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Low-Rank Tensor Approximations for Reliability Analysis

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ABSTRACT: Low-rank tensor approximations have recently emerged as a promising tool for efficiently building surrogates of computational models with high-dimensional input. In this paper, we shed light on issues related to their construction with greedy approaches and demonstrate that meta-models built with small experimental designs can be used to estimate tail probabilities with high accuracy.

1. INTRODUCTION

Advances in computer science in combination with an improved understanding of physical laws lead to the development of increasingly complex computational models for simulating behaviors of physical and engineering systems. Unfortunately, uncertainty propagation through such models becomes intractable in many practical situations when the computational cost of a single simulation is high. A remedy is the use of *surrogate models*, also called *meta-models*, which possess similar statistical properties with the original models, but have simple functional forms and are thus inexpensive to evaluate.

Polynomial Chaos Expansions (PCE) represent the model response as an expansion onto a basis of orthonormal multivariate polynomials obtained as tensor products of appropriate univariate polynomials. Although this meta-modeling approach has proven powerful in a wide range of applications, it suffers from the *curse of dimensionality*, meaning the exponential growth of the basis size - and therefore of the unknown coefficients - with the dimension of the random input.

A promising alternative for efficiently building meta-models in high-dimensional spaces using polynomial functions is offered by Low-Rank Approximations (LRA) (e.g. Nouy (2010), Doostan et al. (2013)). LRA exploit the tensor-product form

of the polynomial basis to express the random response as a sum of a small number of rank-one functions. Such representations drastically reduce the number of unknown coefficients with respect to PCE, with this number growing only linearly with the input dimension.

Existing algorithms for building LRA are based on greedy approaches, where the polynomial coefficients in separate dimensions are alternately updated and the rank of the approximation is progressively increased. These algorithms involve a sequence of error-minimization problems of small size that can be easily solved with standard techniques. However, stopping criteria and selection of optimal rank are open questions that call for further investigations.

The aim of the present paper is to introduce and demonstrate the potential of LRA in the context of reliability analysis as well as to shed light on aspects of their construction. The paper is organized as follows: In Section 2, the mathematical setup of the problem is described. Following a brief review of PCE in Section 3, LRA are presented in Section 4. In Section 5, we employ LRA to develop meta-models of the responses of a beam and a truss structure; in these applications, we investigate properties of the greedy constructions and demonstrate the efficiency of LRA for evaluating small probabilities of failure, also in comparison to PCE.

2. SURROGATE MODELS WITH NON-INTRUSIVE APPROACHES

Let us consider a physical or engineering system whose behavior is represented by a - possibly complex - computational model \mathcal{M} . We denote by $\mathbf{X} = \{X_1, \dots, X_M\}$ the M -dimensional random input and by Y a scalar response quantity of interest. Our goal is to develop a surrogate \hat{Y} of the exact model response $Y = \mathcal{M}(\mathbf{X})$, *i.e.* an approximate model that possesses similar statistical properties, but has a simple functional form.

Non-intrusive methods for building surrogate models are of interest in the present study. Such methods rely on a series of calls to the deterministic computational model, which may be used without any modification. Building a meta-model in a non-intrusive manner requires an Experimental Design (ED) comprising a set of realizations of the input vector, $\mathcal{E} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}\}$, and the corresponding model evaluations at these points, $\mathcal{Y} = \{\mathcal{M}(\mathbf{x}^{(1)}), \dots, \mathcal{M}(\mathbf{x}^{(N)})\}$.

Let us consider a set of realizations of the input vector, $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$. In order to define measures of accuracy of a meta-model, we introduce the semi-inner product

$$\langle a, b \rangle_{\mathcal{X}} = \frac{1}{n} \sum_{i=1}^n a(\mathbf{x}_i) b(\mathbf{x}_i), \quad (1)$$

leading to the semi-norm $\|a\|_{\mathcal{X}} = \sqrt{\langle a, a \rangle_{\mathcal{X}}}$. A good measure of accuracy is the generalization error, $Err_G = \mathbb{E} \left[\left(Y - \hat{Y} \right)^2 \right]$, which can be estimated by

$$\widehat{Err}_G = \left\| Y - \hat{Y} \right\|_{\mathcal{X}_{\text{val}}}^2, \quad (2)$$

where $\mathcal{X}_{\text{val}} = \{\mathbf{x}_1, \dots, \mathbf{x}_{n_{\text{val}}}\}$ is a sufficiently large set of realizations of the input vector, denoted *validation set*. The relative generalization error can be estimated by normalizing \widehat{Err}_G with the empirical variance of $\mathcal{Y}_{\text{val}} = \{\mathcal{M}(\mathbf{x}_1), \dots, \mathcal{M}(\mathbf{x}_{n_{\text{val}}})\}$, *i.e.*

$$\widehat{err}_G = \frac{\widehat{Err}_G}{\text{Var}[\mathcal{Y}_{\text{val}}]}. \quad (3)$$

