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Metaheuristics of Failure Probability Estimation in High Dimensions

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ABSTRACT: In this paper it is attempted to highlight some problems of failure probability estimation in high dimensions. These are the need to find structures and not only numbers, and the need for a solid mathematical foundation by systematic testing. Then two new approaches for such problems are introduced, the onion method and the BMM concept

1. INTRODUCTION

Most articles about failure probability estimation start more or less in the following way:

A basic problem in structural reliability is the computation of failure probabilities:

$$P = \int_{g(\mathbf{x}) \le 0} f(\mathbf{x})\, d\mathbf{x} \tag{1}$$

Here $f(\mathbf{x})$ is a PDF (probability density function) and $g(\mathbf{x})$ is an LSF (limit state function). Transforming the random vector $\mathbf{X}$ into a standard normal random vector $\mathbf{U}$ with independents components gives the standardized form:

$$P = (2\pi)^{-n/2} \int_{g(\mathbf{u}) \le 0} \exp\left(-\frac{|\mathbf{u}|^2}{2}\right)\, d\mathbf{u} \tag{2}$$

Our totally new and highly efficient algorithm ...

Here it will be attempted to look at this problem from a broader point of view.

2. A BROADER VIEW

In a more realistic setting the LSF in Eq. (2) depends on a parameter vector $\boldsymbol{\theta}$. This parameter vector may contain distribution and design parameters as well. So this equation should be written as:

$$P(\boldsymbol{\theta}) = (2\pi)^{-n/2} \int_{g(\mathbf{u}|\boldsymbol{\theta}) \le 0} \exp\left(-\frac{|\mathbf{u}|^2}{2}\right)\, d\mathbf{u} \tag{3}$$

It is important to notice that due to the transformation to the standard normal space the dependence on parameters appears only now in the LSF, not in the standardized PDF.

It should be clear that methods which produce only estimates of the probability $P(\boldsymbol{\theta})$ are not very informative. In fact everybody knows that almost always there are so many uncertainties in the underlying probability distributions that the found values are wrong anyway.

Therefore it makes more sense to see these probabilities more in a operational sense. This means to look at the relations between the results for different parameter values, i.e. to study the relations between parameters and its failure probability values. This requires the calculation of partial derivatives and sensitivities of the failure probabilities. This can be done by differentiating the asymptotic SORM approximations, by approximating the surface (Papaioannou et al. (2018)) or by replacing the surface integral by a domain integral using the divergence theorem (Breitung (1994), p. 23, Breitung (2012)).

This view leads then to a structuralist view of the whole problem. This is explained in the next section.

3. STRUCTURALISM

Some short words about structuralism to begin with. Structuralism is a scientific methodology emphasizing the relations between the elements of the

subject as main topic of the study, for a description see Piaget (1971). In Rickart (1995) *structuralism* is defined as a *method of analyzing a body of information with respect to its inherent structure*.

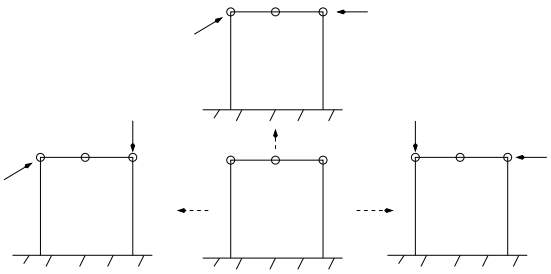


Figure 1: Example of a system: A framework and some potential structures

A *system* is any collection of interrelated objects along with all of the potential structures that might be identified with it, see Fig. 1. So, from a structuralist point of view for structural reliability the focus should be on studying the structure or configuration of components leading to failure.

Whereas in considering structural reliability as a forward mathematical problem, one concentrates on finding probabilities, seeing it a structuralist problem, one concentrates on analyzing the structure related to the failure events, i.e. one sees it more as an inverse problem.

Two main concepts of structuralism are isomorphism and reduction. An *isomorphism* between two structures consists of a one-to-one correspondence between the elements of the two structures such that the sets of objects from one structure are related if, and only if, the corresponding objects from the other structure are related also.

A simple example of isomorphic structures in reliability are all the reliability problems defined in the original space which can be transformed into the same failure domain in the standard normal space using the transformation given in Rackwitz and Fiessler (1977). The structures have all the same failure probability.

