MCS selection criterion (Eq.13), which identifies the point with the highest learning function value.
(2) **Multipoint selection via clustering.** K_1 additional samples $\mathbf{y}_1^*, \ldots, \mathbf{y}_{K_1}^*$ are selected simultaneously from the set of candidates located in the *Limit-State Margin (LSM)* $S_f^{(k)}$.

In the above point, we introduced the LSM which is a natural region for design enrichment, since it focuses on samples that are close to the true limit-state surface. It is defined considering lower and upper boundaries to the accuracy of the predicted LSF values. This is possible thanks to the prediction uncertainty estimation of the Kriging model. More formally, given a set of samples $S = \{y_1, .., y_N\}$, K_1 samples are selected in the set $S \cap S_f^{(k)}$ where $S_f^{(k)}$ is the difference $\mathcal{D}_f^{(k)+} \setminus \mathcal{D}_f^{(k)-}$. Which are described as: $\mathcal{D}_f^{(k)+} = \{\mathbf{y} \in \mathbb{R}^d : \mu_{\hat{G}}(\mathbf{y}) + k\sigma_{\hat{G}}(\mathbf{y}) < u\}$ and $\mathcal{D}_f^{(k)-} = \{\mathbf{y} \in \mathbb{R}^d : \mu_{\hat{G}}(\mathbf{y}) - k\sigma_{\hat{G}}(\mathbf{y}) < u\}$. Here $\mu_{\hat{G}}(\mathbf{y})$ and $\sigma_{\hat{G}}(\mathbf{y})$ are respectively the predictive mean and variance of the Kriging model at $\mathbf{y}$ and k is a constant with value 1.96.

Overall, this multipoint enrichment strategy improves the efficiency of the AK-MCS algorithm by refining the surrogate model in regions of interest and enabling parallel evaluation of multiple samples.

2.5. *MP-AK-IEI-SSIS algorithm*

(1) **Generate the initial design of experiments (DoE).** Randomly generate N samples $\mathbf{x} = \{x_1, x_2, \ldots, x_N\}$ of the variables using Latin Hypercube Sampling (LHS). Then, obtain the real response values $g(\mathbf{x}) = \{g(x_1), g(x_2), \ldots, g(x_N)\}$ and form an initial training sample library S.
(2) **Construct the initial Kriging model based on S.** build and fit the initial Kriging model on the existing DoE
(3) **Generate the candidate sample set Ω_0 in the first level of SSIS.** Using the PDF of the variables, N_1 random samples are drawn.
(4) **Update the Kriging model with sample $\mathbf{x}_{\text{new}}$ from Ω_0.** Using the learning function in Eq. (13), we select a sample $\mathbf{x}_{\text{new}}$ in Ω_0. The true performance function is then used to evaluate $\mathbf{x}_{\text{new}}$, and the true evaluation $g(\mathbf{x}_{\text{new}})$ is added to the DoE to update the Kriging model.
(5) **Check the termination criterion.** The stopping condition is defined as Eq. 13 in $\mathbf{x}_{\text{new}}$ lower equal to 0.1%. If the criterion is not met, the current prediction accuracy of the Kriging model is considered insufficient and the previous point must be repeated. The update process continues until the termination condition is satisfied.
(6) **Execute the SSIS.** If the previous condition is satisfied, the SSIS is executed until the last level samples Ω_L are generated. In each level, k-means clustering is implemented on the conditional samples to identify empirical centers, variances, and weights of clusters, which are deployed to perform importance

sampling for generating candidate samples for the next level. Moreover, the Kriging model is applied to evaluate the response of the samples in SSIS.

(7) **Update the Kriging model with sample $\mathbf{x}_{\text{new}}$ from Ω_L.** This step is almost identical to Step 4. The difference is that $\mathbf{x}_{\text{new}}$ is selected from the last level samples Ω_L of SSIS using the Eq. (13) learning function. Additionally, only in the first iteration of this adaptive loop, more learning samples are chosen by the multiple enrichment algorithm, presented in Section 2.4, using k-means and are added to the DoE for updating the Kriging model.

