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Comparison of Three Versions of Conjugate Gradient Method in Predicting an Unknown Irregular Boundary Profile

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***Abstract*—**An inverse geometry problem is solved to predict an unknown irregular boundary profile. The aim is to minimize the objective function, which is the difference between real and computed temperatures, using three different versions of Conjugate Gradient Method. The gradient of the objective function, considered necessary in this method, obtained as a result of solving the adjoint equation. The abilities of three versions of Conjugate Gradient Method in predicting the boundary profile are compared using a numerical algorithm based on the method. The predicted shapes show that due to its convergence rate and accuracy of predicted values, the Powell-Beale version of the method is more effective than the Fletcher-Reeves and Polak –Ribiere versions.

***Keywords*—**Boundary elements, Conjugate Gradient Method, Inverse Geometry Problem, Sensitivity equation.

I. Introduction

THE inverse heat transfer method (IHTM) has received great attention recently and found many applications in the engineering discipline. In such applications, data such as geometry, boundary and initial conditions and also thermal properties, normally provided in direct approaches to solving the problem, are not known and should be predicted. The IHT method are used in predicting heat flux [1],[2], thermal conductivity [3],[4], internal heat generation [5], and geometry [6],[7].

The problem attended to in this study is one of predicting the unknown boundary profile using the temperature distribution on other boundaries of an object. These types of problems are ill-posed, mathematically non-linear, and highly sensitive to input errors and inevitable measurement noises. In light of this fact, use is made of two approaches in solving inverse problems: the first uses discretization to solve the direct problem and the other is a regularization scheme for the inverse problem. The latter approach usually includes an iterative procedure to minimize the objective function. To obtain the unknown boundary and also solve the ensuing equations, the boundary elements method (BEM) is suggested. In comparison to other segmentation methods such as finite difference and finite elements, BEM is favored since it decreases computation time and memory, while allowing a solution to problems of complicated geometries [8].

Among various types of regularization methods, two which are of more significance are Tikhonov [9] and Beck [10] regularization methods. The other method, which in using a convergence criterion falls in the iterative regularization methods category, is the Conjugate Gradient Method (CGM). The Conjugate Gradient Method (CGM) is a powerful minimization procedure which can be implemented to predict the function or parameter in both linear and non-linear inverse heat transfer problems. There are three common versions of this method whose approaches to calculating the conjugate directions are different [11]. The objective function gradient can be obtained using direct gradient evaluation and adjoint equation methods [12].

In fact, the current work is the extension of [13] in which, the Levenberg-Marquardt method and the Fletcher- Reeves version of CGM have been compared in predicting the unknown boundary in steady-state conditions and the boundary conditions were assumed to be in the form of constant temperature and constant heat flux.

II. Mathematical Formulation

A. Formulating the Direct Heat Conduction Problem

The direct problem is a two-dimensional steady-state conduction equation in region Ω with the known boundary conditions. As shown in Fig. 1, the boundaries at x=0, and x=10 are insulated. At y=0, a constant heat flux, q_0 flows out of the boundary, while the irregular boundary, illustrated as f(x) , is in the constant temperature T_0 .

Two-dimensional, steady-state conduction equation is

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}=0 \qquad \text{in} \quad \Omega \tag{1-a}$$

BC's

$$\partial T/\partial x=0 \qquad \text{at} \quad x=0 \tag{1-b}$$

$$\partial T/\partial x=0 \qquad \text{at} \quad x=L \tag{1-c}$$

$$-\partial T/\partial y=q_0 \qquad \text{at} \quad y=0 \tag{1-d}$$

$$T=T_0 \qquad \text{at} \quad y=f(x) \tag{1-e}$$

The differential equation is discretized using BEM. The boundary integral relation for two-dimensional conduction

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problem with constant properties and steady-state conditions in region Ω bounded by Γ is:

$$cT_M + \int_\Gamma Tq^* d\Gamma = \int_\Gamma qT^* d\Gamma \quad (2)$$

where M is a point, either in region Ω or on the boundary Γ. T and q represent the temperature and heat flux density, respectively. Constant C can take different values based on the position of point M. T*, is the general solution in BEM, and q* represents the normal gradient of T*. The general solution for the two- dimensional, steady-state condition is:

$$T^* = \frac{1}{2\pi} \ln r \quad (3)$$

where r is the distance between point M and any point on boundary Γ.