A main topic is to find for a given structure simpler substructures which retain in some way the important information. This is called in Rickart (1995) a *reduction*, a more appropriate name might be *projection*. In reliability theory it might be necessary to project the original structure on several simpler substructures to get an easier to handle representation of the original structure. Nowadays also the term surrogate model is used in this context.

The FORM/SORM approach can be viewed as a projection method. For arbitrary LSF's $g(\mathbf{u})$ having a unique design point $\mathbf{u}^*$ with $|\mathbf{u}^*| = \beta$, the set of all these LSF's is an affine space of functions.

The functions in this set are projected onto:

1. FORM: the set of all linear functions with $g(\mathbf{u}^*) = 0$ by

$$g \to g_L = \nabla g(\mathbf{u}^*)^T (\mathbf{u} - \mathbf{u}^*) \tag{4}$$

2. SORM: the set of all quadratic functions with $g(\mathbf{u}*) = 0$ by

$$\begin{aligned} g \to g_Q &= \nabla g(\mathbf{u}^*)^T (\mathbf{u} - \mathbf{u}^*) \\ &+ \frac{1}{2}(\mathbf{u} - \mathbf{u}^*)^T \nabla^2 g(\mathbf{u}^*)(\mathbf{u} - \mathbf{u}^*) \end{aligned} \tag{5}$$

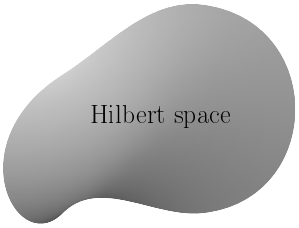
These projections now define new failure domains. So the problem of failure probability calculation is reduced to a calculating it for a simpler substructure, i.e. the reliability problems defined by linear/quadratic functions.

A program for a more structuralist approach is shown in the following Fig. 2. First to derive from the space of the underlying variables a subspace which contains the relevant variables and then to build functional relations there.

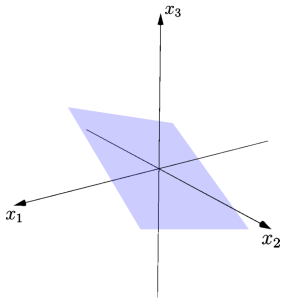
4. ALGORITHMS: ATTEMPTS TO VALIDATE THEM

The algorithms developed for failure probability estimation are mostly based on more heuristic mathematical arguments. This is understandable, since the given problems are often quite complex. However on the other hand, the conclusions some authors draw from this, that it is possible to validate the correct performance of methods by examples, is slightly problematic.

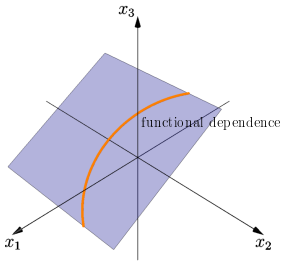
Basically there are two methods for validation. One is a mathematical convergence proof. It shows that under a set of reasonable conditions the algorithm converges to the correct solution in "some



(a) Underlying Hilbert space



(b) Dimension reduction



(c) Building a functional model

Figure 2: A structuralist program for reliability

sense". An example is the SORM approach (Breitung (1994)). Here it is shown that the approximations derived with SORM are asymptotic approximations. This means that for $\beta \to \infty$ the relative error goes to zero.

The second possibility is systematic testing of the procedure. In most cases this is the only possible way. In Bartz-Beielstein et al. (2010) this is outlined in more detail. It is important to distinguish systematic testing from accumulating just a heap of examples. The fact that a method works for hundreds of examples can be very misleading if the examples are all more or less constructed in a similar way so that the algorithm will produce a satisfactory result. This is then a case of self-fulfilling prophecy.

Often the validation of an algorithm in a paper is done in the following way. First two or three toy examples are calculated where the results are obvious anyway. In these cases one can still see what is happening. Then to demonstrate the power of the proposed procedure, two or three very complex examples are studied. These are in general "dark examples" (the author just invented this word). With this he means that one cannot see what is going on during the computations. There is given a correct failure probability found by a Monte Carlo run and then the algorithm produces a result near this value. No further explanations given.

