An efficient global optimization algorithm based on augmented radial basis function[⋆]

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Abstract – In the structural optimization, the accuracy of approximation for the established mathematical model will directly affect the solution efficiency, even the convergence. The global optimization model based on the augmented Gaussian radial basis function h as a high approximation accuracy, but the solution efficiency will not be increased without a matched optimization algorithm. In this paper, we adopt the information at the interpolating points in large extent and the augmented Gaussian radial basis function to construct the approximate mathematical model. Using the explicit derivatives of the model for the sensitivities and sequential quadratic programming (SQP) algorithm for the optimization solving, an efficient algorithm of global optimization is proposed. It is simple to be realized and converges quickly. Two examples will illustrate the stability and efficiency of the present algorithm.

Key words: Structural optimization; approximate model; Gaussian radial basis function; global optimization algorithm

1 Introduction

In 1960, Schmit [1] brought forward the idea which introduced the mathematical programming into the structural optimization by using the systematic synthesis. At that time, he might not realize the importance of the establishment of mathematical models, so the optimal design was found by hundreds structural reanalyses. In fact, the objective function and constraint functions in an engineering problem can be rarely written as the explicit expressions in terms of design variables, the sensitivity analysis is very time-consuming.

In 1974, Schmit and Farshi [2] proposed some approximation concepts including the obtaintion of explicit approximate functions for constraint functions to improve the structural optimization efficiency and the iteration times largely decreased. Essentially, the establishment of an optimization model consists in constructing approximate functions for objective function or/and constraint conditions. From then on, the idea of establishing mathematical model has been accepted by many optimization researchers and is becoming a relative independent research domain. However, some researchers still use the methods without establishing any optimization

model. Although the difficulty of sensitivity analysis can be avoided, the calculations are very time-consuming and the problem of converge often arises.

Therefore, the establishment of an approximate optimization model is a good choice for the structural optimization. The research works on the model establishment can be divided into three parts: the first one is to select suitable approximate functions, the second one is to provide the derivatives of these functions (sensitivity analysis), the third one is to choose an adapted algorithm to solve the optimization model. In the early used methods for mathematic model establishing, the Taylor's expansions of first order and/or second order are usually used, and analytical methods of sensitivity analysis are often adopted. The disadvantages of the sensitivity analysis are that the analytical derivatives is very difficult and the computation of derivatives is too expensive. This may be the reason that some scholars do not establish any optimization model.

Are there some methods to establish the mathematical model without sensitivity analysis? Recently, the Response Surface Methodology (RSM) (Mayer et al. [3]) is largely used for the structural optimization, a lot of research (Venter and Haftka [4], Hosder et al. [5], Jansson et al. [6], Liu et al. [7]) and improved works (Zheng and Das [8], Sui and Li [9]) have been done by using the RSM. The RSM is mainly a polynomial regression method, it usually uses the first order and/or second order polynomials and the approximation accuracy is good only in local domain. It is often combined with QP algorithm by

sequential iterations, so an initial solution should be selected by user. Because this selection is very difficult in a structural optimization, the method can not promise to give the global optimal solution. Although high order polynomials can be used to obtain some global approximations, but a lot of response calculations are needed at the experiment points and this will lead to too expensive calculations.

In recent years, some researchers introduced an accurate global approximate method called Radial Basis Function method (RBF) (Mason and Cox [10], Krishnamurthy [11]). Fang and Horstemeyer [12] demonstrate that the approximation accuracy of the augmented Gaussian RBF is higher than that of other types of RBF and its approximation domain is also wider. How to solve this type of models with high approximation accuracy? From published papers, an optimization algorithm is often taken to solve the model without considering whether the algorithm is adapted to the characteristic of the model. In other word, it is deficient in considering the relation between an establishing approximate optimization model and an adapted algorithm. Consequently, the optimization computation is not efficient. In this paper, we introduce a new sequential algorithm corresponding to the approximation model based on the augmented RBF method. The numerical results illustrate the accuracy and efficiency of the present algorithm.