In cases when one cannot afford the additional model evaluations required to compute \widehat{Err}_G , an error estimate based on the ED may be used instead.

This is the empirical error, \widehat{Err}_E , given by

$$\widehat{Err}_E = \left\| Y - \hat{Y} \right\|_{\mathcal{E}}^2. \quad (4)$$

The respective relative error is obtained by normalizing \widehat{Err}_E with the empirical variance of $\mathcal{Y} = \{\mathcal{M}(\mathbf{x}^{(1)}), \dots, \mathcal{M}(\mathbf{x}^{(N)})\}$, *i.e.*

$$\widehat{err}_E = \frac{\widehat{Err}_E}{\text{Var}[\mathcal{Y}]}. \quad (5)$$

It should be noted that \widehat{Err}_E tends to underestimate Err_G , which might be severe in cases of overfitting.

3. POLYNOMIAL CHAOS EXPANSIONS

Let us assume that the components of \mathbf{X} are independent with joint Probability Density Function (PDF) $f_{\mathbf{X}}(\mathbf{x})$ and marginal PDFs $f_{X_i}(x_i)$, $i = 1, \dots, M$.

Polynomial Chaos Expansions (PCE) approximate the exact model response $Y = \mathcal{M}(\mathbf{X})$ as

$$\hat{Y} = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\mathbf{X}), \quad (6)$$

where $\{\Psi_{\alpha}, \alpha \in \mathcal{A}\}$ is a set of multivariate polynomials with multi-indices $\alpha = (\alpha_1, \dots, \alpha_M)$ that are orthonormal with respect to $f_{\mathbf{X}}(\mathbf{x})$ and y_{α} denotes the corresponding polynomial coefficients. The multivariate polynomials are obtained by tensorization of univariate polynomials, *i.e.*

$$\Psi_{\alpha}(\mathbf{X}) = \prod_{i=1}^M \psi_{\alpha_i}^{(i)}(X_i), \quad (7)$$

where $\psi_{\alpha_i}^{(i)}(X_i)$ is a polynomial of degree α_i in the i -th input variable belonging to a family of polynomials that are orthonormal with respect to $f_{X_i}(x_i)$.

For standard distributions, the associated family of orthonormal polynomials is well-known; for instance, a uniform variable with support $[-1, 1]$ is associated with the family of Legendre polynomials, whereas a standard normal variable is associated with the family of Hermite polynomials. Other cases can be treated through an isoprobabilistic transformation of \mathbf{X} to a basic random vector \mathbf{U} *e.g.* a standard normal or a standard uniform vector. Cases with mutually dependent input variables can

also be treated through an isoprobabilistic transformation (e.g. Nataf transformation) to a vector of independent standard variables.

The set of multi-indices \mathcal{A} is determined by an appropriate truncation scheme. A common scheme consists in selecting multivariate polynomials up to a total degree p^t , i.e. $\{\psi_{\alpha}, \alpha \in \mathbb{N}^M : |\alpha| \leq p^t\}$, where $|\alpha| = \sum_{i=1}^M \alpha_i$. The corresponding number of terms in the truncated series is

$$\text{card.}\mathcal{A} = \binom{M+p^t}{p^t} = \frac{(M+p^t)!}{M!p^t!}. \quad (8)$$

For other advanced truncation schemes, the reader is referred to Blatman and Sudret (2011).

Once the basis has been specified, the set of coefficients $\mathbf{y} = \{y_{\alpha}, \alpha \in \mathcal{A}\}$ may be computed as the solution of

$$\mathbf{y} = \arg \min_{\mathbf{v} \in \mathbb{R}^{\text{card.}\mathcal{A}}} \mathbb{E} \left[\left(\mathcal{M}(\mathbf{X}) - \sum_{\alpha \in \mathcal{A}} v_{\alpha} \Psi_{\alpha}(\mathbf{X}) \right)^2 \right]. \quad (9)$$

By replacing the expectation operator with the empirical mean over a sample set, the above equation becomes a standard least-squares minimization problem, which may be solved with well-known techniques. A more efficient approach leading to sparse PCE is the Least Angle Regression (LAR) method (see Blatman and Sudret (2011) for further details).

