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THE LEAST SQUARES METHOD: KANTOROVICH APPROACH

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Abstract — A version of the least squares method, when adjustable parameters in a trial solution are functions of an independent variable, is presented. Minimization of the least squares residual is done in the sense of the variational calculus. The procedure is applied on a few heat conduction problems. In one example an error estimate of the approximate solution is obtained.

NOMENCLATURE

u,	temperature;
U,	approximation to temperature distribution;
x, y,	position coordinates;
t,	time;
k,	heat source coefficient;
q,	adjustable parameter.

Greek symbols

α,	thermal diffusivity;
γ, β, τ,	parameters defined in text.

1. INTRODUCTION

APPROXIMATE analytical solutions to partial differential equations are useful when exact analytical solutions are either too difficult or impossible to obtain, or when the work to find a numerical solution cannot be justified. There are a lot of such methods, which have appeared in the technical literature in the past 30 years (see for example [1], [2] and [4–10]), for solving the heat conduction problems. One of them is the least squares method.

The basic point of the least squares method is a functional which is attached to the differential equation. The variational principle, based on this functional, is a true minimum principle [9] whose minimum (value of the functional) is zero. The corresponding Euler–Lagrange equation is of a higher order than the differential equation of the process, in our case the heat conduction equation. The equation is a combination between the heat conduction equation and its partial derivatives, but if the heat conduction equation is satisfied then the corresponding first variation is zero. If we substitute a trial solution of the heat conduction equation into the functional, then the functional measures the total squared residual by which the functional fails to satisfy the equation. Minimization of the square residual with respect to adjustable parameters in a trial solution is precisely the least squares method. When the parameters are undetermined constants the minimization can be straightforwardly escorted. According to Finlayson and Scriven [5], the direct extension of the least squares criterion is of doubtful significance when the parameters are a function of time, or some other independent variable. This problem is surpassed by Vujanovic and Baclic [6]. They selected, in a physical way, a group of parameters and minimized the functional with respect to them. However, in both papers [5] and [6], the functional is not minimized in the sense of variational calculus. Hence, the adjustable parameters are not calculated in the optimal way.

In this paper the least squares residual will be minimized in the sense of the variational calculus. Because the adjustable parameters are functions of an independent variable, the method presented here, is in some sense, the Kantorovich approach to the least squares method. The procedure is demonstrated on four heat conduction problems. According to the order of the differential equation, for finding the adjustable parameter, the procedure is unfamiliar with all other approximate methods.

2. BASIC EQUATIONS

Let us consider the following partial differential equation of the second order

$$G(u, u_x, u_t, u_{xx}, u_{tt}, u_{xt}, x, t) = 0, \quad \text{for} \quad x \in [x_0, x_1],\ t \in [t_0, t_1] \quad (1)$$
$$(u_t \equiv \partial u/\partial t, \dots),$$

whose solution u is a function of the independent variables x and t. So far we will assume that the corresponding boundary and initial conditions can be arbitrary. Mikhlin [9] has shown that the classical variational formulation for this equation is equivalent to minimizing the positive definite integral

$$I = \int_{t_0}^{t_1} \int_{x_0}^{x_1} [G(u, u_x, u_t, u_{xx}, u_{tt}, u_{xt}, x, t)]^2 \, dx \, dt, \quad (2)$$

where t_0, t_1, x_0 and x_1 are given values of the independent variables on the boundaries. Indeed, the first variation of the functional (2) is

$$\delta I = 2\int_{t_0}^{t_1}\int_{x_0}^{x_1} \delta u\left[G\frac{\partial G}{\partial u} - \left(G\frac{\partial G}{\partial u_t}\right)_t - \left(G\frac{\partial G}{\partial u_x}\right)_x + \left(G\frac{\partial G}{\partial u_{tt}}\right)_{tt} + \left(G\frac{\partial G}{\partial u_{xx}}\right)_{xx} + \left(G\frac{\partial G}{\partial u_{xt}}\right)_{xt}\right]\mathrm{d}x\,\mathrm{d}t$$
$$+ 2\int_{x_0}^{x_1}\left\{\delta u\left[G\frac{\partial G}{\partial u_t} - \left(G\frac{\partial G}{\partial u_{tt}}\right)_t\right] + \left[G\frac{\partial G}{\partial u_{tt}}\delta u_t + G\frac{\partial G}{\partial u_{tx}}\delta u_x\right]\right\}_{t_0}^{t_1}\mathrm{d}x$$
$$+ 2\int_{t_0}^{t_1}\left\{G\frac{\partial G}{\partial u_{xx}}\delta u_x + \delta u\left[G\frac{\partial G}{\partial u_x} - \left(G\frac{\partial G}{\partial u_{xx}}\right)_x - \left(G\frac{\partial G}{\partial u_{tx}}\right)_t\right]\right\}_{x_0}^{x_1}\mathrm{d}t. \quad (3)$$