2 RBF and augmented RBF methods

The Radial Basis Function (RBF) can be expressed by the linear combination of the functions in terms of radial distance from the considered point to every interpolation point (or sample point or experiment design point) [12]:

$$s(\mathbf{x}) = \sum_{j=1}^{m} \lambda_j \varphi \left(\left\| \mathbf{x} - \mathbf{x}^j \right\|_2 \right) \quad \mathbf{x} \in E^n \qquad (1)$$

where n is the total number of design variables or the dimensional number of the design space, m is the total number of interpolating points, $\lambda_j (j = 1, \ldots, m)$ is the jth coefficient to be determined, $\mathbf{x}$ is the position vector of a design point, $\mathbf{x}^j$ is the position vector of jth interpolating point, $\left\| \mathbf{x} - \mathbf{x}^j \right\|_2$ is the jth radial distance between the two points:

$$r^{0j} = \left\| \mathbf{x} - \mathbf{x}^j \right\|_2 = \sqrt{\sum_{k=1}^{n} (x_k - x_k^j)^2}. \qquad (2)$$

Different forms of the RBF $\varphi(r)$ are listed in Table 1.

Let F_i the real response value at the interpolating point $\mathbf{x}^i$, the formula (1) becomes:

$$\sum_{j=1}^{m} \lambda_j \varphi(r^{ij}) = F_i \quad (i = 1, \ldots, m) \qquad (3)$$

$$r^{ij} = \left\| \mathbf{x}^i - \mathbf{x}^j \right\|_2 = \sqrt{\sum_{k=1}^{n} (x_k^i - x_k^j)^2}. \qquad (4)$$

Table 1. Usually used radial basis functions.

Function name	Expression
Linear	$\phi(r) = cr$
Thrice	$\phi(r) = cr^3$
Thin plate spline	$\phi(r) = r^2 \ln(cr), 0 < c \leqslant 1$
Gaussian	$\phi(r) = e^{-cr^2}, 0 < c \leqslant 1$
Multi-quadratic	$\phi(r) = \sqrt{r^2 + c^2}, 0 < c \leqslant 1$

where the constant c is usually taken as 1.

Then $\lambda_j (j = 1, \ldots, m)$ can be obtained by solving equations (3).

To increase the approximation accuracy and expand the approximation range of the RBF, a polynomial term can be added to the expression (1):

$$s(\mathbf{x}) = \sum_{j=1}^{m} \lambda_j \varphi(\mathbf{r}^{0j}) + \sum_{i=1}^{I} b_i P_i(\mathbf{x}) \qquad (5)$$

where the polynomial functions $p_i(\mathbf{x})(i = 1, ..., I)$ can be $1, x_1, \ldots, x_n, x_1^2, x_1 x_2, \ldots, x_n^2, \ldots$ or a part of them. The above expression is called augmented RBF. Using m interpolating points and their corresponding real response values in expression (5), we obtain:

$$\begin{cases} \lambda_1 0 + \lambda_2 \varphi \left(\mathbf{r}^{12} \right) + \ldots + \lambda_m \varphi \left(\mathbf{r}^{1m} \right) + b_1 p_1 \left(\mathbf{x}^1 \right) + \ldots \\ \qquad + b_I p_I \left(\mathbf{x}^1 \right) = F_1 \\ \lambda_1 \varphi \left(\mathbf{r}^{21} \right) + \lambda_2 0 + \ldots + \lambda_m \varphi \left(\mathbf{r}^{2m} \right) + b_1 p_1 \left(\mathbf{x}^2 \right) + \ldots \\ \qquad + b_I p_I \left(\mathbf{x}^2 \right) = F_2 \\ \qquad \vdots \\ \lambda_1 \varphi \left(\mathbf{r}^{m1} \right) + \lambda_2 \varphi \left(\mathbf{r}^{m2} \right) + \ldots + \lambda_m 0 + b_1 p_1 \left(\mathbf{x}^m \right) + \ldots \\ \qquad + b_I p_I \left(\mathbf{x}^m \right) = F_m. \end{cases}$$
$$(6)$$

