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A Polynomial Chaos Expansion Trust Region Method for Robust Optimization

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Abstract. Robust optimization is an approach for the design of a mechanical structure which takes into account the uncertainties of the design variables. It requires at each iteration the evaluation of some robust measures of the objective function and the constraints. In a previous work, the authors have proposed a method which efficiently generates a design of experiments with respect to the design variable uncertainties to compute the robust measures using the polynomial chaos expansion. This paper extends the proposed method to the case of the robust optimization. The generated design of experiments is used to build a surrogate model for the robust measures over a certain trust region. This leads to a trust region optimization method which only requires one evaluation of the design of experiments per iteration (single loop method). Unlike other single loop methods which are only based on a first order approximation of robust measure of the constraints and which does not handle a robust measure for the objective function, the proposed method can handle any approximation order and any choice for the robust measures. Some numerical experiments based on finite element functions are performed to show the efficiency of the method.

AMS subject classifications: 60H15, 65K05, 62K20, 62K05

Key words: Reliability based design optimization, polynomial chaos expansion, trust region method.

1 Introduction

The design of a mechanical structure is usually formulated as an optimization problem as follows:

$$\begin{aligned} &\min_x f(x) \\ &\text{s.t. } g_i(x) \leq 0, \quad i=1,\cdots,r, \\ &\quad x^l \leq x \leq x^u, \end{aligned} \tag{1.1}$$

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where $x \in \mathbb{R}^M$ is a vector of M design variables (geometry, load,$\cdots$), f is an objective function (weight, cost,$\cdots$) and g_i is a set of r constraint functions representing the mechanical requirements (deformation, buckling load,$\cdots$). Due to the uncertainties in the design variables, the f and g_i functions (the response of the mechanical system) have a deterministic component and a random component. The random component of each function is characterized by a robust measure. This robust measure consists in defining ϕ the probability density functions (pdf) of the design variable uncertainties and propagating them through the mathematical model of the mechanical system in order to characterize the random component of the output functions. In [2–4], a detailed review of the possible mathematical definitions of the robust measures is available. Let ϵ be the vector of the M design variable uncertainties. In this paper, only the case of Gaussian uncertainties is considered, but the proposed algorithm applies to any other continuous uncertainty type. For the objective function, one can define its robust measure $\mathbf{R}_f(x)$ as one of the following possibilities:

- the function itself, $\mathbf{R}_f(x) = f(x)$;
- its mean value with respect to the design variable uncertainties:

$$\mathbf{R}_f(x) = E[f|x] = \int f(x+\epsilon)\phi(\epsilon)d\epsilon;$$

- a combination of its mean value and its variance:

$$\mathbf{R}_f(x) = E[f|x] + var(f|x)$$

  with

$$var(f|x) = \int (f(x+\epsilon) - E[f|x])^2 \phi(\epsilon)d\epsilon;$$

- the probability that f is less than a certain threshold q:

$$\mathbf{R}_f(x) = Pr[f < q|x].$$

The robust measure $\mathbf{R}_{g_i}(x)$ of the constraints can be defined as:

- its statistical feasibility:

$$\mathbf{R}_{g_i}(x) = Pr[g_i \leq 0|x] \geq P_0$$

  for some confidence probability P_0;
- its feasibility robustness:

$$\mathbf{R}_{g_i}(x) = g_i(x) + \sqrt{\sum_j \left(\frac{\partial g_i}{\partial x_j}\right)^2} \leq 0.$$

Robust optimization is an approach for the design of a mechanical structure which takes into account the uncertainty of the design variables. It replaces the objective function and the constraints by their robust measures with respect to the uncertainties of the design variables. The robust optimization problem becomes:

$$\begin{aligned} &\min_x \mathbf{R}_f(x) \\ &\text{s.t. } \mathbf{R}_{g_i}(x) \geq P_0, \quad i=1,\cdots,r, \\ &\quad x^l \leq x \leq x^u. \end{aligned} \tag{1.2}$$

Unlike deterministic optimization in (1.1), where at each iteration the objective function and the constraints are only evaluated for the current values of the design variables, the robust optimization requires at each iteration the evaluation of these functions for all the possible scenarios of the design variable uncertainties. This requires two loops: the outer one for the optimization itself and the inner one for computing robust measures. For example, take the case of a gradient method used to perform the robust optimisation. At each iteration point x_k, the gradient of the robust measures is computed using a finite difference approximation. This requires the evaluation of the robust measures at points x_k and x_k+dx_i for $i=1,\cdots,M$. If the evaluation of the robust measure requires N evaluations of f and g_i, then, each iteration of the gradient method requires $N\times(M+1)$ evaluations of f and g_i. The high number of evaluations of the f and g_i due to the double loop constitutes the main difficulty of the robust optimization.