Now, if equation (1) is satisfied ($G = 0$) then the first variation δI is equal to zero.

Remark I

This is valid for arbitrary boundary conditions which must be satisfied by equation (1).

Remark II

Here, the condition $\delta I = 0$ does not imply that G also must be zero, as is usual in other variational formulations. That is, the solution of (1) is not the only point at which the functional is stationary (2).

Remark III

The Euler–Lagrange equation that follows from (3) if $\delta I = 0$, is of the fourth order. The equation is a combination of equation (2) and its partial derivatives with respect to the independent variables.

Remark IV

The variational principle (2) is a true minimum principle. The corresponding minimal value of (2) is zero.

In our application of the variational principle (2) for obtaining an approximate solution of equation (1) we will need the first variation of the following functional

$$I = \int_{t_0}^{t_1} L(q,\dot{q},\ddot{q},t)\mathrm{d}t, \quad (\dot{q} \equiv \mathrm{d}q/\mathrm{d}t), \quad (4)$$

where q is the 'generalized coordinate' and L is the corresponding Lagrangian function. The first variation of (4) is

$$\delta I = \int_{t_0}^{t_1}\left(\frac{\partial L}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} + \frac{\mathrm{d}^2}{\mathrm{d}t^2}\frac{\partial L}{\partial \ddot{q}}\right)\delta q\,\mathrm{d}t + \left[\left(\frac{\partial L}{\partial \dot{q}} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \ddot{q}}\right)\delta q + \left(\frac{\partial L}{\partial \ddot{q}}\delta\dot{q}\right)\right]_{t_0}^{t_1}. \quad (5)$$

If we substitute a trial solution of equation (1) into the functional (2) then the functional measures the total squared residual by which the function fails to satisfy equation (1). We will assume that the trial solution is a known function of the independent variable x with the adjustable parameter (generalization to more parameters is straightforward) q as an unknown function of another independent variable t. Substituting the trial solution into (2) and performing integration with respect to the variable x, the functional (2) will take the form (4). Now, the so obtained functional will be minimized with respect to $q(t)$, in the sense of the variational calculus; that is $q(t)$ will be forced to satisfy the equation $\delta I = 0$, where δI is given by (5).

3. EXAMPLES

(A) As the first example we shall study the heat conduction problem through semi-infinite slab in one dimension (x-coordinate). The governing differential equation is

$$G \equiv \frac{\partial u}{\partial t} - \alpha\frac{\partial^2 u}{\partial x^2} = 0, \quad (6)$$

where u is the temperature, t is the time and α is the thermal diffusivity. The slab is initially at zero temperature and its face $x = 0$ is suddenly raised to temperature u_0. In accordance with the well-known notion of penetration depth we now define a quantity $q(t)$ called the penetration distance. Its property is that for $x > q(t)$ the slab is at the initial temperature and that there is no heat transfer beyond this distance. Hence the boundary conditions of the problems are,

$$u(0,t) = u_0, \quad u[q(t),t] = 0. \quad (7)$$

In order to obtain an approximate solution of the problem we will assume a temperature profile in the form

$$U = u_0\left[1 - \frac{x}{q(t)}\right]^2. \quad (8)$$

Substituting (8) into (6) and (2) and performing integration with respect to x, from $x_0 = 0$ to $x_1 = q(t)$, the equation (2) yields

$$I = 4u_0^2\int_0^{\infty}\left(\frac{\alpha^2}{q^3} - \frac{\alpha}{3}\frac{\dot{q}}{q^2} + \frac{\dot{q}^2}{30q}\right)\mathrm{d}t, \quad (9)$$