Note that in Eq.(8) the number of basis elements grows exponentially with the input dimension M . Consequently, the number of model evaluations required to compute the polynomial coefficients may be prohibitively large in high-dimensional problems. This limitation, known as the *curse of dimensionality*, constitutes a bottleneck in the PCE approach. A promising alternative is offered by canonical decompositions, described in the sequel.

4. LOW-RANK APPROXIMATIONS

4.1. Canonical decompositions

A rank-1 function of the input vector $\mathbf{X} = \{X_1, \dots, X_M\}$ is a function of the form

$$w(\mathbf{X}) = \prod_{i=1}^M v^{(i)}(X_i), \quad (10)$$

where $v^{(i)}(X_i)$ is a univariate function of X_i . A representation of the random response $Y = \mathcal{M}(\mathbf{X})$ as a sum of rank-1 functions constitutes a canonical decomposition; this reads

$$\hat{Y} = \sum_{l=1}^R b_l \left(\prod_{i=1}^M v_l^{(i)}(X_i) \right), \quad (11)$$

where $v_l^{(i)}(X_i)$ denotes a univariate function of X_i in the l -th rank-1 component, b_l are normalizing constants and R defines the rank of the decomposition.

Herein, we consider decompositions with each univariate function $v_l^{(i)}(X_i)$ expanded onto a polynomial basis that is orthonormal with respect to $f_{X_i}(x_i)$, i.e.

$$\hat{Y} = \sum_{l=1}^R b_l \left(\prod_{i=1}^M \left(\sum_{k=0}^{p_i} z_{k,l}^{(i)} P_k^{(i)}(X_i) \right) \right), \quad (12)$$

where $P_k^{(i)}$ is the k -th degree univariate polynomial in the i -th input variable of maximum degree p_i and $z_{k,l}^{(i)}$ is the coefficient of $P_k^{(i)}$ in the l -th rank-1 term. A representation in the form of Eq.(12) drastically reduces the number of unknowns compared to Eq.(6). In the case when $p_i = p, i = 1, \dots, M$, the number of unknowns in a rank- R decomposition is $P = ((p+1)M+1)R$, which grows only linearly with M . Naturally, decompositions with small R are of interest, leading to the name Low-Rank Approximations (LRA).

4.2. Construction of low-rank approximations

Algorithms proposed in the literature for building LRA are based on greedy approaches, where the polynomial coefficients along each dimension are sequentially updated and the rank of the decomposition is progressively increased. The algorithm proposed by Chevreuril et al. (2013b) involves a sequence of pairs of a *correction step* and an *updating step*. In a correction step, a rank-1 tensor is built, whereas in an updating step, the set of normalizing coefficients b_l is determined. A modified version of this algorithm is employed in the subsequent example applications; details are given next.

Let us denote by \hat{Y}_r the rank- r approximation of

$Y = \mathcal{M}(\mathbf{X})$, i.e.

$$\widehat{Y}_r = \sum_{l=1}^r b_l w_l, \quad (13)$$

where w_l represents the l -th rank-1 component

$$w_l = \prod_{i=1}^M \left(\sum_{k=0}^{p_i} z_{k,l}^{(i)} P_k^{(i)}(X_i) \right). \quad (14)$$

In the r -th correction step, the rank-1 tensor w_r is built by solving the minimization problem

$$w_r = \arg \min_{\omega \in \mathcal{W}} \|R_{r-1} - \omega\|_{\mathcal{E}}^2, \quad (15)$$

where \mathcal{W} is the space of rank-1 tensors and $R_{r-1} = Y - \widehat{Y}_{r-1}$ denotes the residual after the $(r-1)$ -th step. The sequence of \widehat{Y}_r is initiated by setting $\widehat{Y}_0 = 0$. Eq.(15) is solved through successive minimizations along each direction $i = 1, \dots, M$. In the minimization along direction j , the polynomial coefficients in all other directions are "frozen" at their current values and the coefficients $\mathbf{z}_r^{(j)} = \{z_{1,r}^{(j)} \dots z_{p_j,r}^{(j)}\}$ are determined as

$$\mathbf{z}_r^{(j)} = \arg \min_{\zeta \in \mathbb{R}^{p_j}} \left\| R_{r-1} - C^{(j)} \cdot \left(\sum_{k=0}^{p_j} \zeta_k P_k^{(j)}(X_j) \right) \right\|_{\mathcal{E}}^2, \quad (16)$$

where

$$C^{(j)} = \prod_{i \neq j} \sum_{k=0}^{p_i} z_{k,r}^{(i)} P_k^{(i)}(X_i). \quad (17)$$