Papers [2–4] give a review of the possible methods to solve the robust optimization problem (1.2). They are classified in three categories: the double loop methods, the single loop methods and the decoupled methods. The double loop methods solve problem 1.2 without any approximation of the functions $\mathbf{R}_f$ and $\mathbf{R}_{g_i}$. They are the most accurate of the three categories but the most expansive in computations. They are based on the construction of surrogate models or evolutionary algorithms like in [5–8, 16].

The single loop and the decoupled methods make use of some approximations to avoid the double loop (see [2, 9, 10]). The single loop methods are restricted to $\mathbf{R}_f=f$ as a robust measure (the first choice in the previous list) and computes the $\mathbf{R}_{g_i}$ functions using a first-order approximation (the FORM method). In this case, the analytical expressions of the derivatives of the robust measures are available. One does not have to compute the robust measures at x_k+dx_i for $i=1,\cdots,M$, which reduces the number of evaluations of f and g_i to only N evaluations per iteration. In many cases, these methods use a trust region algorithm to solve the optimization problem.

The decoupled methods separate the design variables space from the uncertainty space. They perform a deterministic optimization and add a shift to the design variables in order to comply with the constraints without computing robust measures at each iteration. They are the cheapest of the three categories but also the less accurate.

The Polynomial Chaos Expansion (PCE) method builds a multidimensional polynomial function which approximates f and g_i in order to compute their robust measures.

Such approximation can be computed using an intrusive method like in [18], or non intrusive method like in [20] or [15].

The contribution of this paper is the following. In a previous paper, the authors have proposed a method which efficiently generates a design of experiments with respect to the design variable uncertainties to compute the robust measures using the polynomial chaos expansion. This paper extends the proposed method to the case of the robust optimization. The generated design of experiments is used to build a surrogate model for the robust measures of the objective function and the constraints over a defined trust region. The degree of these surrogates is equal to the degree of the PCE and only requires one evaluation of the design of experiments to build the surrogate model. This leads to a trust region optimization method. Only one evaluation of the design of experiments is required per iteration (no double loops). It has the advantage over the above mentioned single loops methods that it can handle any choice of $\mathbf{R}_f$, any choice of method to compute $\mathbf{R}_{g_i}$ and any surrogate degree. Some numerical experiments based on finite element functions are performed to show the efficiency of the method.

2 Probability space and random variables

Computing the output of a mechanical system with uncertain design variables is considered as a random experiment and can be studied using the PCE. In order to give a mathematical framework of the PCE, a brief review of some definitions regarding probability space and random variables is introduced in the following paragraph.

A probability space is a mathematical entity which models the uncertainty in the input and the output of the mechanical system. Three ingredients $(\Omega,\mathcal{F},P)$ are necessary to define a probability space, where:

- Ω is the set of all possible outcomes;
- $\mathcal{F}$ is a σ-algebra over Ω containing all possible events;
- P is a function $\mathcal{F}\to\mathbb{R}$ which gives a probability measure for each random event.

A random variable X is a function $X:(\Omega,\mathcal{F},P)\to\mathbb{R}$.

Using the preceding definitions, one can also define the expectation and the variance of a random variable:

$$\bar{X}=\mathrm{E}[X]=\int X dP, \tag{2.1}$$

$$var(X)=\mathrm{E}[(X-\bar{X})^2]=\int (X-\bar{X})^2 dP. \tag{2.2}$$

We call $<X,Y>=\int XY dP$ the inner product of two random variables on the probability space and $\mathcal{L}^2(\Omega,\mathcal{F},P)$ the set of random variables having a finite variance.