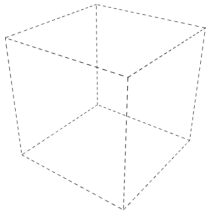
But here are some problems. First, is the Monte Carlo result correct at all? Second, how does the algorithm find the result? Maybe it is only a coincidence that it ended near the correct point? Or were it simply lucky random numbers?

It does not help that it is claimed in many cases that the simple examples show that the algorithm works and then the dark examples that this can be generalized to complex structures.

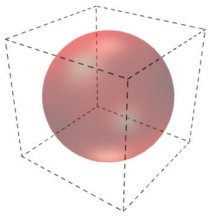
To make meaningful investigations of the performance of such numerical procedures it is necessary to construct complex examples depending on parameters where an analytic or an easily accessible numerical solution is given. These examples should then be studied for systematically varied parameter values to test the behavior of the programs under consideration. Certainly this requires more time and a deeper mathematical understanding than many researcher will or can invest. But only so one can obtain reliable statements. This is important especially now when one studies high dimensional structures where intuitive interpretations and generalization can be misleading.

Now a graphical illustration on the problematic use of examples. Let the cube in Fig. 3a denote a set of problems for which a solution algorithm has to be found. For one algorithm maybe a mathematical proof can be found; it shows that the algorithm converges in the sphere shown in Fig. 3b. For another algorithm working with examples only one can show that it work for the examples in the centers of the green spheres and concludes that it will work also for cases in the neighborhood, i.e. the green spheres, see Fig. 3c. But if only in a non-

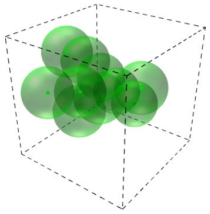
systematic way examples are collected, it might be that all examples share a hidden joint property, see Fig. 3d the grey surface. Then in fact it can be assumed only that the algorithm works on the surface where the problem cases have this hidden property too, see Fig. 3e.



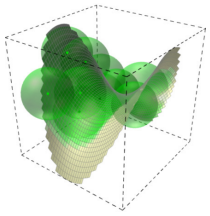
(a) Underlying problem



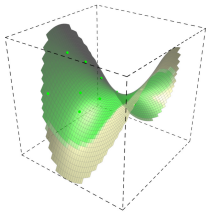
(b) Mathematical proof for an algorithm



(c) Examples



(d) Grey surface= Hidden joint property of examples



(e) Real region of validity of examples

Figure 3: Validation of an algorithm

5. SUBSET SIMULATION

A quite popular approach to find failure probabilities in high dimensional spaces is the subset simulation method, a variant of Monte Carlo methods which tries to avoid the large amount of data points which has to be created in standard Monte Carlo by an iterative procedure. The basic idea of the method (see Au and Wang (2014)) is to write the failure probability $\Pr(F)$ as a product of conditional probabilities

$$\begin{aligned}\Pr(F_n) &= \Pr(F_1|F_0)\cdot\Pr(F_2|F_1)\ldots\cdot\Pr(F_n|F_{n-1}) \\ &= \prod_{k=0}^{n-1}\Pr(F_{k+1}|F_k) \qquad (6)\end{aligned}$$

with $\boldsymbol{R}^n = F_0 \supset F_1 \supset F_2 \supset \ldots \supset F_n = F$. Usually these sets are defined by a sequence of levels for the LSF $G(\mathbf{u})$ in the form $F_1 = \{g(\mathbf{u}) < c_1\}, F_2 = \{g(\mathbf{u}) < c_2\}\ldots, F_n = \{g(\mathbf{u}) < 0\}$ with $c_1 > c_2 > \ldots > 0 = c_n$. Since the respective (suitably chosen) conditional probabilities are relatively large compared with the probability $\Pr(F_n)$ which should be estimated, such an approach has the advantage that these conditional probabilities can be estimated more efficiently with smaller sample sizes. The details how these samples are produced using Monte Carlo Markov Chains can be found in the reference above. This concept is an iterated extrapolation starting from an initial probability estimate $\widehat{\Pr(F_1)}$ and then iterating towards the failure domain.

There are three main flaws in this method:

1. the values of the LSF inside the beta sphere are irrelevant for the calculation of the failure probability. So the sequentially calculated probability integrals are not necessary for the failure probability estimation.

2. the method might not find the relevant design points, see Breitung (2019).

3. the concept produces only numbers no structural relations as design points and alpha factors.

An analysis of some mathematical aspects of this approach can be found in Breitung (2018).