(8) **Check the termination criterion.** The adaptive step in the previous point is repeated until the termination condition of the loop is met. The condition is the same of Step 5.

(9) **Evaluate the failure probability and coefficient of variation.** The final failure probability $\hat{P}_f$ and coefficient of variation COV$(\hat{P}_f)$ are calculated according to Eqs. 9 and 11, respectively.

(10) **Check the termination condition of the entire calculation process.** If COV$(\hat{P}_f) < 5\%$, the reliability analysis process ends. Otherwise, return to point 4.

3. Numerical results

We demonstrate the efficiency of the proposed method through three numerical examples.

3.1. *Example 1: Single failure region 2D*

Table 1.: Example 1 Results Single Failure Region 2D.

Method	N_{calls}	$P_f/10^3$	$COV(P_f)\%$	$\epsilon\%$
MCS[1]	10^8	2.8974	1.8054	–
SSIS[1]	10^8	2.9461	2.1487	1.68
AK-MCS[1]	30.40	2.7040	4.1356	6.67
AK-IEI-SSIS[1]	26.35	2.8890	2.1280	0.29
MP-AK-IEI-SSIS	15.40	2.8827	1.2602	0.51

Source: [1]Liu et al. (2026)

A classical two-dimensional benchmark problem, is first considered to assess the performance of the proposed method. This example is characterized by a very low failure probability, a smooth nonlinear limit-state function, and a single connected failure region.

The performance function in the standard normal space is defined as

$$G(y_1, y_2) = \frac{y_1^2}{2} + \frac{(y_2 - 5)^2}{3} - 1, \qquad (15)$$

where $\mathbf{Y} = (y_1, y_2)$ follows a standard bivariate normal distribution.

The probability of failure is given by

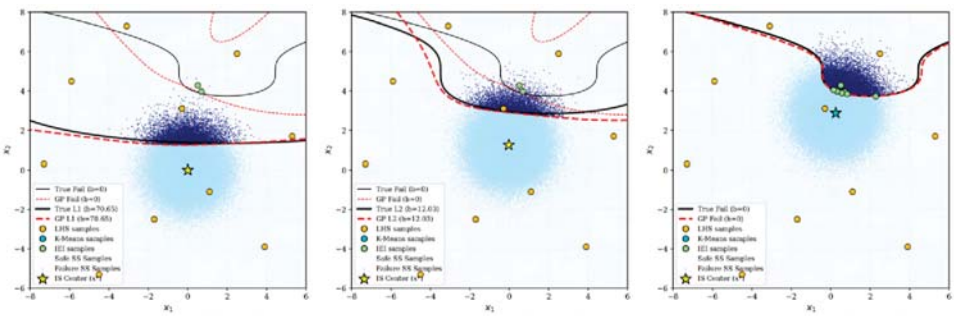
$$P_f = \mathbb{P}\big(G(\mathbf{Y}) \leq 0\big). \qquad (16)$$

A MCS reference failure probability of $P_f = 2.8974 \times 10^{-5}$ with a coefficient of variation (COV) of 1.8054% is reported in Liu et al. (2026).

Table 1 summarizes the results, including the number of calls to the performance function (N_{call}), the estimated failure probability (P_f), the coefficient of variation of the failure probability (COV$_{P_f}$), and the error percentage (ε) relative to the benchmark MCS. Among these metrics, N_{call} and ε are particularly important for evaluating the efficiency and accuracy of each method. The previous performance metrics for MP-AK-IEI-SSIS are averaged over 25 independent experiments.

From Table 1, it is evident that MP-AK-IEI-SSIS outperforms in terms of computational cost while achieving satisfactory accuracy of failure probability prediction. Specifically, it requires 40.7% fewer calls to the performance function than the original AK-IEI-SSIS algorithm while achieving only a 0.51% error. This is mainly due to reducing the dependency on the initial DoE that was reported as a limitation of the original AK-IEI-SSIS method Liu et al. (2026) through adopting the multi-point enrichment algorithm and hyperparameter tuning of the kriging model. Therefore, in this case we managed to use an initial DoE of 10 compared to 19 in Liu et al. (2026), and we enrich it with one k-means sample.