A correction step may involve several iterations over the set of directions $\{1, \dots, M\}$. We propose a stopping criterion that combines the number of iterations over the set $\{1, \dots, M\}$, denoted I_r , with the decrease in the relative empirical error between two successive iterations, denoted $\Delta \widehat{err}_r$, where the empirical error is given by

$$\widehat{err}_r = \frac{\|R_{r-1} - w_r\|_{\mathcal{E}}^2}{\text{Var}[\mathcal{Y}]}. \quad (18)$$

We require that the algorithm exits the r -th correction step if either I_r reaches a maximum allowable value I_{max} or $\Delta \widehat{err}_r$ becomes smaller than a threshold $\Delta \widehat{err}_{min}$.

After the completion of a correction step, the algorithm moves to an updating step, in which the set of coefficients $\mathbf{b} = \{b_1, \dots, b_r\}$ is obtained as

$$\mathbf{b} = \arg \min_{\beta \in \mathbb{R}^r} \left\| Y - \sum_{l=1}^r \beta_l w_l \right\|_{\mathcal{E}}^2. \quad (19)$$

Note that in each updating step, the size of vector \mathbf{b} increases by one. In the r -th updating step, the value of the new element b_r is determined for the first time, whereas the values of the existing elements $\{b_1, \dots, b_{r-1}\}$ are updated.

The above algorithm relies on the solution of several small least-squares minimization problems (of size $p_i + 1$, $i = 1, \dots, M$, in each correction step and of size r in the r -th updating step), which can be solved using the Ordinary Least Squares (OLS) method. More efficient solution schemes can be developed by replacing Eq.(16) and Eq.(19) with respective regularized problems.

The progressive construction results in a set of LRA of increasing rank. Chevreuil et al. (2013a) propose selection of the optimal rank using 3-fold Cross Validation (CV). In the general case of k -fold CV, the ED is randomly partitioned in k sets of approximately equal size. A meta-model is built considering all but one of the partitions (training set) and the excluded set is used to evaluate the generalization error (testing set). By alternating through the k sets, k meta-models are obtained; the average generalization error of those provides an estimate of the error of the meta-model built with the full ED. In the context of LRA, the above technique yields k meta-models of progressively increasing rank as well as the respective error estimates. The rank yielding the smallest average generalization error is identified as optimal and a new decomposition having the indicated rank is built using the full ED. The average generalization error corresponding to the selected rank provides an estimate of the actual error of the final meta-model.

5. EXAMPLE APPLICATIONS

5.1. Beam deflection

We consider a simply supported beam with a rectangular cross section of width b and height h , length L and Young's modulus E . The beam is subjected to

a concentrated load P at the midpoint of the span. The aforementioned quantities are modeled by independent random variables following the distributions listed in Table 1. Of interest is to construct LRA of the mid-span deflection, $u = PL^3/4Ebh^3$, in terms of the $M = 5$ input random variables. We use ED of varying sizes, N , drawn with Sobol sampling and assess the accuracy of the meta-models with a validation set of size $n_{\text{val}} = 10^4$ drawn with Monte Carlo Simulation (MCS).

Table 1: Distributions of random variables.

Variable	Distribution	mean	CoV
b (m)	Lognormal	0.15	0.05
h (m)	Lognormal	0.3	0.05
L (m)	Lognormal	5	0.01
E (MN/m ²)	Lognormal	3e4	0.15
P (MN)	Lognormal	0.01	0.20

First, we investigate rank selection by means of 3-fold CV. After preliminary investigations, we set $p_1 = \dots = p_5 = 5$, $I_{\text{max}} = 50$ and $\Delta\widehat{err}_{\text{min}} = 10^{-8}$. Considered candidate ranks vary from 1 to 20. For different N , Figure 1 compares the rank R selected with 3-fold CV with the actual optimal rank yielding the minimum generalization error estimated with the validation set. The corresponding relative generalization errors are shown in Figure 2. The figures demonstrate that although the two ranks do not coincide in all cases, the corresponding generalization errors have only small differences. Overall, the meta-models are highly accurate; it is noteworthy that an accuracy of the order of 10^{-5} is achieved with an ED of size as small as $N = 50$.