In equations (6), there are m coefficients $\lambda_j (j = 1, \ldots, m)$ and I coefficients $b_i (i = 1, ..., I)$ as unknowns, so I equations have to be added. The added equations may be obtained according to the following orthogonal conditions:

$$\begin{cases} p_1 \left(\mathbf{x}^1 \right) \lambda_1 + \ldots + p_1 \left(\mathbf{x}^m \right) \lambda_m = 0 \\ \qquad \vdots \\ p_I \left(\mathbf{x}^1 \right) \lambda_1 + \ldots + p_I \left(\mathbf{x}^m \right) \lambda_m = 0. \end{cases} \qquad (7)$$

The equations (6) and (7) can be rewritten in a matrix form:

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^{\mathrm{T}} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \lambda \\ \mathbf{b} \end{Bmatrix} = \begin{Bmatrix} \mathbf{F} \\ \mathbf{0} \end{Bmatrix}$$

with $\mathbf{A} = \begin{bmatrix} 0 & \varphi \left(\mathbf{r}^{12} \right) & \ldots & \varphi \left(\mathbf{r}^{1m} \right) \\ \varphi \left(\mathbf{r}^{21} \right) & 0 & \ldots & \varphi \left(\mathbf{r}^{2m} \right) \\ \vdots & \vdots & \vdots & \vdots \\ \varphi \left(\mathbf{r}^{m1} \right) & \varphi \left(\mathbf{r}^{m2} \right) & \ldots & 0 \end{bmatrix}$,

$\mathbf{B} = \begin{bmatrix} p_1 \left(\mathbf{x}^1 \right) & \ldots & p_I \left(\mathbf{x}^1 \right) \\ \vdots & \vdots & \vdots \\ p_1 \left(\mathbf{x}^m \right) & \ldots & p_I \left(\mathbf{x}^m \right) \end{bmatrix}$
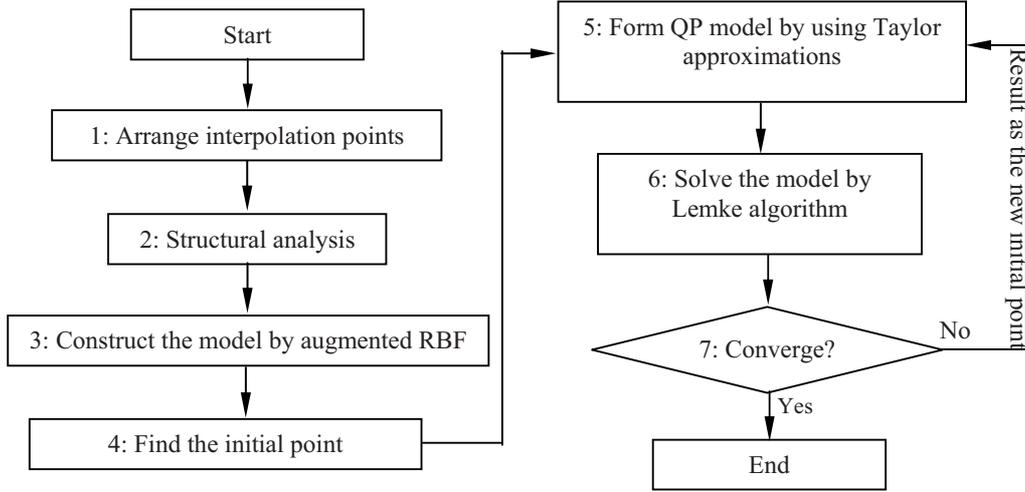
Fig. 1. Flow chart of present new algorithm.

$\lambda = (\lambda_1, \ldots, \lambda_m)^{\mathrm{T}}, \mathbf{b} = (b_1, \ldots, b_I)^{\mathrm{T}}, \mathbf{F} = (F_1, \ldots, F_m)^{\mathrm{T}}$.

