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Literature review on rare event probability estimation in high dimension

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Reliability analysis in high-dimensions without dimension reduction and no surrogates

In the high dimensional context, for the task of estimating the rare event probability:

$$\mathbb{P}_\alpha[h(\alpha) \leq 0]$$

many relatively efficient direct Monte-Carlo approaches have been developed.

Subset simulation (Au and Beck, 2001) has long been the standout algorithm for reliability analysis in high-dimensions. Subset simulation (SbS) uses intermediate thresholds $\rho_1 > \rho_2 > \dots > \rho_n = 0$ such that $\{h(\alpha) \leq \rho_1\}$ and $\{h(\alpha) \leq \rho_{j+1} | h(\alpha) \leq \rho_j\}$ for $j \geq 1$ are no longer rare events. The original paper proposed a component-wise Metropolis-Hasting MCMC (Gaussian random walk) to move particles from one threshold to the next. If the probability of failure is small (i.e., less than 10^{-4}), it has been shown that by optimizing the scaling of the variance of the Gaussian proposal distributions according to a target MCMC acceptance rate, the resulting strategy SbS-aCS (adaptive Conditional Sampling) (Papaioannou et al., 2015) leads to an estimator with smaller (relative) root mean squared error.

Another family of methods for reliability analysis in high-dimensions is based on sequential importance sampling (SIS), where a collection of intermediate biasing densities $q_j(\alpha) \propto p_j(\alpha)q(\alpha)$ are used ($1 \leq j \leq n$). An interesting choice for $p_j(\alpha)$ is a smooth approximation of the indicator function $\mathbb{1}_{h(\alpha) \leq 0}$ that gets increasingly more accurate as j increases, e.g., the Gaussian cdf $p_j(\alpha) := \Phi(-h(\alpha)/\sigma_j)$ with $+\infty = \sigma_1 > \dots > \sigma_j > \dots > \sigma_n$. Note that both SbS and SIS were recently categorized as members of the same family under the framework relaxation-based importance sampling (Xian and Wang, 2023). SIS-aCS (Papaioannou et al., 2016) is based on the same aCS-MCMC strategy with Gaussian proposals as SbS-aCS above in order to move particles from $q_j(\alpha)$ to $q_{j+1}(\alpha)$, but the resulting estimator exhibits larger RMSE on a high-dimensional linear toy model compared with SbS-aCS (Cheng et al., 2023). SIS-aCS can be potentially further improved in high-dimensions by replacing the Gaussian MCMC proposal with a von Mises-Fisher Nakagami proposal distribution (SIS-vMFN, Wagner et al., 2020) that leverages the polar coordinate decomposition (Munoz Zuniga et al., 2012;

Song and Kawai, 2023):

$$\bar{P}_f = \int_{\mathcal{S}^{d-1}} \mathbb{P}_R[h(RV) \leq 0 | V = v] p_V(v) dv, \quad (1)$$

where the Gaussian vector α is decomposed as $\alpha = RV$; the radial component $R = \|\alpha\|$ follows a χ -distribution with d degrees of freedom on $(0, +\infty)$, \mathcal{S}^{d-1} is the unit hypersphere and $V \sim p_V$ is uniformly distributed on \mathcal{S}^{d-1} . While the SIS-vMFN estimator outperforms SbS-aCS in terms of RMSE for large simulation budgets (i.e. $N > 10^4$), SbS-aCS is superior to SIS-vMFN for smaller budgets $N < 10^4$ on a high dimensional linear model (Wagner et al., 2020). The same conclusion applies to other recent methods designed to exploit the polar coordinate decomposition (1) such as Sequential directional importance sampling (SDIS) (Cheng et al., 2023). In high dimension, relaxation-based directional importance sampling methods (Xian and Wang, 2023) have also been shown to outperform Hamiltonian MC based SbS (Wang et al., 2019) with a simulation budget of at least $N > 10^4$.

Alternatively, cost efficient particle-based methods for Bayesian inverse problems such as Ensemble Kalman Filter (Inversion) (EnKF, EKI) (Iglesias and Yang, 2021) and Consensus based sampling (CBS) (Carrillo et al., 2022) have been adapted to the rare event formulation in (Wagner et al., 2022) and (Althaus et al., 2023), respectively. We can notice that these approaches might require a large number of simulations, involve additional tuning parameters and to the best of our knowledge convergence proof have not been derived so far in dimension greater than one. In particular when facing multi-modal failure problems the Gaussian approximation of the importance distribution seems unreasonable. On a high-dimensional linear model example, these methods require an order of magnitude more simulations than their SIS-vMFN counterpart. Another cost-efficient option for Bayesian inverse problems is to use the cross-entropy method based on Kullback-Leibler divergence minimization, which has been adapted to high-dimensional reliability analysis in (Wang and Song, 2016) and (Papaioannou et al., 2019b). To summarize, as the dimensionality increases all these methods require a large number of particles, and thus a large number of simulations. Indeed, for a fixed simulation

budgets $N \leq 10^4$ and high-dimensional problems ($d > 50$), none of these methods have outperformed SIS-vMFN or SbS-aCS in terms of RMSE on a few literature test cases.