Next, we examine optimal values of the error threshold in the correction step. Other parameters are fixed to their values above. For three different sizes of ED and $\Delta\widehat{err}_{\text{min}}$ varying from 10^{-9} to 10^{-4} , Figure 3 shows the relative generalization errors for ranks selected with 3-fold CV. It is observed that the accuracy of LRA strongly depends on $\Delta\widehat{err}_{\text{min}}$, particularly for the smaller ED. Selection of the optimal error threshold is a compromise between the desired accuracy and the number of iterations in the correction step.

In the following, LRA are confronted with PCE,

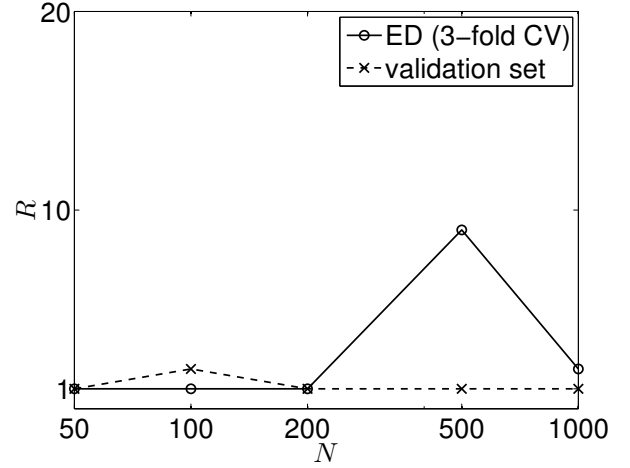


Figure 1: Rank selected with 3-fold CV and actual optimal rank based on validation set.

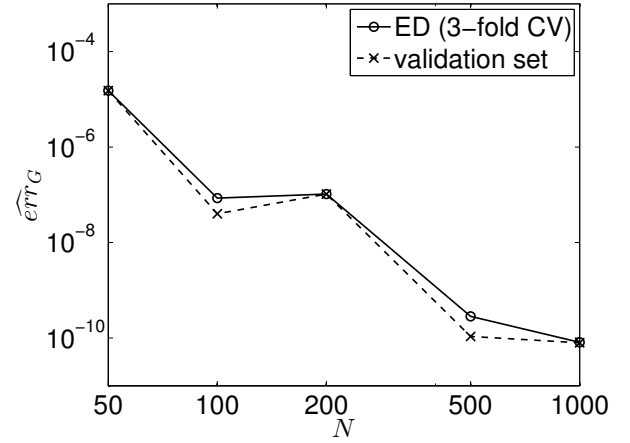


Figure 2: Relative generalization errors for rank selected with 3-fold CV and for actual optimal rank.

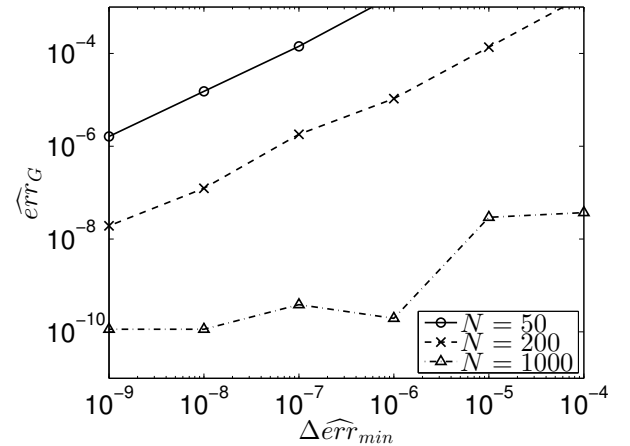


Figure 3: Relative generalization errors for different stopping criteria.

considering meta-models of optimal polynomial degrees for both approaches. In LRA, the optimal common maximum degree p is selected using 3-fold CV (other parameters are same as in Figures 1 and 2). In PCE, the candidate basis is determined by setting a maximum total degree p^t and then, evaluating the coefficients with the LAR method (see Section 3); the optimal p^t is selected by means of the Leave-One-Out (LOO) error (see Blatman and Sudret (2011) for details). Figure 4 shows the relative generalization errors of the resulting meta-models for N varying in 50 – 1,000 (the corresponding optimal p varies in 3 – 6, whereas optimal p^t varies in 2 – 5). Clearly, LRA outperform PCE for all considered N , yielding meta-models that are 2 to 3 orders of magnitude more accurate. It is remarkable that LRA achieve an accuracy of the order of 10^{-6} with only $N = 50$ points ($p = 3$).