The RBF and augmented RBF have no error at the interpolating points. In order to evaluate their approximation accuracy, K other points are selected in the design space. We calculate the approximate response $\overline{F}_i (i = 1, ..., K)$ using (5) and the real response $F_i^{real}(i = 1, ..., K)$ using the structural analysis solver, then the following root of mean square errors can be the evaluate index:

$$RMSE = \sqrt{\sum_{i=1}^{K} \left(\overline{F_i} - F_i^{\mathrm{real}} \right)^2 / K}. \qquad (8)$$

3 Implementation of algorithms of modelling and optimization

The optimization problem of a mathematical programming or a structural optimization can be described by:

$$\begin{cases} \text{find} & \mathbf{x} \in E^n \\ \min & f(\mathbf{x}) \\ \text{s.t.} & c_k(\mathbf{x}) \leqslant b_k(k = 1, \ldots, K) \\ & \underline{x}_i \leqslant x_i \leqslant \bar{x}_i(i = 1, \ldots, n) \end{cases} \qquad (9)$$

where K is the total number of behaviour constraints. The above mentioned Augmented RBF (Eq. (5)) can be used to approach the objective function and constraints functions in order to obtain an optimization model in global domain. But it is difficult to solve this mathematic model because of its high nonlinearity.

In order to find an efficient optimization algorithm matched with high order nonlinear characteristics of the model (9), the following solving strategy including the sequential quadratic programming (SQP) is proposed. It is carried out in 7 steps:

(1) Arrange a set of interpolating points evenly in the global domain representing the experiment design variables. Their feasible properties are not considered.

(2) A series of structural analysis at the interpolating points are carried out to obtain the corresponding response values.

(3) The objective function and constraint conditions based on the Augment Gaussian RBF are established and their corresponding coefficients λ_j and b_i are determined according to the response values.

(4) The vector of design variables giving the minimal value of the objective function at one of all feasible interpolating points is taken as an initial point for SQP.

(5) At the initial point, a standard QP model is formed by using the second order Taylor's expansion for the objective function and the first order Taylor's expansions for the constraint conditions.

(6) Combined with the rational move limits of design variables, the QP model is solved by Lemke algorithm.

(7) Checking the convergence criterion, if it is satisfied then exit, otherwise return to the 5th step and use the obtained result as a new initial point for the next step.

In 5th step, for the solution convenience, the objective function and the constraint conditions adopt different order Taylor's expansions (Sui et al. [13]). In 6th step, the rational move limits of design variables is a method considering accumulated information (Sui et al. [14]) and Lemke algorithm can efficiently solve a standard QP.

The flow chart in Figure 1 shows our new algorithm, named Augmented Gaussian RBF-SQP (AG-RBF-SQP) method.

In the QP model, the first order and second order Taylor's approximations of an arbitrary function $f(\mathbf{x})$ are given by the following expressions

$$f(\mathbf{x}) \approx f(\mathbf{x}^0) - \sum_{i=1}^{n} \frac{\partial f(\mathbf{x}^0)}{\partial x_i} x_i^0 + \sum_{i=1}^{n} \frac{\partial f(\mathbf{x}^0)}{\partial x_i} x_i \qquad (10)$$

$$f(\mathbf{x}) \approx f(\mathbf{x}^0) - \sum_{i=1}^{n} \frac{\partial f(\mathbf{x}^0)}{\partial x_i} x_i^0$$
$$+ \frac{1}{2} \sum_{j=1}^{n} \sum_{k=1}^{n} \frac{\partial^2 f(\mathbf{x}^0)}{\partial x_j \partial x_k} x_j^0 x_k^0 + \sum_{i=1}^{n} \left(\frac{\partial f(\mathbf{x}^0)}{\partial x_i} \right.$$
$$\left. - \sum_{j=1}^{n} \frac{\partial^2 f(\mathbf{x}^0)}{\partial x_i \partial x_j} x_j^0 \right) x_i + \frac{1}{2} \sum_{j=1}^{n} \sum_{k=1}^{n} \frac{\partial^2 f(\mathbf{x}^0)}{\partial x_j \partial x_k} x_j x_k.$$
$$(11)$$