One special mention goes to the recent cross-entropy based strategy (Chiron et al., 2023), which significantly outperformed the existing cross-entropy methods and SbS in terms of RMSE for an equal (and small) simulation budget, at the expense of requiring gradients of the simulator for a sequence of optimization problems, according to a few reliability test problems. Each optimization run has the purpose of finding (quickly, if gradients are available) different failure regions; the optimization solutions are known as ‘critical points’, around which cross-entropy leveraging the polar decomposition (1) is performed (gradient-free optimization methods would increase the simulation cost significantly, and the paper outlines that it is important for the optimization solutions to be accurate).

So far we have presented a collection of general reliability analysis methods for high dimensional problems that require no hypothesis on the simulator such as weakly nonlinear structure for h . In case there exists such a structure, algorithms under the name of first-order reliability (FORM) (Der Kiureghian and Dakessian, 1998) are the most cost efficient. Classical FORM methods can be combined with sampling and this results in good estimators with small c.o.v. in weakly nonlinear high-dimensional problems (Wang and Kiureghian, 2017). The observation that SbS-aCS is the best (gradient-free) method in high-dimensions for small simulation budgets $N < 10^4$ is based on a collection of numerical experiments with smooth, well-behaved simulators $g(x)$ (e.g., linear function or maximum between two linear functions in opposite sides of the origin, hence two failure regions (Cheng et al., 2023), 1D diffusion equation or 2D flow cell (Wagner et al., 2020)). In these experiments, SbS-aCS returned a c.o.v. of around 0.3 using $N < 10^4$ simulations. If a smaller c.o.v. is desired, SbS can be very costly (Chiron et al., 2023) and for some simulators SbS can require $5 \cdot 10^4$ simulations to reach a c.o.v. of around 0.3 (Munoz Zuniga et al., 2021). It is known that c.o.v. for SbS scales as $O(1/\sqrt{N})$ (Au and Beck, 2001), and the estimated c.o.v. returned by SbS generally underestimates the SbS true c.o.v. (Papaioannou et al., 2015).

A last family of approach focuses on estimating the distribution tail of the output maximum. An envisaged strategy was to build a KL expansion of the non-Gaussian time dependent output s . Indeed this latter can be used to sample at reduced cost the output. For this purpose the joint distribution of the KL coefficients have to be estimated and in particular its tail. Finally with the KL samples the probability of failure or a bound can be estimated. But the task of estimating the tail of a joint distribution in high dimension seems too difficult.

To sum up, for small failure probabilities involving a high dimensional random vector and a moderately complex simulator, the approach offering the best c.o.v (~ 0.3) for a simulation budget $N \leq 10^4$ appears to be SbS-aCS. When the model is linear, equivalent or smaller c.o.v can be reached with a smaller simulation budget by using an optimization based method (FORM) but no confidence interval is then available.

Reliability analysis in high-dimensions with surrogates

In order to mitigate the cost of reliability estimation, a large number of publications focus on combining the Monte Carlo method with surrogate modelling.

Surrogate models (meta-models) for expensive simulators can greatly alleviate the computational cost of reliability analysis in low-dimensions, and many such methods have been proposed. The review paper ([Moustapha et al., 2022](#)) compares the performance of these methods on a relatively large benchmark of 20 reliability problems. The review focuses on two popular families of meta-models, i.e., kriging (Gaussian Process modelling) and Polynomial Chaos Expansion (PCE); see e.g., [Bect et al. \(2017\)](#) for kriging within SbS, and [Dubourg et al. \(2013\)](#) for kriging within IS. Out of the 20 reliability problems, 5 problems are of medium to high-dimensionality ($D \in [20, 100]$), for which sparse PCE ([Blatman and Sudret, 2011](#)), kriging (with standard covariance functions) and PC-kriging ([Schobi et al., 2015](#)) (which uses sparse PCE as trend function for kriging) gave remarkable performances for estimating P_f with only approximately hundred of simulations. Nevertheless, it is difficult to draw conclusions on the ranking between kriging, PC-Kriging and sparse PCE in high-dimensional reliability