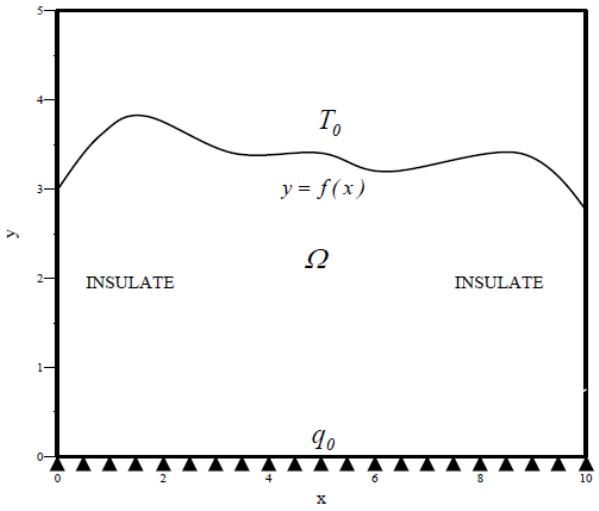

Fig. 1 The studied geometry and region

Dividing boundary Ω into k elements, allows for setting up (2) for any boundary element. Subsequently, a set of linear algebraic equations for all elements can be set up so that:

$$CT + HT = Gq \quad (4)$$

In this equation, T is the temperature vector of boundary elements, q represents the heat flux density vector, G and H are geometry-dependent matrices, and C is a diagonal matrix. With the boundary conditions dually noted, (4) simplifies to:

$$AX=B \quad (5)$$

where X is the vector comprised of the unknown parameters. Matrix B is the result of multiplying the prescribed values matrix, by the geometry-dependent matrices. The set of linear equations with obtained boundary segmentation can be used to evaluate the unknown temperature and heat flux.

B. Formulating the Inverse Heat Conduction Problem

In the inverse approach, boundary f(x) pertinent to region Ω is unknown. The measured temperatures are represented in the form $Y(x_i,0) = Y_i$, where i=1, …, m. The approach used in the inverse method is such that an initial guess is made as to the profile of the unknown boundary, and the ensuing direct conduction problem is solved. An objective function of the form below is defined:

$$J[f(x)] = \sum_{i=1}^{m} [T_i - Y_i]^2 \quad (6)$$

where T_i is the temperature obtained from the solution of the two-dimensional, steady-state conduction problem using the estimated boundary, f^(x). The «^» sign is used to depict estimated values.

C. Conjugate Gradient Method

By obtaining the conjugate direction at each point and the optimum step size in this direction, through an iterative procedure adhering to (7), CGM evaluates the minimum value for the desired objective function (6).

$$\hat{f}^{n+1}(x) = \hat{f}^n(x) + \beta^n P^n(x) \quad , \quad n = 0,1,2,\dots \quad (7)$$

Based on the procedures undertaken in finding the conjugate direction, CGM takes on three different versions. The general form of the conjugate direction is:

$$P^n(x) = -J'^n(x) + \gamma^n P^{n-1}(x) + \varphi^n P^q(x) \quad (8)$$

With this notation, the angle between the decreasing and negative directions of the conjugate direction will be less than 90°. This guarantees the finding of a minimum value. Index q in (8) represents the iteration in which a restart has taken place to optimize CGM. Conjugate coefficients $\gamma^n$and φ^n contribute to each version of CGM in the following manner. The first version of CGM is known as the Fletcher-Reeves version [11]. Coefficients $\gamma^n$and φ^n in this version are defined as:

$$\gamma^n = \frac{\int_{x=0}^{L} (J'^n)^2 dx}{\int_{x=0}^{L} (J'^{n-1})^2 dx}; \ \gamma^0 = 0 \ , \ \varphi^n = 0 \quad (9)$$

In the second version, known as Polak-Ribiere, the coefficients are in the following form:

$$\gamma^n = \frac{\int_{x=0}^{L} (J'^n - J'^{n-1}) J'^n dx}{\int_{x=0}^{L} (J'^{n-1})^2 dx}; \ \gamma^0 = 0 \ , \ \varphi^n = 0 \quad (10)$$

In problems of non-linear parameter prediction, the Polak-Ribiere version performs better than the Fletcher-Reeves version [14].