For our algorithm, the Gaussian functions and linear functions are taken in the formula (5). In order to improve the computation efficiency, the analytical explicit derivatives are deduced. The partial derivatives of first order and second order are calculated as follows:

$$\partial s(\mathbf{x})/\partial x_l = -2 \sum_{j=1}^{m} \lambda_j e^{-\sum_{k=1}^{n}(x_k - x_k^j)^2}(x_l - x_l^j) + b_l \quad (12)$$

$$\frac{\partial^2 s(\mathbf{x})}{\partial x_l \partial x_p} = \begin{cases} 4 \sum_{j=1}^{m} \lambda_j e^{-\sum_{k=1}^{n}(x_k - x_k^j)^2}(x_l - x_l^j)(x_p - x_p^j) \\ \qquad \text{if } l \neq p \\ 2 \sum_{j=1}^{m} \lambda_j e^{-\sum_{k=1}^{n}(x_k - x_k^j)^2}[2(x_l - x_l^j)^2 - 1] \\ \qquad \text{if } l = p. \end{cases}$$
$$(13)$$

Finally, the model (9) can be transformed to a standard QP model:

$$\begin{cases} \text{find} & \mathbf{x}^{(v)} \in E^n \\ \min & \mathbf{x}^{\mathrm{T}} \mathbf{H}^{(v)} \mathbf{x}/2 + \mathbf{C}^{(v)} \mathbf{x} \\ \text{s.t.} & \mathbf{A}^{(v)} \mathbf{x} \leqslant \mathbf{B} - \mathbf{A}_0^{(v)} \\ & \underline{x}_i^{(v)} \leqslant x_i \leqslant \bar{x}_i^{(v)} \end{cases} \quad (14)$$

where v denotes the vth iteration. The objective function is expanded into the second order Taylor expansion: $\mathbf{H}^{(v)}$ is the Hessian matrix, given by the fifth term in the expression (11), $\mathbf{C}^{(v)}$ is a vector, given by the fourth term in (11). The first three terms in (11) have no influence on the minimization of $f(\mathbf{x})$. The constraint functions in (9) are expanded into the first order Taylor expansion: $\mathbf{A}^{(v)}$ is a matrix given by the third term in (10), $\mathbf{A}_0^{(v)}$ is a vector given by the first two terms in (10), $\mathbf{B}$ represents b_k in (9).

4 Numerical examples

In order to evaluate the accuracy and efficiency of the present algorithm, a lot of mathematical functions and practical engineering examples have been treated, we just present two of them in this paper: a mathematical example, an engineering application, whose models are established by the Augmented Gaussian RBF and solved by the present algorithm. The optimal results of the first example is compared with the results obtained by using the
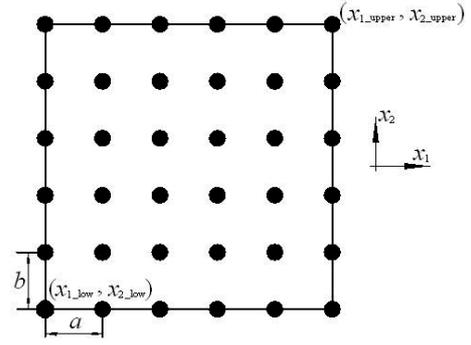
Fig. 2. 36 Interpolating points.
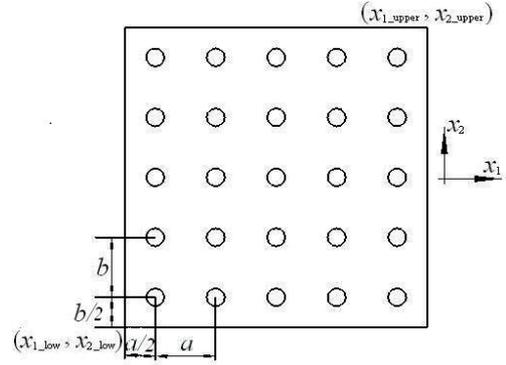
Fig. 3. 25 Non- interpolating points.

Genetic Algorithm (GA) (Xuan et al. [15]) and Simulated Annealing Algorithm (SAA) (Yang and Gu [16]), implemented by the 7D-Soft High Technology Inc. and published in the software 1stOpt1.5 (Website [17]). The optimal results of the second example is compared with that of SRSM-QP (sequential response surface methodology and quadratic programming) algorithm (Yang et al. [18]).