based on these numerical experiments alone given that it seems strongly case and tuning dependent. For instance, an ANOVA decomposition type of kernel could be used which would mimic the sparse PCE approach. Moreover results are averaged over different toy problems which makes difficult to distinguish which method is better suited to which test case. Another conclusion of the paper is that IS is significantly worse than Monte Carlo and SbS for these high-dimensional surrogate-based experiments might be simply due to the presence of the importance ring in high-dimensional reliability; one option is to do IS on the unit hypersphere instead (Wagner et al., 2022) (unless the simulator has a latent low-dimensional structure). One important simulator omitted is the classical nonlinear oscillator (i.e., hysteretic oscillator under random loading), which is widespread in the high-dimensional reliability literature (e.g., Wang and Song (2016)). For this simulator, Papaioannou et al. (2019a) shows that sparse PCE fails to produce a good surrogate, and dimension reduction via nonlinear Partial Least Squares (PLS) is necessary for an accurate surrogate. Another possible argument for the inferior performance of kriging in high-dimensions is that the kriging variance (predictive uncertainty), which is also used to guide further simulator evaluations via active learning, hardly shrinks as the experimental design (training set) is enriched.

Alternatively, we can try to directly model $Y = g(X)$ using an approximate density \hat{p}_Y , easy to sample from, followed by estimating P_F via a MC estimator of $\bar{P}_f = \mathbb{P}_{\hat{p}_Y}[Y \leq 0]$. An approach based on the Laplace transform $\mathcal{L}(s) := \mathbb{E}[\exp(-sY)]$ is proposed in Dang and Xu (2020). For a small $s \approx 0$, $\mathcal{L}(s)$ can be well-estimated in high-dimensions using relatively few simulator evaluations via Monte Carlo samples $x \sim q(x)$; the approximate density $\hat{p}_Y(y)$ is then chosen from a parametric family, such that its Laplace transform matches the one estimated via Monte Carlo. The parameteric family proposed in Dang and Xu (2020) is a mixture of skew Normal distributions. In case the simulator output an extreme value over a time interval e.g., $g(x) = \max_{t \in [0, T]} h(x, t)$, it has been shown that the above method can return extremely inaccurate estimates of P_F , and other parametric families from the Extreme Value Distribution (EVD) literature should be used, e.g., mixture of two generalized inverse Gaussian distributions (Dang et al., 2021).

Another promising strategy is the one proposed in [Gramstad et al. \(2020\)](#) which directly infer the distribution of the maximum of the output:

$$Y = \max_{[0,T]} s(t; U)$$

and then estimate the failure probability directly by MC or a reduced variance MC strategy if necessary. The difficulty boils down to the estimation of the marginal distribution that can be written as

$$g_Y = \int g_{Y|\xi}(y|\xi) f_\xi(\xi) d\xi.$$

Following [Gramstad et al. \(2020\)](#) this estimation can be achieved with first a parametric choice of the conditional distribution. Then the distribution parameters can be learned with a GP model between the long term inputs and these parameters. Finally [Gramstad et al. \(2020\)](#) proposes to estimate the integral for the calculation of g_Y with the strategy introduced in [Mohamad and Sapsis \(2018\)](#). This method has been evaluated in HIPERWIND ([REF report](#)). The main issue is the selection of an appropriate parametric family for the conditional distribution $g_{Y|\xi}$. Moreover the learning design of experiment must be representative of the output extreme to be estimated.

Reliability analysis in high-dimensions via dimension reduction with surrogates

If the high-dimensional simulator exhibits a global low-dimensional structure, various dimension reduction methods can be combined with surrogates such as kriging or PCE. In this way, we can benefit from the remarkable performance of surrogate methods for low-dimensional reliability problems. Indeed, [Moustapha et al. \(2022\)](#) shows that for a fixed target RMSE and a variety of simulators, surrogate-based reliability methods require a much smaller number of simulator evaluations compared with methods such as SbS or IS without surrogates.

The popular dimension reduction method Active Subspaces (AS) ([Constantine et al., 2014](#)) has been used to construct surrogates and perform reliability analysis via PCE ([Navaneeth and Chakraborty, 2022](#)) and kriging ([Jiang and Li, 2017](#); [Ji et al., 2022](#); [Kim et al., 2023](#)).

One disadvantage of AS is that it requires gradient evaluations for the simulator. [Wycoff et al. \(2021\)](#) proposes a gradient-free version of AS; however, this requires performing high-dimensional kriging prior to estimating the active subspace, and thus a large computational budget might be necessary.