Moreover, Figures 1a, 1b, and 1c show the gradual subset partitioning of the MP-AK-IEI-SSIS at levels 1, 2, and 3 of SSIS, respectively.



(a) SSIS Level 1 (b) SSIS Level 2 (c) SSIS Level 3

Fig. 1.: Example 1 SSIS Levels 1–3 in MP-AK-IEI-SSIS

These findings confirm that MP-AK-IEI-SSIS is a practical and effective approach for tackling small failure probability problems.

3.2. *Example 2: Two failure regions 2D*

Table 2.: Example 2 Results Two failure regions 2D.

Method	N_{calls}	$P_f/10^3$	$COV(P_f)\%$	$\epsilon\%$
MCS[1]	1.2×10^5	3.35	0.05	–
Au & Beck[2]	600	2.47	0.08	26.3
MetaAL-OIS[1]	44	3.53	0.001	5.37
MP-AK-IEI-SSIS	27.48	3.52	2.733	5.07

Source: [1]Razaaly and Congedo (2018) [2]Au and Beck (2001)

The second example considers a two-dimensional reliability problem featuring two disconnected failure regions.

The performance function in the standard normal space is given by

$$G(y_1, y_2) = \min \left\{ \begin{array}{l} c - 1 - y_2 + \mathrm{e}^{\frac{-y_1^2}{10}} + \left(\frac{y_1}{5}\right)^4 \\ \frac{c^2}{2} - y_1 y_2 \end{array} \right\}. \tag{17}$$

Where, the parameter $c = 3$ and $\mathbf{Y} = (y_1, y_2)$ follows a standard bivariate normal distribution.

The method manages to detect disconnected failure regions although the failure boundary is nonlinear with a sharp edge. Moreover, it overperforms in terms of 37.6% faster convergence rate while maintaining a low accuracy error of 5.07% relative to the standard MCS, as shown in Table 2. The previous performance metrics for MP-AK-IEI-SSIS are averaged over 25 independent experiments.

Moreover, as for the previous example, Figures 2a, 2b, and 2c show the gradual subset partitioning of the MP-AK-IEI-SSIS at levels 1, 2, and 3 of SSIS, respectively.

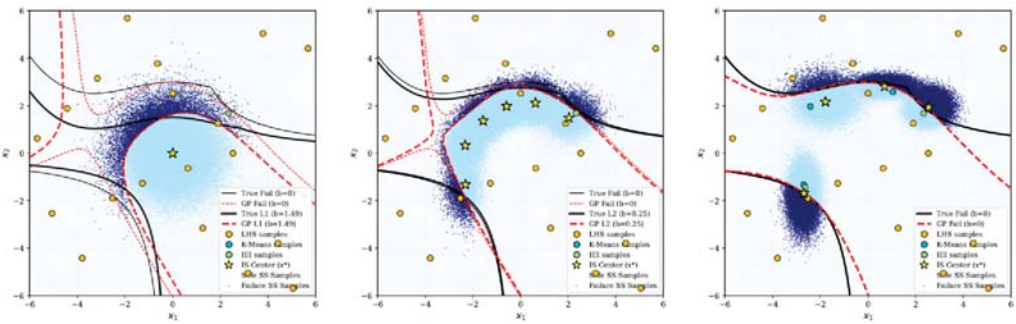
3.3. *Example 3: Four-branch series 2D*

Table 3.: Example 3 Results Four-branch Series 2D.

Method	N_{calls}	$P_f/10^3$	$COV(P_f)\%$	$\epsilon\%$
MCS[1]	10^6	2.231	2.115	–
AK-SS[1]	119	2.192	4.372	1.75
AK-SSIS[1]	115	2.241	3.216	0.45
RVM-SSIS[1]	101	2.237	3.152	0.27
MetaAL-OIS[2]	69	2.210	0.001	0.94
MP-AK-IEI-SSIS	39.7	2.282	1.646	2.29