where we selected the time interval to be $t \in [0, \infty]$. If we want to minimize the functional (9) then the corresponding first variation must be zero. Hence from (9), (4) and (5) and assuming that $q(0) = 0$ [$\delta q(0) = 0$] and that $q(t)$ is not specified for $t = \infty$ [$\delta q(\infty) \neq 0$] we have the following differential equation

$$2q^3\ddot{q} - q^2\dot{q}^2 + 90\alpha^2 = 0 \quad (10)$$

and the next natural boundary condition

$$\frac{\dot{q}}{5q} - \frac{\alpha}{q^2} = 0, \quad \text{for } t_1 = \infty. \quad (11)$$

Remark I

The differential equation (10) is of the second order. All other approximate methods for the same problem and same trial function (8), give the first order differential equation for finding $q(t)$.

Remark II

Structure of the boundary condition (11) is the same as the differential equation for $q(t)$ that can be obtained by the Galerkin method.

Solution of equations (10) and (11), for $q(0) = 0$, is

$$q = (120)^{1/4}\sqrt{(\alpha t)}. \tag{12}$$

The graphical comparison between the exact solution $u = u_0[1 - \mathrm{erf}(z/2)]$ the present method solution $U = u_0[1 - z/(120)^{1/4}]^2$, Galerkin solution $U^G = u_0[1 - z/\sqrt{10}]^2$ and the integral method solution $U^I = u_0[1 - z/\sqrt{12}]^2$, where $z = x/\sqrt{(\alpha t)}$, is plotted on Fig. 1.

(B) Let us consider the temperature distribution in a finite insulated rod of the length 2. The ends of the rod are maintained at a constant temperature, say 0. Assume that the initial temperature is given by $u_0(1 - x^2)$, where u_0 is a constant. If the physical properties of the rod are independent of the temperature then the process of cooling is described by the differential equation (6) subject to the following initial and boundary conditions

$$u = u_0(1 - x^2) \quad \text{at } t = 0 \quad \text{for } x \in [-1, 1] \tag{13}$$

$$u = 0 \quad \text{at } x = \pm 1 \quad \text{for } t \geq 0. \tag{14}$$

Let us suppose the trial solution as

$$U = u_0 q(t)(1 - x^2). \tag{15}$$

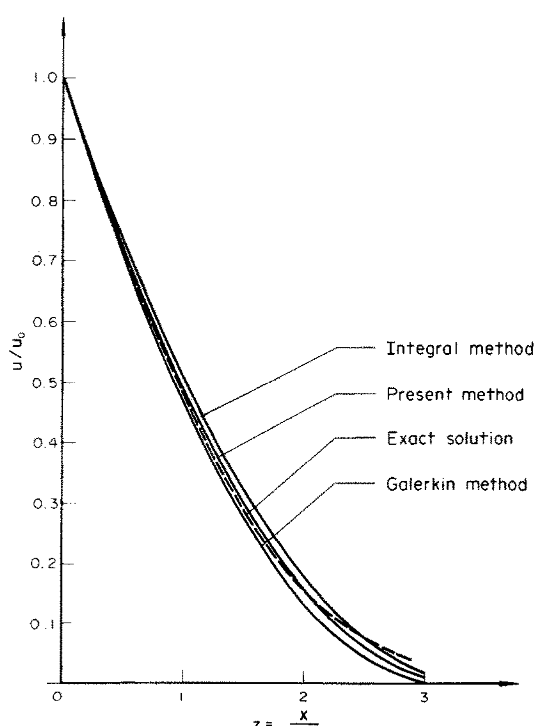

FIG. 1. Comparisons of various solutions for problem (A).