4.1 Maximization problem of a highly nonlinear objective function

$$\begin{cases} \text{find} & \mathbf{x} \in E^2 \\ \max & f(\mathbf{x}) \\ \text{s.t.} & 0.01 \leqslant x_1 \leqslant 1 \\ & 0 \leqslant x_2 \leqslant 1 \end{cases} \quad (15)$$

with $f(\mathbf{x}) = [0.8\sqrt{x_1^2 + x_2^2} + 0.35\sin(2.4\pi\sqrt{x_1^2 + x_2^2})/\sqrt{2}]$ $[1.5\sin(1.3\arctan(x_2/x_1))]$. The real response surface is illustrated in Figure 4. The exact solution gives the maximum value 1.6519 at the point (0.4276, 1.0). To establish an approximate model and evaluate the error, we evenly arrange 36 interpolating points and 25 non-interpolate points respectively in the global design space (Figs. 2 and 3, $a = 0.198$, $b = 0.2$). The approximate model obtained by using the Augmented Gaussian RBF and the given 36 sample points gives an approximate response surface (Fig. 5). The RMSE using the augmented RBF at the given 25 points is 0.0108 and that using RBF at the given 25 points is 0.0112. Table 2 gives the comparison of the results of different algorithms.
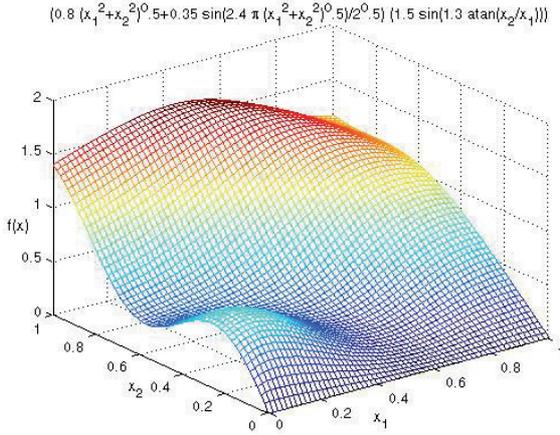
$\{0.8\ (x_1{}^2+x_2{}^2)^{0.5}+0.35\ \sin\{2.4\ \pi\ (x_1{}^2+x_2{}^2)^{0.5}\}/2^{0.5}\}\ \{1.5\ \sin(1.3\ \mathrm{atan}(x_2/x_1))\}$

Fig. 4. Real function image of example 4.1.
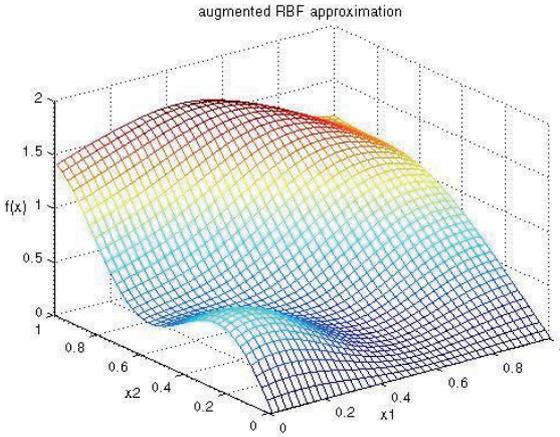

augmented RBF approximation

Fig. 5. Approximate function image of example 4.1.

Table 2. Comparison of the results of different algorithms.

Algorithm	Optimal point		Objective value	Number of
	x_1	x_2	$f(x)$	objective calculations
GA	0.4262	0.9999	1.6518	1304
SAA	0.4276	0.9999	1.6518	416
AG-RBF-SQP	0.4050	1.0000	1.6507	37