Before introducing the PCE, one must also have a look at the Hermite polynomials. These polynomials of degree n are defined in a recursive way as follows:

$$H_0 = 1, \tag{2.3}$$

$$H_{n+1}(x) = xH_n(x) - (n)H_{n-1}(x), \tag{2.4}$$

and they have the property of being orthogonal with respect to the Gaussian measure. If H_i and H_j are two Hermite polynomials of degrees i and j respectively, we have:

$$\int H_i(x)H_j(x)e^{-x^2/2}dx = i!\delta_{ij}\,, \tag{2.5}$$

where δ_{ij} is the Dirac function. Thus, if ξ is a Gaussian random variable, the two random variables $H_i(\xi)$ and $H_j(\xi)$ are orthogonal with respect to the above inner product and the Gaussian measure. This orthogonality property constitutes the basis of the PCE.

Note that, if ξ is a Gaussian random variable, the Hermite polynomials must be replaced by the Legendre polynomials and the density function $e^{-x^2/2}$ by 1.

3 The polynomial chaos expansion (PCE)

The PCE method consists in considering a set of orthogonal multivariate polynomials with respect to the previous inner product. Let M be the number of uncertain design variables in the mechanical system and $\xi = \{\xi_i\}_{i=1}^M$ be a set of M independent Gaussian random variables. Each random variable is associated to an uncertain design variable and represents its perturbation. Consider Γ_p the space of multivariate polynomials of degree less or equal to p and $\tilde{\Gamma}_p$ the space of polynomials of degree equal to p and orthogonal to Γ_{p-1}. We have $\Gamma_p = \oplus_{i=1}^p \tilde{\Gamma}_i$. If the inner product is considered with the Gaussian measure, $\tilde{\Gamma}_p$ is spanned with the multivariate Hermite polynomials $\{\psi_\alpha(\xi)\}$ of degree p, where $\alpha \in \mathbb{N}^M$ and $\sum_{i=1}^M \alpha_i = p$. These multivariate Hermite polynomials $\{\psi_\alpha(\xi)\}$ are defined as the product of M univariate Hermite polynomials of degree α_i:

$$\psi_\alpha(\xi) = \prod_{i=1}^M H_{\alpha_i}(\xi_i). \tag{3.1}$$

Let S be the random output of the mechanical system. If S has a finite variance ($S \in \mathcal{L}^2(\Omega,\mathcal{F},P)$), it can be expressed as an infinite series of multivariate Hermite polynomials (see [12, 13]):

$$S(x+\xi) = \sum_{|\alpha|=0}^{|\alpha|=\infty} \sigma_\alpha(x)\psi_\alpha(\xi) = \sum_{i=0}^{\infty} \sigma_i(x)\psi_i(\xi). \tag{3.2}$$

Here, the multi-index α of ψ is replaced by an index i given the univocal relationship between these two notations. σ_i are the deterministic coefficients of the PCE.

One of the advantages of such a representation of the random output S is that computing the mean and variance of S is straight-forward. From the orthogonality property of ψ_i, one can deduce that:

$$\bar{S} = \sigma_0, \tag{3.3}$$

$$var(S) = \sum_{i=1}^{\infty} \sigma_i^2. \tag{3.4}$$

For computational reasons, the space of multivariate polynomials must be truncated to degree p and S is replaced by $\tilde{S}$ with:

$$S(x+\xi) = \tilde{S}(x+\xi) + \epsilon = \sum_{i=0}^{N} \sigma_i(x)\psi_i(\xi) + \epsilon, \tag{3.5}$$

where $N = \frac{(M+p)!}{M!p!}$ is the number of terms involved in $\tilde{S}$ and ϵ is the truncation error.

In this paper, we consider the regression method to compute the coefficients σ_i of the PCE (see [14, 15]). This method consists in defining a design of experiments, $\Xi(x,\xi) = \{x+\xi^j\}^{j=1,\cdots,Q}$, which is a set of Q different perturbations of the design variables and then computing (by simulation) the output of S for each value $x+\xi^j$ of the design of experiment. These output values are gathered in a vector $S^{sim}(\Xi) \in \mathbb{R}^Q$ and the following equation can be deduced:

$$S^{sim}(\Xi(x,\xi)) = \Psi(\Xi(x,\xi))\sigma(x) + \epsilon, \tag{3.6}$$

where $\Psi(\Xi(x,\xi))$ is a rectangular matrix in $\mathbb{R}^{Q,N}$ defined by $\Psi_{ji} = \psi_i(\xi^j)$. Each row j of this matrix is the set of all ψ_i's computed for the experiment ξ^j. The computation of σ from equation (3.6) corresponds to a linear least squares problem which is detailed in [11].