Beale and Powell, based on the second version of CGM, presented a new version of CGM with the following relations for the conjugate coefficients.

$$\gamma^n = \frac{\int_{x=0}^{L}(J'^n - J'^{n-1})J'^n dx}{\int_{x=0}^{L}(J'^n - J'^{n-1})P^{n-1} dx};\ \gamma^0 = 0 \quad (11)$$

$$\varphi^n = \frac{\int_{x=0}^{L}(J'^{q+1} - J'^q)J'^n dx}{\int_{x=0}^{L}(J'^{q+1} - J'^q)P^q dx};\ \varphi^0 = 0 \quad (12)$$

Powell notes that the use of (11) and (12) necessitates using the restart technique. This technique is used when the gradients in the relevant iteration are non-orthogonal which, is a reason for the local non-linearity. Furthermore, when the direction obtained does not bring about the necessary decrease in the function, the conjugate direction is corrected using the restart technique. This comes about by using $\varphi^n = 0$ in (8). The extent to which a gradient is non-orthogonal in iteration "n" is calculated using the condition below:

$$\left|\int_{x=0}^{L}(J'^{n-1} - J'^n)\,dx\right| \geq 0.2\int_{x=0}^{L}(J'^n)^2 dx \quad (13)$$

The degree to which a function is minimized (largeness of angle between the direction of decrease and negative of the gradient) in iteration "n" can be studied using any of the following relations:

$$\int_{x=0}^{L} P^n J'^n dx \leq -1.2\int_{x=0}^{L}(J'^n)^2\,dx \quad (14)$$

$$\int_{x=0}^{L} P^n J'^n dx \geq -0.8\int_{x=0}^{L}(J'^n)^2 dx \quad (15)$$

In the Powell-Beale version of CGM, the direction of the function reduction defined in (8) is obtained using the following algorithm:

1. Analysis of the inequality mentioned in (13). In the event of both sides being equal, assuming q=n-1
2. Evaluation of γ^n from (11)
3. Where n=q+1, assuming φ^n=0, and for all other cases, calculating φ^n from (12)
4. Evaluating the direction of decrease, using (8)
5. When n≠q+1, checking (14) and (15). In the case of either one holding, setting φ^n, and re-evaluating the direction of reduction from (8)

Setting γ^n=φ^n=0 in each iteration, the direction of reduction for $P^n(x)$ turns out to be the gradient direction. This fact characterizes the quick decrease method. Since the extent of non-linearity of the problem is studied using (13), the Powell- Beale version of CGM proves to be productive in dealing with problems of a non-linear nature. In cases where (13) holds for inverse problems having a high degree of non-linearity, by restarting the calculations, the algorithm can speed up attainment of the minimum more than the other two methods.

D. Sensitivity Equation

The sensitivity equation can be evaluated from (1) by assuming boundary f(x) to move in direction "y" by an amount of Δf. Temperature T(x,y) changes to T+ΔT. Replacing f by f+Δf and T by T+ΔT in (1) produces a new equation. By deducting (1) from the new one, and neglecting the second degree terms which arise, the sensitivity equation for the sensitivity function ΔT(x,y) takes the form:

$$\frac{\partial^2\Delta T}{\partial x^2} + \frac{\partial^2\Delta T}{\partial y^2} = 0 \qquad \text{in} \quad \Omega \quad (16)$$

$$\frac{\partial\Delta T}{\partial x} = 0 \qquad \text{at} \quad x=0 \quad (16\text{-a})$$

$$\frac{\partial\Delta T}{\partial x} = 0 \qquad \text{at} \quad x=L \quad (16\text{-b})$$

$$\frac{\partial\Delta T}{\partial y} = 0 \qquad \text{at} \quad y=0 \quad (16\text{-c})$$

$$\Delta T = \Delta f\frac{\partial T}{\partial y} \qquad \text{at} \quad y=f(x) \quad (16\text{-d})$$

To find the optimum step size, the boundary is corrected to have the form $\hat{f}^n + \beta^n P^n$. The value of β^n is corrected using the steps outlined below. In iteration n+1, the objective function defined using (6) becomes

$$J\left[\hat{f}^{n+1}(x)\right] = \sum_{i=1}^{m}[T_i(\hat{f}^n + \beta^n P^n) - Y_i]^2 \quad (17)$$

Expanding temperature $T_i(\hat{f}^n + \beta^n P^n)$ using the Taylor series bounding$\hat{f}^n$, and neglecting the second and higher degree terms, gives

$$J\left[\hat{f}^{n+1}(x)\right] = \sum_{i=1}^{m}[T_i(\hat{f}^n) - \beta^n\Delta T(P^n) - Y_i]^2 \quad (18)$$