In Table 2, the right column shows the number of objective calculations with different algorithms. We note that the present algorithm is very fast with respect to the two others. The convergence is attained with only two times of model establishment and 37 calls of objective calculations. The first model is established by using the 36 calls at the 36 chosen interpolating points; in the second model, the previously calculated objective functions and constraint functions at the 36 chosen points are kept and one more call is carried out at the optimal point obtained with the first model. We can use all these 37 points or 36 points by removing the nearest point from the optimal point of the first model to establish the second model. Two SQP calculations are needed for the first and second models, respectively.
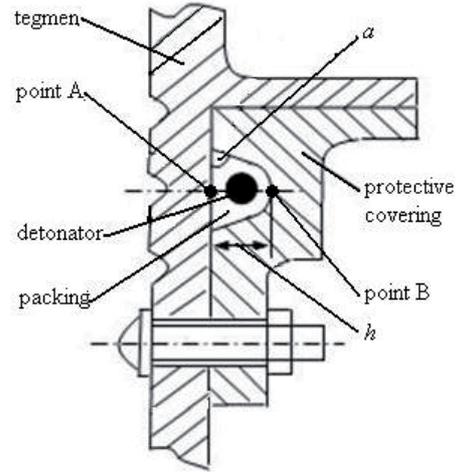
Fig. 6. 2D Section of axisymmetrical device for cutting off by explosion.

4.2 Cavity shape optimization charged detonator of equipment cutting off by explosion

An axisymmetrical device for cutting off by explosion is taken as an industrial application. Only its 2D section is illustrated (Fig. 6) and calculated. The cavity is charged with the detonator, so its shape and dimensions will determine the intensity and direction of the maximal cutting force. The cavity shape is defined by an arc and two segments, the height h of the cavity and the obliquity α of the segments are taken as the design variables. For the initial design, h is 0.36 cm, α is 1.56 rad. The structure is divided into 1635 elements. The aim of the optimization is to give the maximal effective stress at the point A (element No. 1377) to cut of the tegmen and a effective stress inferior to the allowable limit (310 MPa) at B (element No. 941) to preserve the protective covering. Therefore, the effective stress σ_{EA} at point A is taken as objective function and should be maximized, and the effective stress σ_{EB} at point B is taken as behaviour constraint. The following expression (16) describes this optimization problem:

$$\begin{cases} \text{find} & \alpha, h \\ \max & \sigma_{\mathrm{EA}}(\alpha, h) \\ \text{s.t.} & \sigma_{\mathrm{EB}}(\alpha, h) \leqslant 310 \\ & 0.8 \leqslant \alpha \leqslant 1.56 \\ & 0.33 \leqslant h \leqslant 0.43. \end{cases} \tag{16}$$

Two similar schemas of interpolating points (6×6, $a = 0.152$, $b = 0.02$ in Fig. 2) and non interpolating points (5×5 in Fig. 3) are used for this example. At the 25 non-interpolate design points, the RMSEs of objective function and constraint condition obtained by using augmented RBF are 2.658 and 2.349, respectively. They are a little better than those obtained by using RBF (2.734 and 2.408). Table 3 shows the comparison with SRSM-QP.

Similar to Example 4.1, this engineering application has two model establishing and two SQP calculations for every model. The AG-RBF-SQP algorithm use 37 structural analyses. From Table 3 and Figure 7, we note that

Table 3. Result comparison with SRSM-QP.

| Algorithm | Optimal point | | Objective value | Constraint value | Number of |
	$\alpha/$(rad)	$h/$(cm)	$\sigma_{EA}/$MPa	$\sigma_{EB}/$MPa	structural analyses
SRSM-QP [18]	0.9914	0.3300	262.2200	296.5100	85
AG-RBF-SQP	1.2371	0.3300	314.8250	295.8280	37
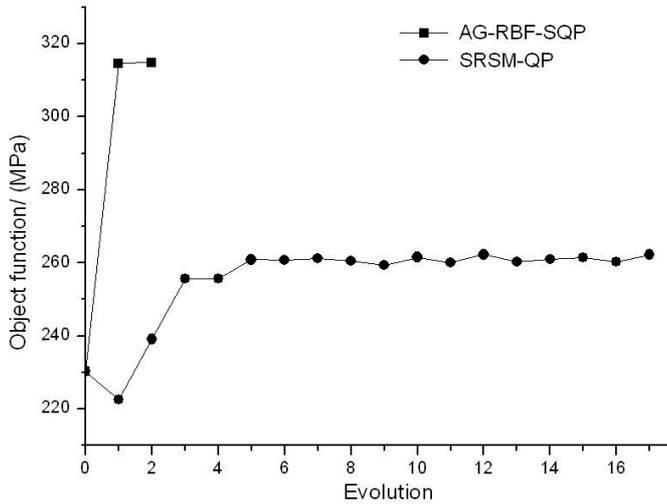
Fig. 7. Evolution of the objection function.

the global optimal objective value calculated by AG-RBF-SQP is 20.1% larger than the local one by SRSM-QP, and the number of structural analyses is much smaller than that by SRSM-QP.