In brief, the evaluation of the robust measure of an output function using the regression PCE requires:

1. defining a design of experiments Ξ like in [1];
2. computing the output function S^{sim} at each point of the design of experiments;
3. computing the coefficients σ of the PCE by the least squares method;
4. computing the robust measure from these coefficients.

It is assumed that step 2, the computation of S^{sim} by simulation, is the most expensive one.

In [1], the generation of the design of experiments is based on maximising the determinant of its information matrix (the D-optimal criterion). It is a coupling between the Fedorov algorithm with the genetic algorithms. The advantage of this method is being able to generate accurate design of experiments with the fewest possible number of simulations.

4 The optimization method

The optimization method proposed in this paper is based on a trust region one. It consists in solving an optimization subproblem at each iteration where the objective function and the constraint are replaced by some surrogate models which approximate these functions over a trust region. This trust region is defined by a hypersphere of radius Δ_k and centered at x_k the current values of the design variables. The optimization subproblem is the following:

$$\begin{aligned} &\min_x \tilde{\mathbf{R}}_f(x) \\ &\text{s.t. } \tilde{\mathbf{R}}_{g_i}(x) \geq P_0, \quad i=1,\cdots,r, \\ &\text{and } |x-x_k| \leq \Delta_k, \end{aligned} \tag{4.1}$$

where the $\tilde{\mathbf{R}}_f$ and $\tilde{\mathbf{R}}_{g_i}$ are the surrogate models of the robust measures of f and g_i respectively. At each iteration, x_k is updated with the solution of this optimisation subproblem. In order to guarantee the efficiency of the trust region method, the construction of these surrogate models and the resolution of the optimization subproblem must not be expensive in terms of computations.

The construction of the surrogate model takes advantage of the regression based PCE. Unlike other non-intrusive methods, the regression method does not require a fixed design of experiments for the perturbations. One can use any design of experiments to perform the PCE.

Let S be any function of f and g_i. At iteration k, define the design of experiments $\Xi(x_k,\xi)=\{x_k+\xi^j\}^{j=1,\cdots,Q}$ and compute $S^{sim}(\Xi)$ the values of S corresponding to the perturbations Ξ. Using the regression method, compute $\mathbf{R}_s(x_k)$ the robust measure of s at x_k. Now, we want to compute the robust measure at another point x. There are two possibilities. Either compute a new vector $S^{sim}(\Xi)$ corresponding to a new $\Xi(x,\xi)=\{x+\xi^j\}^{j=1,\cdots,Q}$ or change the design of experiments such that it can reuse the same vector S_k^{sim}. The second possibility has advantage of not requiring a reevaluation of $S^{sim}(\Xi)$ for each value of x in the trust region. Define $h=x-x_k$. The new design of experiments is $\Xi(x,\xi-h)=\{x+\xi^j-h\}^{j=1,\cdots,Q}$, centered about x and the perturbations are ξ^j-h. One can see that this new design of experiments is such that it defines the same points of $\Xi(x_k,\xi)$. Thus, it can reuse the vector $S^{sim}(\Xi(x_k,\xi))$. Eq. (3.6) can be written as

$$S^{sim}(\Xi(x,\xi-h))=\Psi(\Xi(x,\xi-h))\tilde{\sigma}(x)+\epsilon, \tag{4.2}$$

where $\tilde{\sigma}(x)$ are the PCE coefficients computed at point x using $\Xi(x,\xi-h)$ and ϵ is the truncation error.

4.1 Computer implementation

The optimization algorithm is summarized as follows.