For $q(0) = 1$ the profile (15) will satisfy both the initial and the boundary conditions. Substituting (15) into (6) and (2) and performing integration with respect to x, from $x_0 = -1$ to $x_1 = 1$, we have

$$I = u_0^2 \int_0^{t_1} 8\left(\frac{2}{15}\dot{q}^2 + \frac{2}{3}\alpha q\dot{q} + \alpha^2 q^2\right)\mathrm{d}t, \tag{16}$$

where t_1 is a specified instant of time. Assuming that the adjustable parameter $q(t)$ is arbitrary for $t = t_1$, the condition $\delta I = 0$ in (5) yields the following differential equation

$$\ddot{q} - \frac{15}{2}\alpha^2 q = 0, \tag{17}$$

and the natural boundary condition

$$2\dot{q} + 5\alpha q = 0, \quad \text{for } t = t_1. \tag{18}$$

Remark I

The boundary condition (18) is of the same form as the differential equation for finding q which is obtained by the Local Potential method (see [2] p. 259). The solution of (17) and (18), for $q(0) = 1$, is

$$q = \mathrm{e}^{-\gamma\alpha t} + \frac{(4\gamma - 10)\sinh \gamma\alpha t}{\mathrm{e}^{2\gamma\alpha t_1}(5 + 2\gamma) + (2\gamma - 5)}, \quad \gamma = \sqrt{\frac{15}{2}}. \tag{19}$$

If we select a logical value for t_1 to be $t_1 = \infty$, then the solution (19) becomes $q = \mathrm{e}^{-\gamma\alpha t}$. This solution is in good agreement with the solution of the same problem obtained by the local potential method, where $\gamma = 5/2$. The values of the functional (16), which are certain measures of the error involved in approximate solution, are $I[\gamma = \sqrt{(15/2)}] = \alpha u_0^2 0.25452$ and $I(\gamma = 5/2) = \alpha u_0^2\, 0.26666$.

(C) Let us consider the same problem as (B) but with arbitrary initial temperature distribution $u(x, 0) = f(x)$ and with the heat conductivity linearly dependent on temperature. We take the length of the rod to be equal to π so that boundary conditions become

$$u(0, t) = 0, \quad u(\pi, t) = 0. \tag{20}$$

The differential equation describing the process becomes

$$G \equiv \frac{\partial u}{\partial t} - \alpha\frac{\partial}{\partial x}\left[(1 + \beta u)\frac{\partial u}{\partial x}\right], \tag{21}$$

where α and β are given constants. Choosing the trial function as

$$U = q(t) \sin x, \tag{22}$$

substituting this expression into (21) and (2) and integrating with respect to x from $x_0 = 0$ to $x_1 = \pi$, we have

$$I = \alpha \int_0^{\tau_1} \left[\frac{\pi}{2}\left(\frac{\mathrm{d}q}{\mathrm{d}\tau}\right)^2 + \left(\pi q + \frac{4}{3}\beta q^2\right)\frac{\mathrm{d}q}{\mathrm{d}\tau} + \frac{\pi}{2}q^2 + \frac{4}{3}\beta q^3 + \frac{\pi}{2}\beta^2 q^4\right]\mathrm{d}\tau, \tag{23}$$

where,

$$\tau = \alpha t, \tag{24}$$

and τ_1 is given value of the new independent variable. Again, the minimizing condition $\delta I = 0$, together with $\delta q(0) = 0$ and $\delta q(\tau_1) \neq 0$, yields the following differential equation

$$\frac{d^2 q}{d\tau^2} = q + \frac{4}{\pi}\beta q^2 + 2\beta^2 q^3, \tag{25}$$

and the natural boundary condition,

$$\frac{dq}{d\tau} + q + \frac{4}{3\pi}\beta q^2 = 0, \quad \text{for } \tau = \tau_1. \tag{26}$$

The solution of the equations (25) and (26) for $\tau_1 = \infty$ and $q(0) = q_0$ is given as:

(a) for small values of the parameter β

$$q = q_0 e^{-\tau} + \beta\frac{4}{3\pi}q_0^2 e^{-\tau}(e^{-\tau} - 1) + \beta^2 q_0^3 e^{-\tau}\left[\left(\frac{1}{4} + \frac{4}{3\pi^2}\right)e^{-2\tau} - \frac{32}{9\pi^2}e^{-\tau} - \frac{1}{4} + \frac{20}{9\pi^2}\right] + O(\beta^3); \tag{27}$$

(b) for arbitrary β which is larger than zero $\beta > 0$,

$$q = \frac{3\pi}{\beta[(9\pi^2 - 16)^{1/2}\sinh(\tau + C_1) - 4]}, \tag{28}$$

where,

$$C_1 = \operatorname{arcsinh}\frac{2 + \frac{8\beta}{3\pi}q_0}{\frac{2\beta}{3\pi}q_0(9\pi^2 - 16)^{1/2}}. \tag{29}$$

