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BRIEF NOTE

A generalized "max-min" sample for surrogate update

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Abstract This brief note describes the generalization of the "max-min" sample that was originally used in the update of approximated feasible or failure domains. The generalization stems from the use of the random variables joint distribution in the sampling scheme. In addition, this note proposes a numerical improvement of the max-min optimization problem through the use of the Chebychev norm.

Keywords Max-min sample · Chebychev norm · Adaptive sampling · Reliability

1 Introduction

The use of surrogates has become omnipresent in reliability assessment, design optimization, and reliability-based design optimization. In many cases, the surrogates are initially constructed from a design of experiments and refined using an adaptive sampling scheme. This idea is used for example in Efficient Global Optimization (Jones et al. 1998, EGO), Efficient Global Reliability Assessment (Bichon et al. 2008, EGRA), and Explicit Design Space Decomposition (Basudhar and Missoum 2010, EDSD).

Sparsity of data is often the basis for the choice of an adaptive sampling scheme. For instance, the Kriging update scheme for optimization, EGO, uses the sparsity information through a distance-based correlation function (Jones 2001). EDSD uses it more explicitly through a "max-min" sample (Basudhar and Missoum 2008, 2010) that maximizes the minimum distance to existing samples (i.e., maximum sparsity). In Regis and Shoemaker (2005), a minimum distance between samples is enforced through a constraint.

The max-min sample, which is the focus of this paper, was mostly used to refine approximations of the feasible or failure domain using Support Vector Machines (SVMs). However, its formulation did not account for the various probabilistic distributions of the variables. As a consequence, this was an issue for probability of failure estimates since samples were wasted in regions with low probabilistic content. For this reason, this article introduces a generalization of the max-min sample which accounts for the joint distribution of the variables. Note that the use of such a sample is not restricted to SVM surrogates. A similar idea was used in Wang and Wang (2013), where an estimated improvement criterion is used to draw more attention in high probabilistic content region.

In addition, this note presents a substantial numerical improvement by replacing the max-min problem using the Chebychev norm. This norm has the advantage of transforming the problem into a traditional differentiable and unconstrained optimization problem.

This article is structured as follows: Section 2 provides a background on the max-min samples and presents the generalized formulation. Section 3 describes the implementation using the Chebychev norm. Finally, Section 4 describes a 10 dimensional reliability example.

2 Background and basic formulation

The primary objective of this work is to extend and generalize the notion of max-min sample that was introduced by Basudhar and Missoum (2010). The sample was used

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to update an approximation of the boundary of feasible or failure domain constructed using an SVM. The max-min sample was chosen as far away from the N_s existing training samples while lying on the SVM. It was found by solving the following global optimization problem:

$$\begin{aligned} \max_{\mathbf{x}} \quad & \min_{i=1,\ldots,N_s} \left|\left|\mathbf{x}-\mathbf{x}^{(i)}\right|\right| && (1)\\ \text{s.t.} \quad & \mathbf{x} \in \partial\tilde{\Omega}_F \\ & l_i \leq x_i \leq u_i \qquad\qquad i=1,\ldots,N_v \end{aligned}$$

where $\partial\tilde{\Omega}_F$ is the boundary of the approximation $\tilde{\Omega}_F$ of the feasible or failure domain Ω_F.

This formulation distributes samples "uniformly" on the boundary. This is an attractive feature if one wants to approximate Ω_F globally over the whole space or in the case of deterministic optimization. However, the approach was also used for reliability assessment. In this case, a uniform distribution of samples is no longer efficient since a higher accuracy of the failure domain should be obtained in places where the probabilistic content is larger. For this purpose, the objective function in (1) was generalized by introducing the joint probability density function (PDF), $\mathbf{f_X}$, of the variables:

$$\max_{\mathbf{x}} \quad \mathbf{f_X}(\mathbf{x})^{\frac{1}{N_v}} \min_{i=1,\ldots,N_s} \left|\left|\mathbf{x}-\mathbf{x}^{(i)}\right|\right| \qquad (2)$$

This novel formulation is constructed so that the max-min samples follow the joint PDF $\mathbf{f_X}$ while enforcing maximum spread. To demonstrate this feature, consider the case where the samples are not constrained to lie on the boundary. Figure 1a depicts the case where samples are sequentially added using the original formulation. In this case, the result is similar to what would be obtained using an optimal Latin Hypercube sampling algorithm (Park 1994). Figure 1b depicts samples generated using the generalized formulation with normal uncorrelated variables. Note that the generalized formulation reduces down to the original one (1), in the case of uniform distributions.