6. THE BETA SPHERE

Returning now to the original problem in the standard normal space, with the help of asymptotic analysis some basic results about the structure of the problem can be found.

The concept of the *beta sphere* seems to be to introduced by Grooteman(2008). Let be defined fro $t > 0$ the centered spheres:

$$S(t) \quad = \quad \{\mathbf{u}; |\mathbf{u}| = t\} \tag{7}$$

and let β be defined by

$$\beta \quad = \quad \min\{t > 0; \min_{\mathbf{u} \in S(t)} g(\mathbf{u}) \leq 0\} \tag{8}$$

Then the beta sphere is defined as $S(\beta)$. It is obvious that the values of the LSF inside the beta sphere are irrelevant for the calculation of the failure probability.

The conclusion is that therefore one has to find the beta sphere in a first step; then starting from the surface on this sphere one has to find more precise estimates of the failure probability. From the definition of $S(\beta)$ one gets the following upper bound:

$$\Pr(g(\mathbf{U})) \leq 0) \leq \Pr(|\mathbf{U}| \geq \beta) = 1 - \chi_n(\beta^2) \tag{9}$$

with $\chi_n(.)$ the chi-square distribution with n degrees of freedom.

The second step is then to make a more precise estimate of the conditional probability

$$\Pr(g(\mathbf{U}) \leq 0) \;\big|\; ||\mathbf{U}| \geq \beta) \tag{10}$$

It will now be shown that the main probability mass in the failure domain outside the beta sphere is concentrated near it. To derive the conditional distribution in Eq. 10 results from Olver et al. (2017), chap. 8.2, are used. For the n-dimensional standard normal random vector $\mathbf{U}$ one has

$$\Pr\left(|\mathbf{U}|^2 > \beta^2\right) \propto \beta^{n-2} \exp(-\beta/2),\ \beta \to \infty \tag{11}$$

This gives then for $d > 0$ neglecting the lower order terms:

$$\Pr(|\mathbf{U}|^2 > (\beta + d)^2 \;\big|\; |\mathbf{U}|^2 > \beta^2) \propto e^{-\beta \cdot d} \tag{12}$$

This demonstrates that if the beta sphere for a reliability problem defined by a LSF $g(\mathbf{u})$ has been determined, in high dimensions and for small probabilities the most probability weight of the distribution outside of the sphere is concentrated on a shell around it. In Breitung (1994) more precise results for the distribution in the failure domain were derived.

For this second step there are different possibilities. One can use different Monte Carlo approaches or asymptotic approximation methods.

7. THE ONION METHOD

To find the beta sphere one has to locate the design points, i.e. the points with

$$|\mathbf{u}^*| = \min_{g(\mathbf{u}) \leq 0} |\mathbf{u}|. \tag{13}$$

In the original FORM/SORM concept the design point is determined by solving the Lagrangian system:

$$\begin{aligned} \mathbf{u} + \lambda \nabla g(\mathbf{u}) &= \mathbf{0} \\ g(\mathbf{u}) &= 0 \end{aligned} \tag{14}$$

Now, instead one searches the extrema of the LSF on a centered sphere with radius γ in an iterative way

$$\begin{aligned} \nabla g(\mathbf{u}) + \mu \mathbf{u} &= \mathbf{0} \\ |\mathbf{u}|^2 - \gamma^2 &= 0 \end{aligned} \tag{15}$$

This is done in the following scheme:

1. choose an initial estimate $\hat{\beta}$,
2. Start the algorithm from the sphere $S_n(\hat{\beta})$,
3. minimize the LSF on this sphere $S_n(\hat{\beta})$,
4. by extrapolation find from the minimum a new approximation value $\hat{\beta}$ for the beta sphere (see Fig. 4).
5. return to step 2) if convergence has not yet be reached.

The second step can be made simpler with stereographic projection. In complex analysis the Riemann sphere is used to project all points lying in the complex plane onto the unit sphere S_3 in $\boldsymbol{R}^3$ defined by $S_3 = \{(x,y,z); x^2 + y^2 + z^2 = 1\}$. But the

inverse of this projection can be used to project the points on this sphere — with the exception of the north pole $(0,0,1)$ — onto the complex plane.