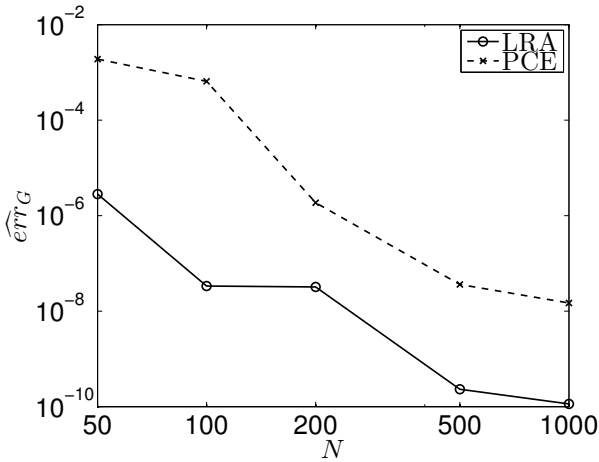


Figure 4: Comparison of relative generalization errors of LRA and PCE.

Finally, we assess LRA versus PCE in the evaluation of tail probabilities required in reliability analysis. Of interest is the probability that the beam deflection exceeds a prescribed threshold u_{lim} , called failure probability. We compare the failure probabilities evaluated using the actual model to the failure probabilities evaluated using LRA and PCE; these are respectively denoted P_f , \hat{P}_f^{LRA} and \hat{P}_f^{PCE} . Because u follows a lognormal distribution, an analytical solution is available for P_f . \hat{P}_f^{LRA} and \hat{P}_f^{PCE} are evaluated with a MCS approach as N^f/N^t , where $N^t = 10^7$ is the total number of points in

MCS and N^f is the number of points at which $u > u_{lim}$. For u_{lim} varying between 4mm and 10mm, Figure 5 compares the three failure probabilities considering the LRA and PCE meta-models in Figure 4 for $N = 50$. Obviously, the approximation of all failure probabilities using LRA is excellent, whereas use of PCE considerably underestimates small failure probabilities when $P_f < 10^{-3}$. We note that although the PCE meta-model has a relatively small relative generalization error (of the order of 10^{-3}), it provides particularly poor approximations at the tails of the response distribution.

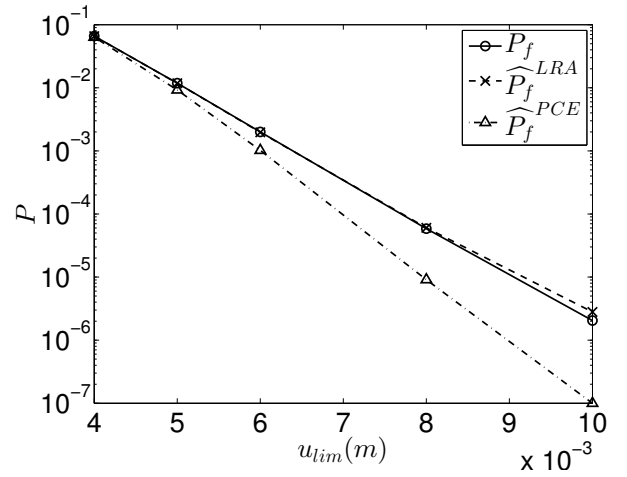


Figure 5: Comparison of failure probabilities evaluated with LRA and PCE to a reference value ($N = 50$).

5.2. Truss deflection

We now consider the simply supported truss in Figure 6, loaded with vertical loads P_1, \dots, P_6 . The cross-sectional area and Young's modulus of the horizontal bars are respectively denoted A_1 and E_1 , whereas the cross-sectional area and Young's modulus of the vertical bars are respectively denoted A_2 and E_2 . The aforementioned quantities are modeled by independent random variables following the distributions listed in Table 2. The response quantity of interest is the mid-span deflection, u , which is computed with a finite-element analysis code. We construct LRA of u in terms of the $M = 10$ input variables using Sobol-sampling based ED of varying sizes, N . The accuracy of the meta-models is assessed with a MCS-based validation set of size $n_{val} = 10^4$.