At each iteration k, a design of experiments $\Xi(x_k,\xi)$ is defined as for example in [1]. The objective function and the constraints are evaluated with respect to this design of experiments in order to have the vectors $f^{sim}(\Xi(x_k,\xi))$ and $g_i^{sim}(\Xi(x_k,\xi))$. Then, the optimization subproblem (4.1) is solved and x_k is updated by the solution of the subproblem. In this paper, it is chosen to use the local search method coupled with the penalty method to solve this optimization sub-problem. It is an inner loop of the optimization algorithm which does not require any additional evaluation of f and g. The values of $\tilde{\mathbf{R}}_f(x)$ and $\tilde{\mathbf{R}}_{g_i}(x)$ needed by the local search method at point x are computed as follows. A new design of experiments is generated such that it can reuse the same vectors $f^{sim}(\Xi(x_k,\xi))$ and $g_i^{sim}(\Xi(x_k,\xi))$. Then, the PCE coefficients at point x are computed based on this generated design of experiments. Finally, these PCE coefficients give the polynomial approximations of f and g_i. The value of $\tilde{\mathbf{R}}_f(x)$ is deduced from Eqs. (3.3) and (3.4) and $\tilde{\mathbf{R}}_{g_i}(x)$ is computed using this approximation with a Monte Carlo method.

Note that one can choose any optimization method to solve the optimization subproblem other than the local search method and any other method than Monte Carlo to compute the constraints. The proposed optimization method is not restricted to these choices.

5 Numerical experiment

The test case used in this paper is the design of a stiffener shown in Fig. 1. It is composed of two panels and one stringer and it is subjected to a compression load parallel to the stringer (10 N/cm). The uncertain parameters of this model are the thickness of both panels (1cm), the thickness of the stringer (1cm), and the height of the stringer (10cm). In total, we have three uncertain parameters. They are the solid arrows in Fig. 1. The uncertain outputs are the mass of the structure and the first six buckling modes of the structure. The finite elements model and the first three buckling modes are in Fig. 2. These finite element based functions are commonly used in structural analysis and structural optimization.

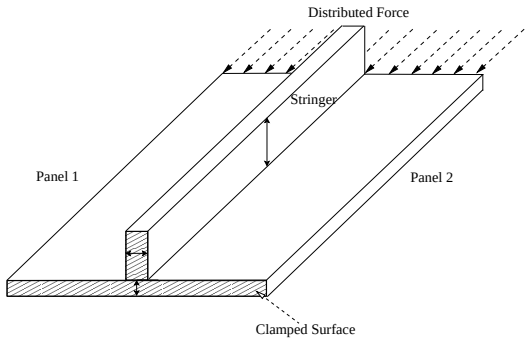

Figure 1: Description of the finite element based test: the solid arrows are the uncertain variables.

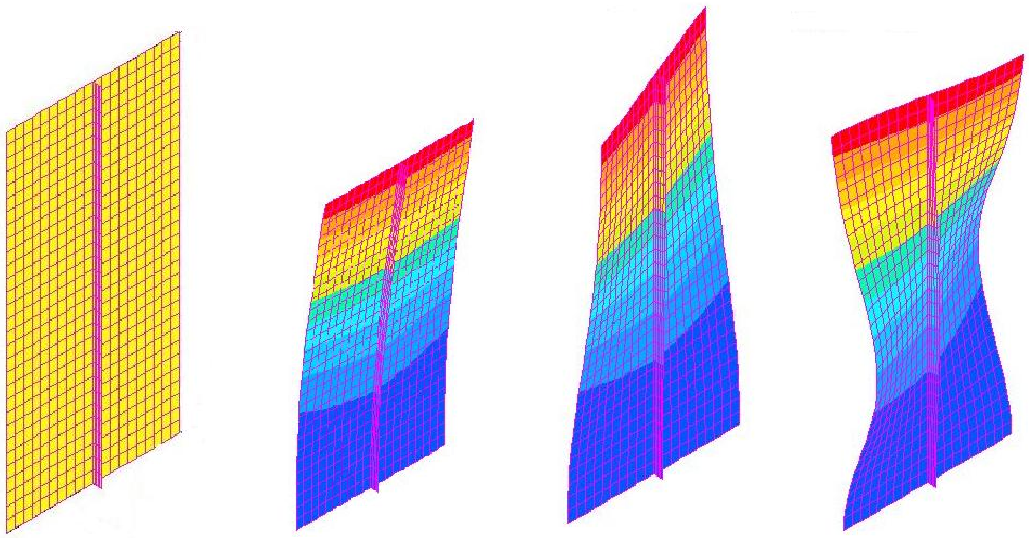

Figure 2: The finite elements model and the first three buckling modes of the structure.