The simulated explosive process lasts 21 μs. Figure 8 shows the curves of the effective stresses versus time before and after optimization, the maximum effective stress at point A is 314.825 MPa after optimization, it increase 36.7% compared with 230.31 MPa before optimization, the maximum effective stress at point B changes very little, from 298.11 MPa before optimization to 295.828 MPa after optimization, it also satisfies the constraint.

5 Conclusion

In this paper, the augmented Gaussian Radial Basis Function is used to establish an approximate model for a global optimization procedure. This approximate model expressed explicitly in terms of the design variables allows to easily obtain the derivatives of the objective function and constraint functions, required in many optimisation algorithms. Taking into account the characteristics of the augmented Gaussian RBF, the method of Sequential Quadratic Programming (SQP) is adopted as optimisation solver. Since the derivatives of the objective function and constraint functions are calculated analytically without structural reanalyses, the present optimisation procedure is very fast. Furthermore, it does not require the user to provide any initial solution. The numerical tests show that the optimal results given by the present algorithm are very close to those obtained by the usually used GA
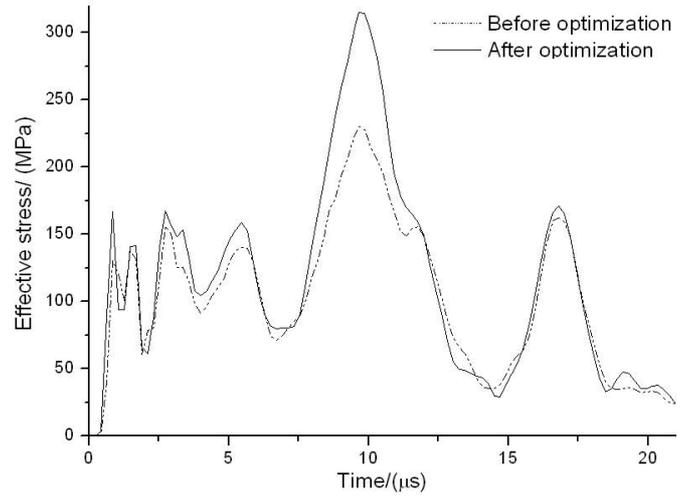
(a)
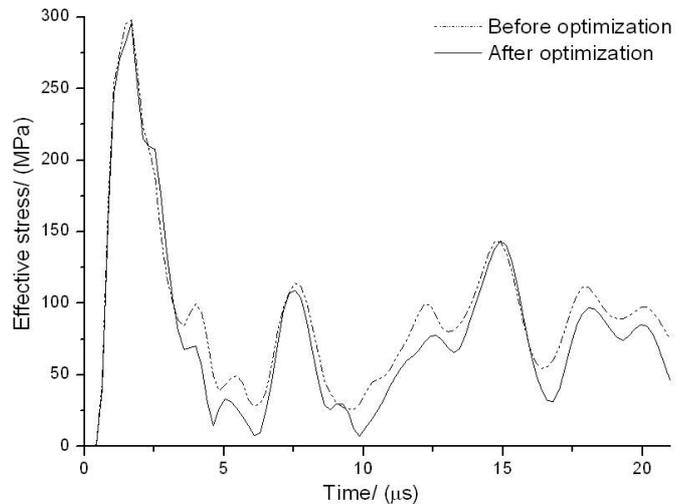
(b)

Fig. 8. Curves of the effective stress versus time. (a) Point A. (b) Point B.

and SAA, but it is much more efficient than these two optimisation algorithms and SRSM-QP algorithm.

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