A proof of concept of the ability of the proposed formulation to actually follow the joint distribution $\mathbf{f_X}$ is proposed using numerical experiments of up to 30 dimensions in the case of a joint normal PDF. This was done both graphically (Fig. 2) and numerically by means of a Kolmogorov-Smirnov test at the 5 % significance level.

3 Implementation using the Chebychev norm

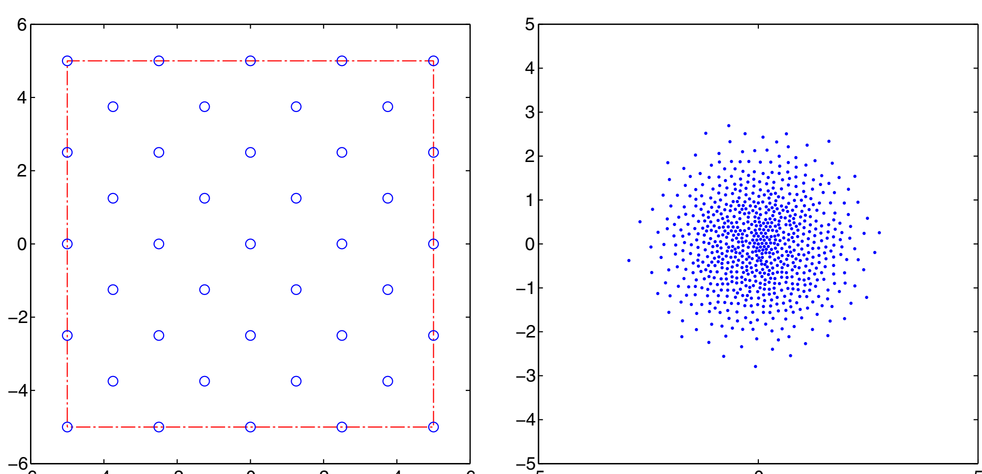
In the previous work by Basudhar and Missoum (2010), the non-differentiability of the max-min problem was removed using the following constrained problem:

$$\begin{aligned} \max_{\mathbf{x},\, z} \quad & z && (3)\\ \text{s.t.} \quad & z-\left|\left|\mathbf{x}-\mathbf{x}^{(i)}\right|\right| \leq 0 \qquad i=1,\ldots,N_s \\ & \mathbf{x} \in \partial\tilde{\Omega} \\ & l_i \leq x_i \leq u_i \qquad\qquad i=1,\ldots,N_v \end{aligned}$$

which transforms (1), an N_v dimensional optimization problem with one constraint into (3), a N_v+1 dimensional optimization problem with N_s+1 constraints.

In order to remove the N_s additional constraints and keep (2) as an unconstrained formulation, the max-min problem is formulated using the Chebychev distance $||\mathbf{v}||_\infty = \max(\mathbf{v})$. It can easily be shown that the Chebychev distance

Fig. 1 Example of classic and generalized max-min sample patterns



a Classic max-min, equivalent to generalized max-min with $X_i \sim U(-5,5)$.

b Generalize max-min with $X_i \sim N(0,1)$.