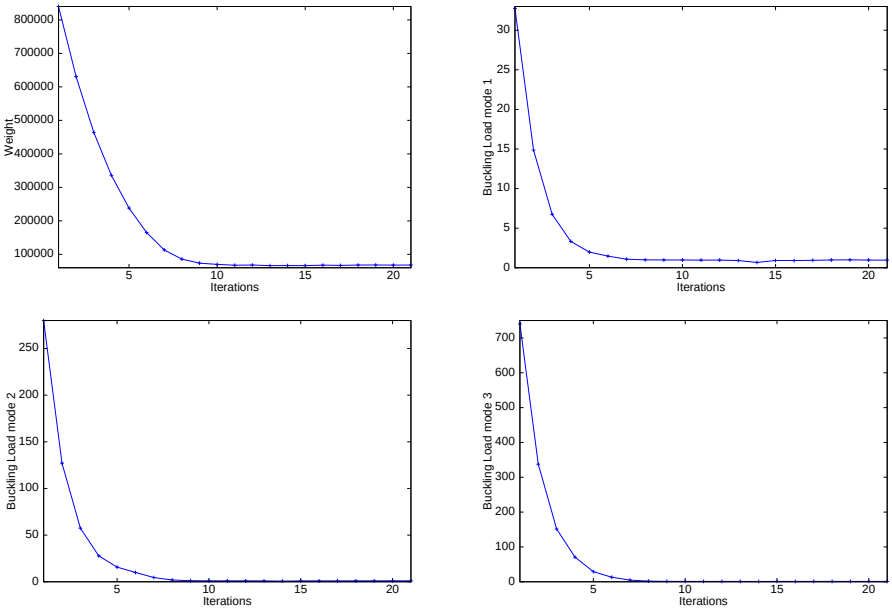

Figure 3: Deterministic optimization: evolution of the mass and the first three critical loads with respect to the number of iterations.

The optimization problem consists in minimizing the weight of the structure while ensuring that the first six buckling loads are higher than one.

A deterministic optimization (1.1) is performed using the GCM method, described in [17]. Fig. 3) shows the evolution of the mass and the first three critical buckling modes

Table 1: The results obtained with the deterministic and the two robust optimizations.

	Deterministic	Degree 1	Degree 2
Panel thickness	0.70	0.719	0.722
Stringer thickness	3.19	3.188	3.26
Stringer height	9.18	9.32	9.32
Weight	68196	69578	70000
Prob. of viol. Cri. Load 1	-	0.011	0.009
Prob. of viol. Cri. Load 2	-	0.005	0
size of DoE $\times$ #iterations	-	4×30	10×30

with respect to iterations. The solution is shown in Table 1.

The initial point for the robust optimization is taken as the deterministic optimum. Given that in this point the constraints are active and the violation probability is equal to 1%, this point is necessarily a non admissible solution for the robust optimization. Therefore during the optimization, the weight increases to find the robust optimum.

Two numerical tests have been performed for the robust optimization with PCE of degree one and two. The Gaussian variables have a standard deviation equal to 1% of their nominal values. The probability of violation is equal to 1%. With degree one and two, the trust region radii Δ_k are equal to 0.25 and 0.5 respectively in the normal Gaussian space. The sizes of the design of experiments are 4 and 10 respectively. This means that each iteration only requires 4 and 10 evaluations respectively. Figs. 4 and 5 show the evolution of the robust measures of the weight and the first three critical loads with degree one and two. The results of the robust optimizations are shown in Table 1. Note that the two optimal solutions satisfy the constraints. They show that we have an increase in the weight of the structure of 2% and 2.6% due to the 1% uncertainty in the three design variables and the 1% probability of violation. One can see that these results are obtained with designs of experiments of small sizes which allows to take small trust regions and perform a lot of iterations (30 iterations) which demonstrates the efficiency of the proposed method.