$T_i(\hat{f}^n)$ results from the direct problem solution for the boundary $\hat{f}^n(x)$. By minimizing the objective function relevant to β^n in the direction of P^n, the optimum step size can be evaluated

$$\beta^n = \frac{\sum_{i=1}^{m}(T_i - Y_i)\Delta T_i}{\sum_{i=1}^{m}(\Delta T_i)^2} \quad (19)$$

E. Adjoint Equation

Obtaining the gradient of the objective function using a method other than normal differentiation is possible through the definition of the Lagrange Coefficient, denoted by λ(x,y). It is also known as the adjoint function. In this way, the change of the objective function, ΔJ, will be obtained from:

$$\Delta J = \sum_{i=1}^{m}\int_{x=0}^{L} 2(T-Y)\Delta T\delta(x-x_i)dx + \int_{x=0}^{L}\int_{y=0}^{f(x)}\lambda\left(\frac{\partial^2\Delta T}{\partial x^2} + \frac{\partial^2\Delta T}{\partial y^2}\right)dydx \quad (20)$$

To cancel out terms including ΔT, λ is assumed to be the solution to the differential equation:

$$\frac{\partial^2\lambda}{\partial x^2}+\frac{\partial^2\lambda}{\partial y^2}=0 \qquad \text{in} \quad \Omega \tag{21}$$

$$\frac{\partial\lambda}{\partial x}=0 \qquad \text{at} \quad x=0 \tag{21-a}$$

$$\frac{\partial\lambda}{\partial x}=0 \qquad \text{at} \quad x=L \tag{21-b}$$

$$\frac{\partial\lambda}{\partial y}=-2\sum_{i=1}^{m}(T-Y)\delta(x-x_i) \quad \text{at} \quad y=0 \tag{21-c}$$

$$\lambda=0 \qquad \text{at} \quad y=f(x) \tag{21-d}$$

By performing some algebraic manipulations one can reach the objective function gradient:

$$J'(x)=-\left(\frac{\partial\lambda}{\partial y}\frac{\partial T}{\partial y}\right)_{y=f(x)} \tag{22}$$

F. Convergence Criterion

Considering the significant fluctuations in the inverse approach which result from noises in input data, CGM does include a criterion which considers difference between temperatures as a measure to abort the algorithm, thus making the problem well-posed. This criterion is:

$$|T_i-Y_i|\approx\sigma_i \tag{23}$$

where σ_i is the standard deviation of measurement and is assumed to take on a value of $\sigma_i=\sigma$. By using this value in (6), the following relation is obtained for ε:

$$\varepsilon=\sum_{i=1}^{m}{\sigma_i}^2=m\sigma^2 \tag{24}$$

III. Computer Algorithm

An algorithm can be presented to aid in shape prediction using CGM along with the adjoint equation. The steps are outlined below:

1. Solve the direct heat conduction problem and evaluate values of T(x,y)
2. Analyze the convergence criterion
3. Solve the adjoint equation and evaluate values of γ(x,y)
4. Obtain objective function gradient and values of $J'(x)$
5. Evaluate conjugate coefficient $\gamma^n$and the direction of decrease
6. Solve the sensitivity equation for $\Delta f=P^n$and evaluate values of ΔT(x,y)
7. Evaluate the optimal step size, β^n
8. Evaluate the new boundary $\hat{f}^{n+1}(x)$and repeat the calculations from step 1

IV. Results and Discussion

In this section, function f(x) is predicted for a problem with sinusoidal boundary, with the aid of the temperature of some points on the boundary at y=0 being known.

In order to compare the results with those in a situation where measurement is reported with error, an error having normal distribution and zero mean-value with constant standard deviation is assumed for the data. The temperature with reporting error is assumed to have the form:

$$Y=Y_{exact}+\omega\sigma \tag{25}$$

where Y_{exact} results from the solution to the direct conduction problem for the precise boundary $f(x)$. σ is the value of standard deviation, while ω is the random variable produced by the DRNNOR sub-routine, present in the function library of FORTRAN.

A. Comparison of Three Versions of Conjugate Gradient Method in Predicting an Unknown Boundary

To investigate the ability of different versions of CGM, they are used to predict unknown sinusoidal boundary for the accurate measurement and zero-error ($\sigma=0.0$) situation. It should be noted that the mean relative error can be evaluated using the accurate and computed values of the unknown boundary, with the equation below:

$$ERR=\sum_{i=1}^{M}\left|\frac{f(x_i)-\hat{f}(x_i)}{f(x_i)}\right|\div M*100\% \tag{26}$$

In (26), M is the number of parameters predicted by the algorithm or, alternatively, the number of unknown points.