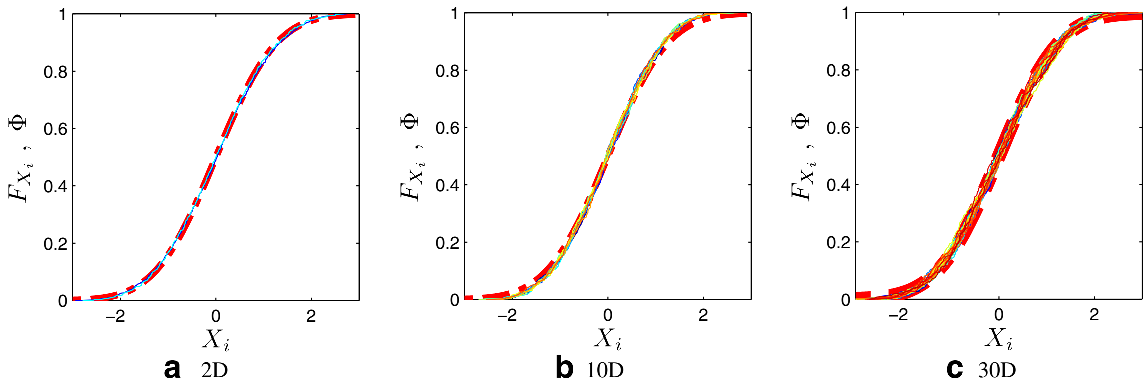


Fig. 2 Graphical proof of concept of the ability of the generalized formulation to draw samples from a given joint distribution. Empirical marginal CDFs $\mathbf{F}_{X_i}$ compared to standard normal CDF Φ (red thick dotted line) for 2, 10, and 30 dimensions based on 400 generalized max-min samples

("norm infinity") can be approximated using the Minkowski metric ("p-norm") for large p (e.g., $p = 40$):

$$||\mathbf{v}||_\infty = \max(\mathbf{v}) \underset{p \gg 1}{\approx} ||\mathbf{v}||_p = \left(\sum_{i=1}^{N_s} v_i^p \right)^{\frac{1}{p}} \tag{4}$$

where each v_i are positive. Noting that

$$\min_{i=1,\ldots,N_s} v_i = \left(\max_{i=1,\ldots,N_s} v_i^{-1} \right)^{-1} \approx \left(\sum_{i=1}^{N_s} v_i^{-p} \right)^{-\frac{1}{p}},$$

and defining $v_i = \left|\left|\mathbf{x} - \mathbf{x}^{(i)}\right|\right|$, we obtain:

$$\min_{i=1,\ldots,N_s} \left|\left|\mathbf{x} - \mathbf{x}^{(i)}\right|\right| \approx \left(\sum_{i=1}^{N_s} \left|\left|\mathbf{x} - \mathbf{x}^{(i)}\right|\right|^{-p} \right)^{-\frac{1}{p}}$$

Finally, the generalized formulation (2) can be written as:

$$\max_{\mathbf{x}} \quad \frac{1}{N_v} \log \mathbf{f_X}(\mathbf{x}) - \frac{1}{p} \log \sum_{i=1}^{N_s} \left|\left|\mathbf{x} - \mathbf{x}^{(i)}\right|\right|^{-p} \tag{5}$$

which, in addition of being unconstrained, is also differentiable. In fact, analytical sensitivities can easily be derived and the optimization problem can be solved efficiently using a gradient-based method.

Note that logarithms have been introduced because as the dimension increases, the numerical values of $\mathbf{f_X}$ drops to 0. Consider the maximum value of the multidimensional standard normal joint PDF $\boldsymbol{\phi}$, which is obtained at the origin. For $N_v = 2$, $\boldsymbol{\phi}(\mathbf{0}) \approx 0.16$ whereas for $N_v = 50$, $\boldsymbol{\phi}(\mathbf{0}) \approx 1.11 \times 10^{-20}$.

4 Application to reliability assessment

For reliability assessment, the boundary of the failure domain needs to be properly approximated by constraining the max-min sample on the boundary. Figure 3 depicts the differences between the original and generalized max-min formulation for a two-dimensional joint standard normal distribution and a given limit-state. The probability of failure is defined as

$$P_f = \mathbb{P}\left[\mathbf{X} \in \Omega_F\right], \tag{6}$$

and is iteratively obtained by refining an SVM as described in Algorithm 1.