This projection method can be generalized to n dimensions. This gives a projection of the n-dimensional unit sphere onto the $(n-1)n$-dimensional plane $\boldsymbol{R}^{n-1}$ (see Fig. 5). For a given point $\mathbf{x} = (x_1, \ldots, x_n)$ on the unit sphere $S_n = \{\mathbf{x} \in \boldsymbol{R}^n; |\mathbf{x}| = 1\}$ the stereographic projection on a point $\mathbf{X} = (X_1, \ldots, X_{n-1})$ in the $(n-1)$-dimensional plane is given by

$$X_i = \frac{x_i}{1 - x_n} \tag{16}$$

The inverse of this projection is from the plane onto the sphere given by

$$x_i = \frac{2X_i}{S^2+1}, \; x_n = \frac{S^2-1}{S^2+1} \tag{17}$$

with $S^2 = \sum_{j=1}^{n-1} X_i^2$.

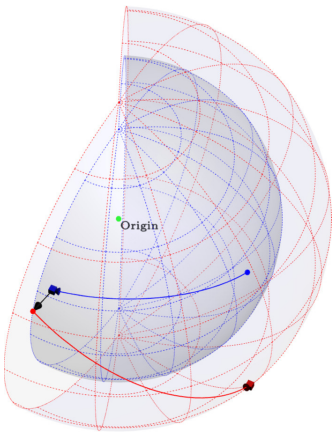


Figure 4: The onion method: one step

Using now these transformations it is possible to replace a constrained minimization problem on the unit sphere S_n by an unconstrained minimization problem in the $(n-1)$-dimensional space. Depending on the location of the iteration points the projection should be switched to a projection from the south pole if necessary.

8. THE BMM CONCEPT

Now, another method for calculating failure probabilities will be described shortly. It avoids the

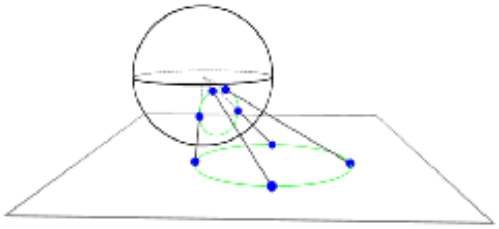


Figure 5: Stereographic projection of a circle

pitfalls of SuS, but seems to be more efficient, at least at the first glance.

Let $\varphi_n(\mathbf{u}) = (2\pi)^{n/2} \exp(-|\mathbf{u}|^2/2)$ denote the n-dimensional standard normal density. For a given failure domain $F = \{g(\mathbf{x}) < 0\}$ one can write

$$P(F) = \int_{g(\mathbf{x})<0} \varphi_n(\mathbf{x})\, d\mathbf{x} =$$

Making the substitution $\mathbf{x} \mapsto \mathbf{u} = \beta^{-1}\mathbf{x}$ yields

$$= \beta^n \int_{g(\beta\mathbf{u})<0} \varphi_n(\beta\mathbf{u})\, d\mathbf{u} \tag{18}$$

This can be split up into the product of two normal densities. Neglecting the integration constants, one gets

$$\propto \int_{g(\beta\mathbf{u})<0} \varphi_n(\sqrt{\beta^2-1}\cdot\mathbf{u}) \cdot \varphi_n(\mathbf{u})\, d\mathbf{u} \tag{19}$$

Multiplying nominator and denominator by $P(1) = \Pr(g(\beta\mathbf{U}) < 0)$ yields

$$\propto P(1) \int_{g(\beta\mathbf{u})<0} \varphi_n(\sqrt{\beta^2-1}\cdot\mathbf{u}) \left[\frac{\varphi_n(\mathbf{u})}{P(1)}\right] d\mathbf{u} \tag{20}$$

Given the probability measure $\pi(\mathbf{u})$ with Radon-Nikodym derivative $\varphi_n(\mathbf{u})\mathbf{1}_{\{g(\beta\mathbf{u})<0\}}/P(1)$ with respect to the Lebesgue measure on the set $g(\beta\mathbf{u}) < 0$ the term in the square brackets can be interpreted as this derivative. So this can be written as

$$\propto \int_{g(\beta\mathbf{u})<0} \varphi_n(\sqrt{\beta^2-1}\cdot\mathbf{u})\, \pi(d\mathbf{u}) \tag{21}$$

Now, if one has a set of (maybe dependent) data points in the domain $\{g(\beta\mathbf{u}) < 0\}$ having this stationary probability distribution $\pi(d\mathbf{u})$, the integral above can be estimated by the MC method. This can be done by running MCMC algorithms having $\pi(\mathbf{u})$ as stationary distribution. This leads to the following approximation method for failure probabilities.