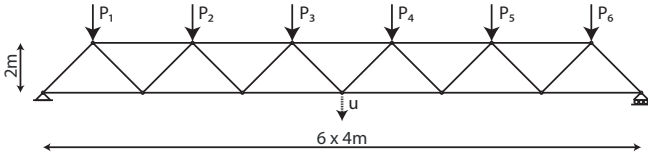


Figure 6: Truss structure.

Table 2: Distributions of random variables.

Variable	Distribution	mean	CoV
A_1 (m)	Lognormal	0.002	0.10
A_2 (m)	Lognormal	0.001	0.10
E_1, E_2 (N/m ²)	Lognormal	2.1e11	0.10
P_1, \dots, P_6 (N)	Gumbel	5e4	0.15

Figure 7 compares the rank $R \in [1, 20]$ selected with 3-fold CV with the actual optimal rank (based on the validation set) for the case $p_1 = \dots = p_{10} = 3$, $I_{max} = 50$ and $\Delta\widehat{err}_{min} = 10^{-5}$. The corresponding relative generalization errors are shown in Figure 8. We observe that 3-fold CV always selects $R = 1$, which is the actual optimal rank except for $N = 1,000$. Note that in this case, the size of ED only slightly affects the accuracy of the meta-model.

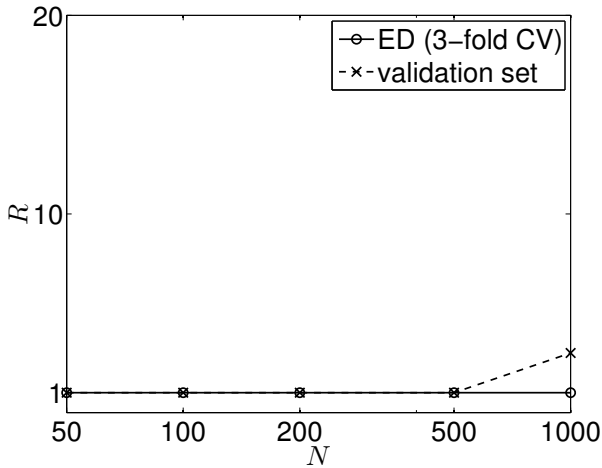


Figure 7: Rank selected with 3-fold CV and actual optimal rank based on validation set.

Figure 9 shows the relative generalization errors of LRA with rank selected with 3-fold CV for $\Delta\widehat{err}_{min}$ varying from 10^{-6} to 10^{-1} and other parameters fixed to their previous values. It is observed that $\Delta\widehat{err}_{min}$ has a significant effect on the

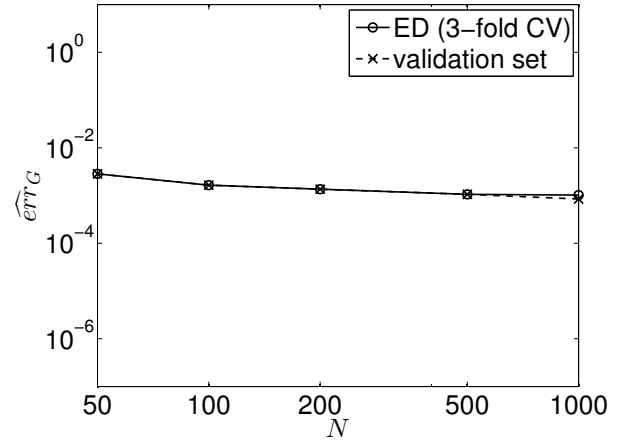


Figure 8: Relative generalization errors for rank selected with 3-fold CV and for actual optimal rank.

meta-model accuracy only for the smallest considered ED.