B. Sinusoidal Boundary

The function which is to be predicted for a sinusoidal boundary is

$$f(x)=1.5+0.8\sin\left(\frac{\pi x}{5}\right),\ \ 0\le x\le L \tag{27}$$

In all the cases dealt with, the geometric specifications and boundary conditions are: $L=10$, $T_0=100$ and $q_0=20$.

The number of boundary elements on either side of the region Ω is 3, while on the top and bottom boundaries, 20 elements are foreseen. The inverse analysis is based on the temperatures obtained using 21 heat sensors (m=21), placed $\Delta x=0.5$ apart.

Based on Figs. 2 and 3, the differences between the predicted boundary geometry using various versions of CGM are negligible. However, comparison of results set out in Tables I and II shows that even though the Polak-Ribiere version of CGM for higher iterations predicts the boundary more accurately than the other two versions, its performance in lower iterations doesn't fare well when compared to the Powell-Beale version which converges more quickly. The analyses which follow are all based on the Powell-Beale version of CGM.

TABLE I
COMPARISON OF THREE VERSIONS OF CGM IN PREDICTING THE BOUNDARY FOR PRESCRIBED CONVERGENCE RATE

Version	Initial Guess	ε	No. of Iterations	Objective Function	Mean Error(%)
Fletcher-Reeves	1.5	0.03	21	0.0267	2.5381
Polak-Ribiere	1.5	0.03	29	0.0241	2.3844
Powell-Beale	1.5	0.03	20	0.0235	2.5569

TABLE II
COMPARISON OF THREE VERSIONS OF CGM IN PREDICTING THE BOUNDARY FOR PRESCRIBED NUMBER OF ITERATIONS

Version	Initial Guess	ε	No. of Iterations	Objective Function	Mean Error(%)
Fletcher-Reeves	1.5	-	50	0.0138	2.0936
Polak-Ribiere	1.5	-	50	0.0035	1.7583
Powell-Beale	1.5	-	50	0.0091	2.2042

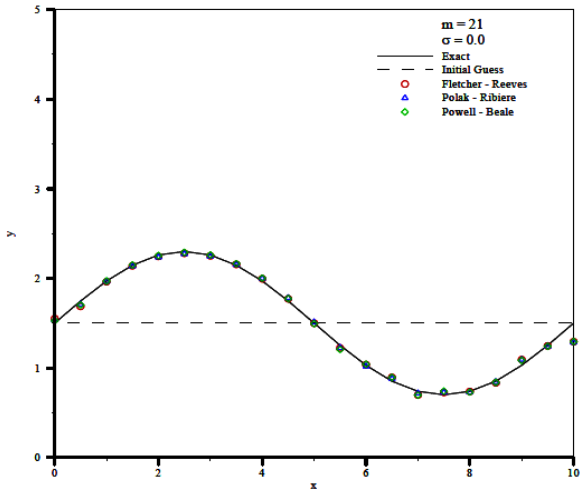

Fig. 2 Sinusoidal boundary predicted using three versions of CGM for σ=0.0 and ε=0.03

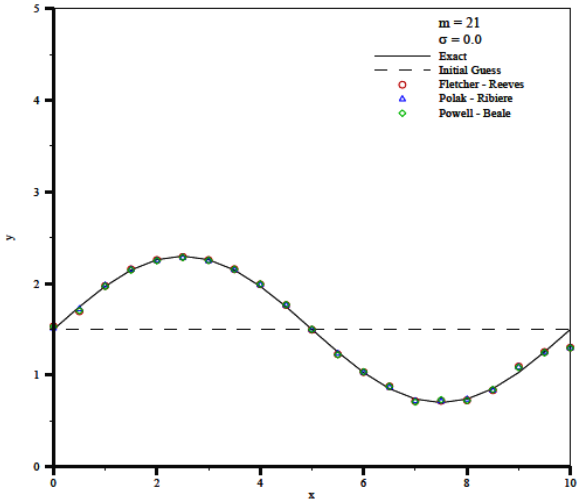

Fig. 3 Sinusoidal boundary predicted using three versions of CGM for σ=0.0 and 50 iterations

C. Study of the Effect of Reduction in Number of Sensors on Inverse Algorithm

Numerical analyses have been done to study the effect of reducing the number of sensors on the accuracy of prediction of the unknown boundary for the case of σ=0.0.