1. Calculate the reliability index $\beta = \min_{g(\mathbf{u})=0} |\mathbf{u}|$.

2. Run an MC estimate of the probability content of the set $\{g(\beta\mathbf{u}) < 0\}$ under the standard normal distribution; i.e. produce a sample of k_1 points with an n-dimensional standard normal distribution and estimate the probability by the percentage of points in this set. The estimate will be denoted by $\widehat{P(1)}$. In the MC data denote the set of all the points $\mathbf{u}$ with $g(\beta\mathbf{u}) < 0$ by S.

3. From the data points in the set S take k points $\mathbf{u}_1^0, \ldots, \mathbf{u}_k^0$. Run for each of these points an MCMC with length n_c having the stationary distribution with density $\varphi_n(\mathbf{u})\mathbf{1}_{\{g(\beta\mathbf{u})<0\}}/P(1)$, see Fig. 6. Denote the set of all these points including the starting points by S_1.

4. Calculate:

$$I(\beta) = k_s^{-1} \sum_{i=1}^{k_s} \varphi_n(\sqrt{\beta^2 - 1} \cdot \mathbf{u}_i). \qquad (22)$$

   Here $k_s = n_c \cdot k$ and $S_1 = \{\mathbf{u}_1, \ldots, \mathbf{u}_{k_s}\}$ is the set of all the points produced by the Markov chains in step 3) including the starting points.

5. Estimate $P(F)$ by

$$\widehat{P(F)} = \beta^n (2\pi)^{n/2} \widehat{P(1)} I(\beta) \qquad (23)$$

Here the integers k_1, k_2 and n_c have to be chosen appropriately. For the third step it is important to note that in this case the starting points have already the stationary distribution, since they come from an MC run. If points are produced by MCMC methods as in the further steps of the SuS concept, this is not always the case as outlined in Breitung (2018).

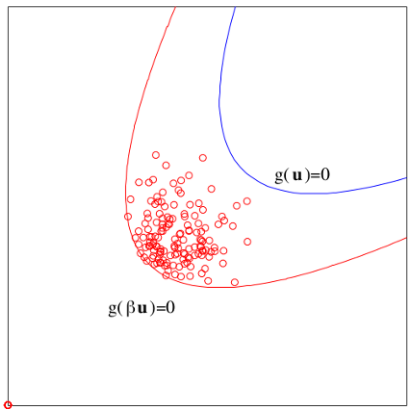


Figure 6: The stationary distribution in $\{g(\beta\mathbf{u}) < 0\}$

For the MCMC step it appears to be useful to use an algorithm which works well also for high dimensions. Appropriate seems to be the preconditioned Crank-Nicolson algorithm (see Wikipedia contributors (2019)), proposed first in Neal (1999) and in Cotter et al. (2013). Later it was used in SuS by Papaioannou et al. (2015).

This approach can be generalized to non-normal probability densities. Consider a standardized and centered n-dimensional random distribution. Then one takes $\lambda = \min_{g(\mathbf{u})=0} |\mathbf{u}|$ instead of the reliability index and modifies the following steps accordingly.

This approach can be modified by varying the parameter for the uniform scaling and by trying to optimize the MCMC runs in the second step.

Since the trick with splitting the integrand reminds of the famous Münchhausen maneuver of pulling himself out of the mud, the author named this approch BMM (Breitung's Münchhausen Method).

Certainly there will be cases where this is no optimal and critics will soon point out those; however it seems — at least at the first look — that this method is more efficient and not so prone to errors appearing in the sequential approach of SuS.

9. CONCLUSIONS

This is only an attempt to try to look at the problem of faulure probability calculation from different viewpoints and an appeal to experiment with vari-

ous methods and concepts. Here two new concepts were outlined, the onion and the BMM approach.

Since science is — as Feyerabend (1993) says — in principle an anarchistic enterprise. And as he said also, all methodologies have their limits even the most obvious ones. What should be done is — as proposed in Bartz-Beielstein et al. (2010) — a systematic testing of various methods

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