Algorithm 1 Reliability assessment algorithm

Compute an initial DOE with m samples
k=m+1;
while Not Converged **do**
  Define labels $l^{(i)}$ as:

$$l^{(i)} = \begin{cases} -1 & \text{if } \mathbf{x}^{(i)} \in \Omega_F \\ +1 & \text{else} \end{cases} \qquad i = [1, k-1]$$

  Build the current approximation of the failure domain $\tilde{\Omega}_F^{(k)}$
  Compute $P_f^{(k)} = \mathbb{P}\left[\mathbf{X} \in \tilde{\Omega}_F^{(k)}\right]$
  Find the next adaptive sample(s) and add them to the data base
  k=k+1;
end while

4.1 Use of the generalized max-min

After the training of the SVM at iteration k, the generalized max-min sample to update the SVM approximation of the failure domain is given by:

$$\max_{\mathbf{x}} \quad \frac{1}{N_v} \log \mathbf{f_X}(\mathbf{x}) - \frac{1}{p} \log \sum_{i=1}^{N_s} \left|\left|\mathbf{x} - \mathbf{x}^{(i)}\right|\right|^{-p} \tag{7}$$
$$\text{s.t.} \quad \mathbf{x} \in \partial \tilde{\Omega}_F^{(k)}$$

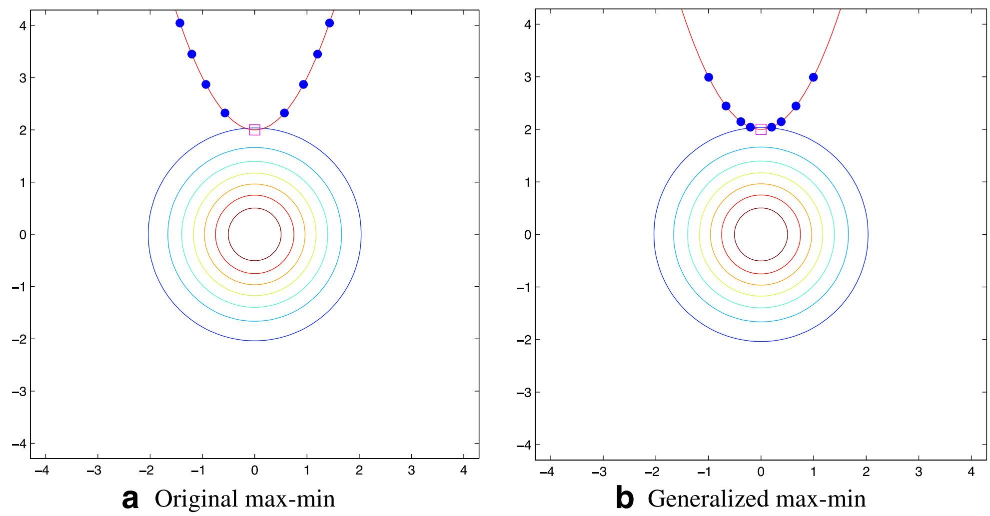


Fig. 3 Distribution of original and generalized max-min samples along a given limit state for a two-dimensional joint standard normal distribution

4.2 Use of the original max-min

For comparison purpose, we will also use the original version of the update:

$$\begin{aligned} \max_{\mathbf{x}} \quad & \min_{i=1,\dots,N_s} \left\|\mathbf{x}-\mathbf{x}^{(i)}\right\| \\ \text{s.t.} \quad & \mathbf{x} \in \partial\tilde{\Omega}_F \\ & \mathbf{x} \in \Omega_U \end{aligned} \tag{8}$$

where Ω_U is an update region. The need for an update region comes from the fact that max-min samples in the case of infinite support distributions are ill-defined. The type and characteristics of the update region is discussed in Appendix. It is noteworthy that the generalized max-min formulation does not require any update region as this information is embedded within $\mathbf{f_X}$.