6 Conclusions

A trust region method is proposed to solve a robust optimization problem. This method is based on the polynomial chaos expansion method to compute the robust measures of the objective function and the constraints. Here, the coefficients of the polynomial chaos expansion are obtained by defining a design of experiments and solving a regression problem. The advantage of this method is that it only requires one evaluation of the design of experiments per iteration. Therefore, it can be classified as a single loop method.

The efficiency of the proposed method is demonstrated with a test case using a finite element model to optimize (design) a stringer. The method is able to generate an optimal

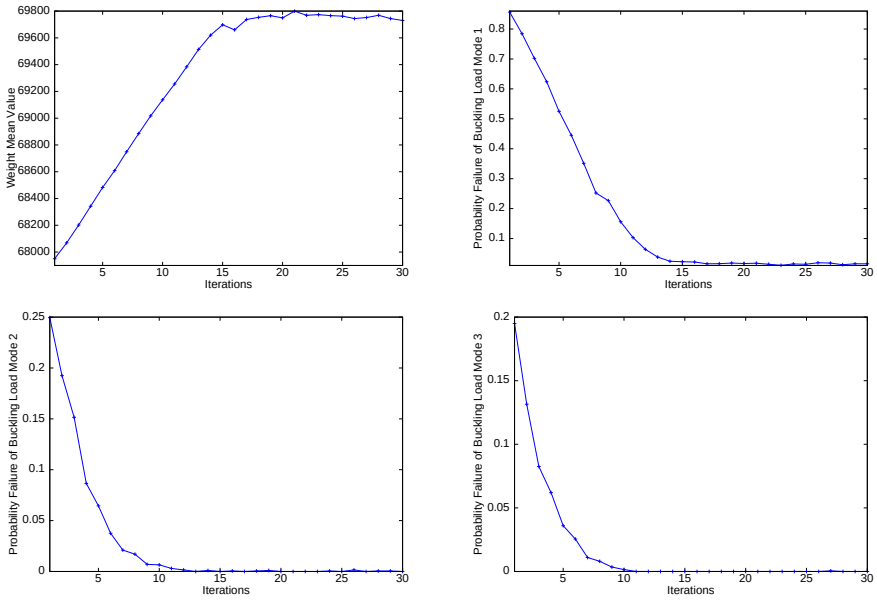

Figure 4: Robust optimization with PCE degree 1: evolution of the weight and the first three critical loads with respect to the number of iterations.

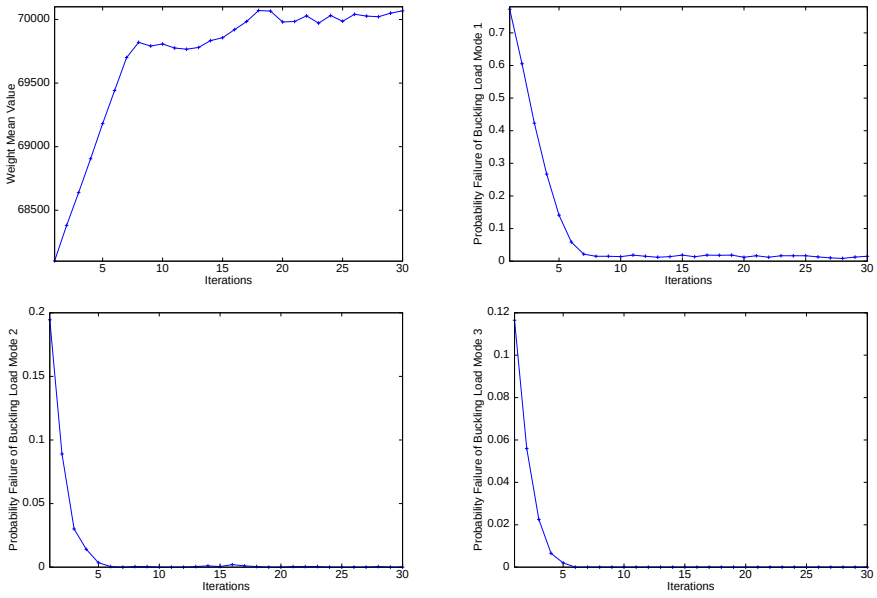

Figure 5: Robust optimization with PCE degree 2: evolution of the weight and the first three critical loads with respect to the number of iterations.

design for the stringer with a relatively low cost in computations and satisfy all design constraints.

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