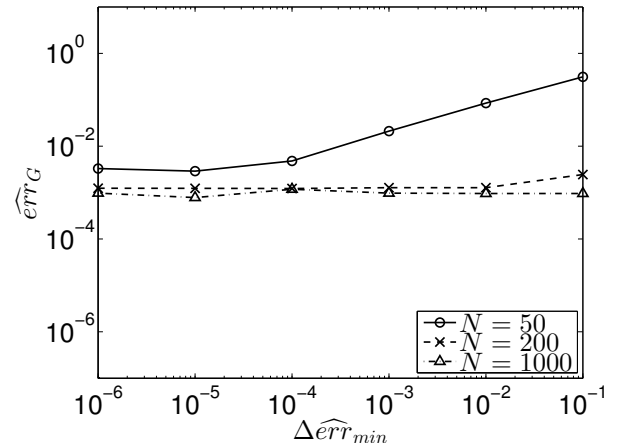


Figure 9: Relative generalization errors for different stopping criteria.

As in the former example, LRA are confronted with PCE, considering meta-models of optimal polynomial degrees (common degree p of univariate polynomials in LRA and total degree p^t of multivariate polynomials in PCE). Figure 10 shows the relative generalization errors of the resulting meta-models for N varying in 50 – 1,000 (the corresponding optimal p varies in 2 – 3, whereas optimal p^t varies in 2 – 4). In this case, LRA perform better than PCE for the smaller ED, whereas the reverse is true for the larger ones. Note however that although LRA yield fairly accurate meta-models for all N , this is not true for PCE and the smaller N .

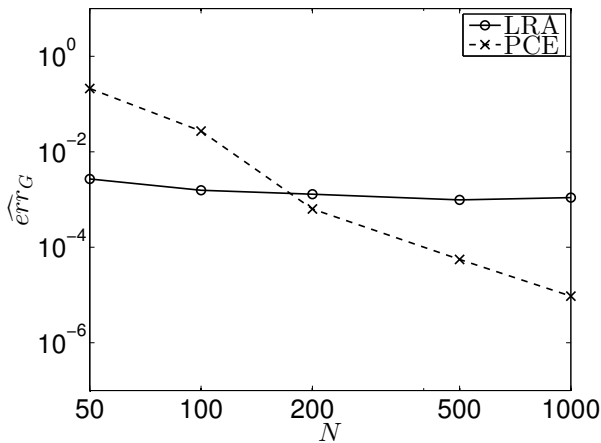


Figure 10: Comparison of relative generalization errors of LRA and PCE.

We conclude the example by assessing LRA versus PCE in reliability analysis. Of interest is the probability $u > u_{lim}$, where u_{lim} varies between 10cm and 16cm. The reference failure probabilities P_f are taken from Sudret (2007), whereas \hat{P}_f^{LRA} and \hat{P}_f^{PCE} are computed with a MCS sample of size $N^t = 10^7$. Figure 11 compares the three failure probabilities considering the LRA and PCE meta-models in Figure 10 for $N = 100$. We observe that use of LRA leads to fairly accurate estimates of the reference probabilities, whereas use of PCE is largely inaccurate (for $u_{lim} = 14cm$ and $u_{lim} = 16cm$, use of PCE yields $N^f = 0$).

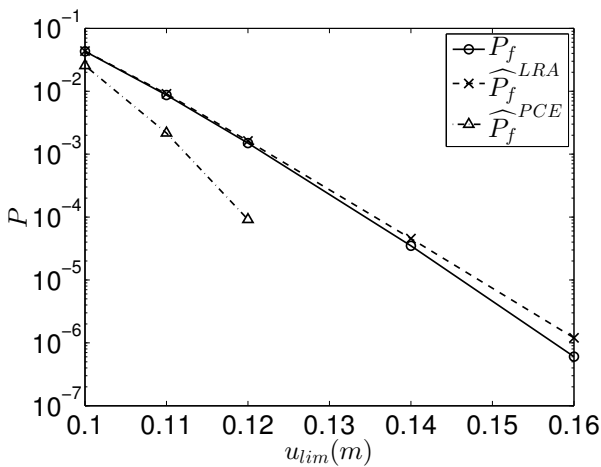


Figure 11: Comparison of failure probabilities evaluated with LRA and PCE to a reference value ($N = 100$).

6. CONCLUSIONS

By drastically reducing the number of unknowns with respect to Polynomial Chaos Expansions (PCE), Low-Rank Approximations (LRA) comprise a promising tool against the curse of dimensionality. After examining issues in their construction with greedy approaches, we have shown that LRA may be used to accurately evaluate tail probabilities in reliability analysis with experimental designs that prove inadequately small for the PCE approach.

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