4.3 Example

As a numerical example, consider the following 10 dimensional highly non-linear analytical limit state where failure is defined as (Engelund and Rackwitz 1993):

$$\frac{\sum_{i=1}^{10} \log X_i}{2} + 12 \leq 0 \quad , \quad X_i \sim N(0,1) \tag{9}$$

Figure 4 shows the convergence of the estimated probability of failure using the generalized and original max-min updates. In addition, the generalized max-min sample was run in parallel by adding 10 samples per iteration before updating the SVM. All probabilities are calculated using Monte-Carlo simulations with a 5 % coefficient of variation. The dashed black line shows the actual probability of failure (estimated using the actual limit state). Note that

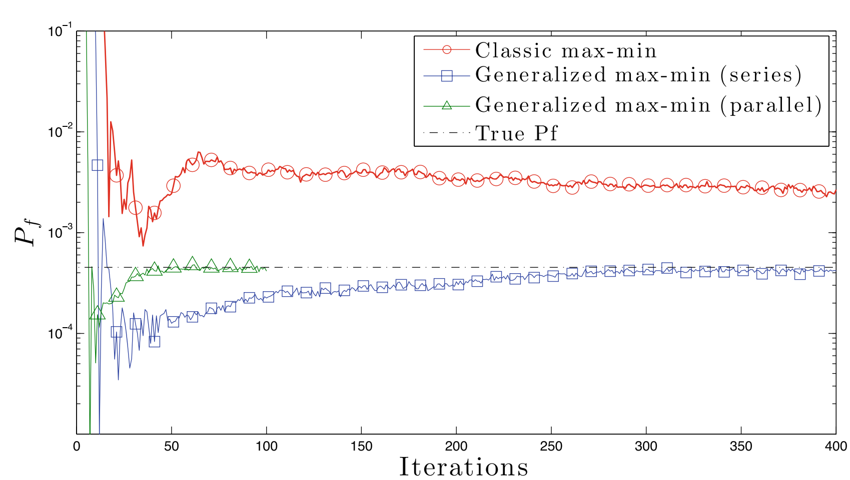


Fig. 4 Convergence of the probability of failure estimate using the original max-min sample (*red line with circles*), the generalized max-min sample (*blue line with square*), and 10 generalized max-min samples in parallel (*green line with triangles*). The black dashed line represents the estimated probability using the actual limit state

the problem in (2) was solved using a sequential quadratic programming (SQP) with multiple starting points.

The figure clearly shows the advantage of using the generalized max-min formulation over the traditional one. In addition, the convergence of the green line clearly shows the potential of using this sample in parallel.

Note that the original max-min sample, represented by the red line, exhibits a slow convergence, which is a well known result due to a phenomenon referred to as locking of the SVM. This was solved in previous work using an additional sample referred to as the "anti-locking" sample (Basudhar and Missoum 2010).

5 Conclusion

In this note, the orignal max-min sample is generalized to account for the joint distribution of the variables. In addition, a novel efficient implementation based on an approximation of the Chebychev distance is proposed. Application to an analytical limit state shows promising results for reliability assessment with both serial and parallel updates.

The next step of this work will involve the use of the generalized max-min within a reliability-based design optimization algorithm as well as for reliability assessment with correlated variables.

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Appendix

Update region size for original max-min

For reliability assessment, the traditional max-min samples need to be constrained within an update region. The nature and size of the update region are related to the distributions chosen as well as the probability of failure value. In the case of uncorrelated standard normal distributions (as in this paper), the update region should be an hypersphere. The radius of the hypersphere, R, can be linked to the probability of failure based on the fact that the norm of standard normal variables follows a χ^2 distribution (Katafygiotis and Zuev 2008):

$$\text{If } X_i \sim N(0,1) \text{ and } X_i \perp\!\!\!\perp X_j,\ \forall i \neq j \Rightarrow ||\mathbf{X}||^2 \sim \chi^2_{N_v} \tag{10}$$

From this, one can define R, such that, for instance, the hypersphere excludes a fraction (10 % in this note) of the estimated probability of failure. This way, the update region, is iteratively defined as:

$$\Omega_U^{(k)} = \left\{ \mathbf{x} \;\middle|\; ||\mathbf{x}|| \leq R^{(k)} \right\} \text{ with } R^{(k)} = \sqrt{\chi^{2^{-1}}_{N_v}\left(1 - 0.1 P_f^{(k)}\right)} \tag{11}$$

where $P_f^{(k)}$ is the probability of failure calculated using the failure domain approximation at iteration k.

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