Alternative gradient-free dimension reduction methods such as Partial least squares (PLS) or (gradient) kernel dimension reduction (gKDR, KDR) have been considered in the reliability literature. Kriging with PLS strategies for reliability were proposed in [Zuhal et al. \(2021\)](#), [Liu et al. \(2022\)](#); Moreover, as mentioned, [Papaioannou et al. \(2019a\)](#) shows that sparse PCE fails to produce a good surrogate, and dimension reduction via nonlinear Partial Least Squares (PLS) is necessary for an accurate surrogate named PCE-PLS. The follow-up paper ([Ehre et al., 2022](#)) shows that PCE-PLS produces good results in a diverse collection of reliability problems in medium-high dimensions. Kriging strategies for reliability with both KDR ([Fukumizu et al., 2003](#)) and gKDR ([Fukumizu and Leng, 2014](#)) were proposed in [Munoz Zuniga et al. \(2021\)](#). Both KDR and gKDR are part of the Sufficient Dimension Reduction (SDR) family, together with e.g., Sliced Inverse Regression (SIR); see [Pan and Dias \(2017\)](#), [Xu and Wang \(2019\)](#) for PCE strategies with SIR dimension reduction for reliability.

To summarize, if the high-dimensional simulator exhibits a global low-dimensional structure, it may be beneficial to perform dimension reduction prior to constructing surrogates in general ([Liu and Guillas, 2017](#)), and for reliability analysis in particular ([Munoz Zuniga et al., 2021](#)). If only a local low-dimensional structure can be found, one reliability strategy with local surrogates via kriging with PLS was proposed in ([Šehić and Karamehmedović, 2020](#)). In this local case, kriging with PLS might not necessarily return a more accurate surrogate compared with performing high-dimensional kriging directly; it is simply faster to train the surrogate hyperparameters in low-dimensions.

We finish this section with a warning. It is well-known that performing linear dimension reduction (e.g., PLS, KDR, AS) prior to applying kriging is equivalent to performing high-dimensional kriging with a particular kernel; the lengthscales of this high-dimensional kernel as a function of the dimension reduction matrix can be found in [Bouhlef et al. \(2016\)](#).

This suggests that if the low-dimensional subspace is not accurately estimated (e.g., due to computational budget limitations), we suffer from the same problem of large kriging variance as in high-dimensional kriging in general, as exemplified by [Seshadri et al. \(2019\)](#).

Reliability analysis in high-dimensions via dimension reduction without surrogates

Cross-entropy-based importance sampling with failure-informed dimension reduction (iCEred) ([Uribe et al., 2021](#)), which addresses the short-comings of the standard cross-entropy method discussed before, i.e., as the dimensionality increases, the standard cross-entropy method ([Papaoannou et al., 2019b](#)) requires a large number of particles and thus a large number of simulator evaluations. As in sequential importance sampling (SIS), a collection of intermediate biasing densities $q_j(x) \propto h_j(x)q(x)$ are used ($1 \leq j \leq n$); $h_j(x)$ is a smooth approximation of the indicator function $\mathbb{1}_{g(x) \leq 0}$ that gets increasingly more accurate as j increases, e.g., the Gaussian cdf $h_j(x) := \Phi(-g(x)/\sigma_j)$ with $+\infty = \sigma_1 > \dots > \sigma_j > \dots > \sigma_n$. Given that for all j , a local low-dimensional approximation $d_j \ll D$ exists: $h_{j+1}(x) \approx v(W_j^T x)$ for $x \sim q_j(x)$ and $W_j \in \mathbb{R}^{D \times d_j}$, we can exploit it to essentially perform cross-entropy in low-dimensions. The dimension reduction matrix W_j is estimated with a certified accuracy via [Zahm et al. \(2022\)](#); however, gradients of the simulators are required. An alternative gradient-free method could be possible following ([Wycoff et al., 2021](#)) but as discussed in the previous section, ([Wycoff et al., 2021](#)) requires performing high-dimensional kriging prior to estimating the dimension reduction matrix, and thus a large computational budget might be necessary. If instead a global dimension reduction exists for $d \ll D$: $g(x) \approx v(W^T x)$ for $x \sim q(x)$ and $W \in \mathbb{R}^{D \times d}$, the low-dimensional subspace can be exploited for more efficient sampling from $\tilde{q}(x) \propto \mathbb{1}_{v(W^T x) \leq 0} q(x)$ compared with sampling from the high-dimensional space directly (see [Munoz Zuniga et al. \(2021\)](#) where such $\tilde{q}(x)$ is used for reliability via IS).

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