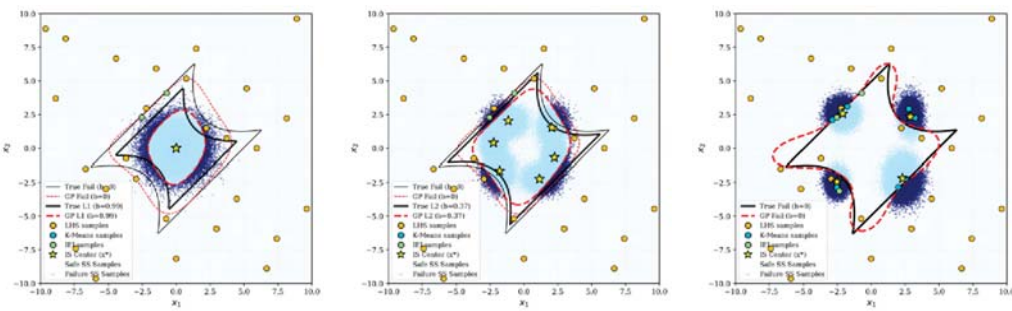
Source: [1]Xie et al. (2023) [2]Razaaly and Congedo (2018) .

The third example is a classical structural reliability test problem, where the failure threshold is modified in order to further reduce the failure probability. The system consists of four failure modes arranged in a series configuration.



(a) SSIS Level 1 (b) SSIS Level 2 (c) SSIS Level 3

Fig. 2.: Example 2 Results SSIS Levels 1–3 in MP-AK-IEI-SSIS



(a) SSIS Level 1 (b) SSIS Level 2 (c) SSIS Level 3

Fig. 3.: Example 3 SSIS Levels 1–3 in MP-AK-IEI-SSIS

The performance function is defined as

$$\begin{aligned} G(y_1, y_2) = \min \Big\{ & 3 + \frac{(y_1 - y_2)^2}{10} - \frac{y_1 + y_2}{\sqrt{2}}, \\ & 3 + \frac{(y_1 - y_2)^2}{10} + \frac{y_1 + y_2}{\sqrt{2}}, \\ & (y_1 - y_2)^2 + \frac{y_1 + y_2}{\sqrt{2}} - 7, \\ & (y_1 - y_2)^2 - \frac{y_1 + y_2}{\sqrt{2}} - 7 \Big\}, \end{aligned} \tag{18}$$

where $\mathbf{Y} = (y_1, y_2)$ follows a standard normal distribution. The objective is to estimate the failure probability

$$P_f = \mathbb{P}\big(G(\mathbf{Y}) \leq 0\big). \tag{19}$$

The proposed method extends the original AK-IEI-SSIS method to identify the four failure regions consistently through the SSIS enhanced with k-means clustering. The clustering at SSIS levels 1, 2, and 3 can be shown in Figures 3a, 3b, and 3c, respectively. In addition, the number of clusters, k, is optimized through Akaike Information Criterion (AIC). This is a valuable advantage, as in most real-world engineering problems, little information exists a priori on the true number of failure regions.

Moreover, the method achieves the lowest number of calls to the performance function, indicating 42.5% faster convergence than the MetaAL-OIS algorithm presented in Razaaly and Congedo (2018). The method reports an accuracy error of 2.29% compared to the MCS standard as shown in Table 3. The previous performance metrics for MP-AK-IEI-SSIS are averaged over 10 independent experiments.

4. Conclusion

This work presents an efficient framework for estimating rare failure probabilities in complex systems governed by computationally intensive models. The proposed method successfully identifies multiple failure regions while requiring, on average, 40% fewer calls to the performance function. Moreover, unlike traditional approaches, it does not require prior knowledge of the number of failure regions and is less sensitive to the quality of the initial design of experiments than the original AK-IEI-SSIS method Liu et al. (2026), which can otherwise slow convergence. Our framework integrates a multi-point active-Kriging approach with an improved expected improvement learning function, k-means-based clustering, and subset-simulation importance sampling. This combination allows efficient prediction of multiple failure regions while accelerating convergence rate. Overall, our results indicate that the MP-AK-IEI-SSIS method can serve as a practical tool for reliability analysis and reliability-design optimization in engineering applications.

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