As shown in Table III, the predicted values for the inverse solution when m=11 have more error than the case of m=21. However, a closer look at Fig. 4 shows that there are no significant differences between the predicted boundaries in two cases.

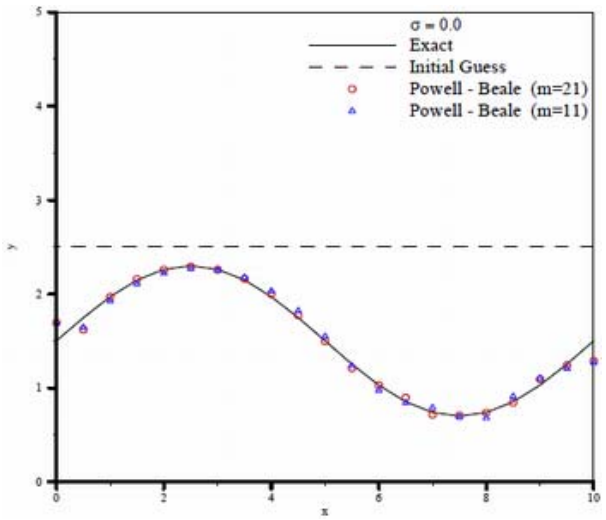

Fig. 4 Boundary predicted using third version of CGM for σ=0.0 with m=21 and m=11

TABLE III
EFFECT OF NUMBER OF SENSORS ON CONVERGENCE PARAMETERS OF THIRD VERSION OF CGM FOR σ=0.0

No. of Sensors	ε	No. of Iteration	Objective Function	Mean Error (%)
21	0.04	21	0.0379	2.8925
11	0.24	16	0.2365	4.4710

D. Study of the Effect of Measurement Errors on the Inverse Algorithm

One of the ways which can be used in studying the effect of measurement errors on the results obtained from the inverse algorithm is to add error to the temperatures evaluated using the direct algorithm. Here the standard deviation of temperature obtained for predicting the boundary for all the sensors used assumed to be $\sigma = 1.0$ and then the effect of simultaneously reducing the number of sensors while increasing measurement error has been studied.

Fig. 5 shows that the reduction in the number of sensors, coupled with an increase in error has not resulted in the error in the predicted data to intensify. That through the addition of error to the acquired data, it is not expected that the inverse algorithm reduces the value of objective function to much lower values, as well, data in Table IV show that the convergence rate increases.

TABLE IV
EFFECT OF SIMULTANEOUS INCREASE IN ERROR AND DECREASE IN NUMBER OF SENSORS ON THE CONVERGENCE PARAMETERS OF THIRD VERSION OF CGM

No. of Sensors	ε	No. of Iteration	Objective Function	Mean Error (%)
21	21	7	20.3769	4.6222
11	11	6	10.7691	7.8993

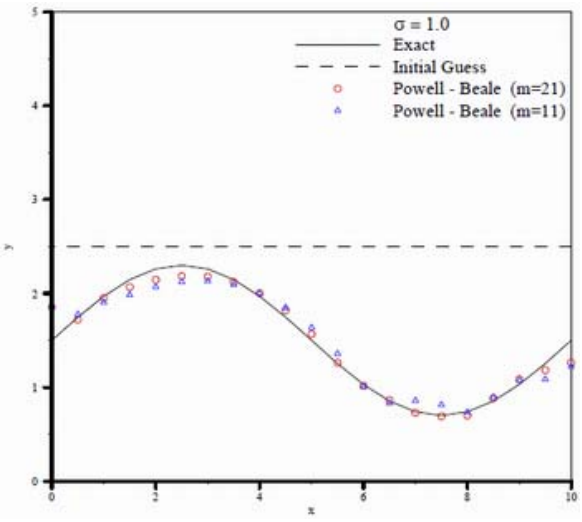

Fig. 5 Sinusoidal boundary predicted using third version of CGM for σ=1.0 with m=21 and m=11

The difference between the error present in this table and that of Table III provides that the error for evaluated values is of the same degree of those for input values, and the inverse algorithm, even in the presence of errors for input data, is able to predict the unknown boundary well.

V. CONCLUSION

Three different versions of Conjugate Gradient Method used in determining the unknown boundary geometry, which is one of the function determination inverse problems. The presented results clearly indicate that CGM utilizing the boundary elements method can predict the optimum profile conveniently, and the Powell-Beale version of CGM shows higher convergence rate and accuracy of the other ones. Also, the results obtained through this method are not sensitive to the measurement errors and the number of used temperature sensors.

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