We note that the initial value q_0 can be found by minimizing the initial square residual of the form

$$J = \int_0^\pi [u(x,0) - q_0 \sin x]^2 dx, \tag{30}$$

with respect to q_0. This standard procedure for finding q_0 was applied previously (see for example [8]). Applying the condition $\partial J/\partial q_0 = 0$, we have,

$$q_0 = \frac{2}{\pi}\int_0^\pi f(x)\sin x\, dx, \tag{31}$$

where $u(x, 0) = f(x)$ is given initial condition.

(D) As a last example we consider the problem of determining the stationary temperature field in a plate with, on one coordinate linearly dependent, heat sources. Namely, we take

$$G \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - ky = 0, \tag{32}$$

where k = constant. Also we choose

$$u = 0 \quad \text{for } (x, y) \in C, \tag{33}$$

where C is the boundary of the plate defined by $x = \pm a$ and $y = \pm b$. The differential equation (32) with the boundary conditions (33) also arises in the elasticity theory. In that context u represents the stress function for the bending of rectangular beams (see [11], Section 124).

Let us take the approximate solution to the problem (32), (33) in the form

$$U = (x^2 - a^2)q(y), \tag{34}$$

where $q(y)$ is a function to be determined by minimizing (2). Substituting (34) into (2) and performing the integration with respect to x from $x = -a$ to $x = a$, the equation (2) becomes

$$I = 2a\int_{-b}^{b}\left[\frac{8}{15}a^4 q''^2 + \frac{4}{3}a^2 kyq'' - \frac{8}{3}a^2 qq'' + 4q^2 - 4kyq + k^2y^2\right]dy. \tag{35}$$

The Euler–Lagrange equation for the functional (35) is

$$\frac{4}{15}a^4 q^{iv} - \frac{4}{3}a^2 q'' + 2q - ky = 0, \tag{36}$$

while the natural boundary conditions are

$$q(y = b) = q(y = -b) = 0,$$
$$\frac{4}{15}a^2 q'' + ky - 2q = 0 \quad \text{for } y = \pm b. \tag{37}$$

Remark I

The boundary conditions $(37)_2$ are of the same form as the differential equation for finding q by the Galerkin method. The solution to the equation (36) with the boundary conditions (37) is

$$q = C_1 \cosh\frac{n}{a}y \sin\frac{m}{a}y + C_2 \sinh\frac{n}{a}y \cos\frac{m}{a}y + \frac{k}{2}y, \tag{38}$$

where $n = 1.61842$, $m = 0.345407$ and where C_1 and C_2 are constants that can be easily determined for specified a, b and k. If we take $a = b = 1$ and $k = 0.2$, then $C_1 = -0.01482$, $C_2 = -0.03808$ so that the approximate solution to the problem (32), (33) becomes

$$U = (x^2 - 1)[-0.01482\cosh 1.61842y \sin 0.345407y - 0.03808\sinh 1.61842y \cos 0.345407y + 0.1y]. \tag{39}$$

For the differential equation (32) an error estimate may be constructed, based on the value of the functional (2). To do this, we define the error δu as

$$\delta u = U - u, \tag{40}$$

where U is approximate and u exact solution to the boundary value problem (32), (33). Expressing u in (2) by (40) we get

$$I = \int_{-b}^{b}\int_{-a}^{a}\left[\frac{\partial^2 \delta u}{\partial x^2} + \frac{\partial^2 \delta u}{\partial y^2}\right]^2 dx\, dy. \tag{41}$$

The Fourier series corresponding to δu can be written as

$$\delta u = \sum_n \sum_m C_{nm} \Phi_{nm}(x, y), \tag{42}$$

where C_{nm} are constants (Fourier coefficients) and Φ_{nm} are solutions of the following spectral problem

$$\frac{\partial^2 \Phi_{nm}}{\partial x^2} + \frac{\partial^2 \Phi_{nm}}{\partial y^2} + \lambda_{nm}^2 \Phi_{nm} = 0. \tag{43}$$

$$\Phi_{nm} = 0 \quad \text{for } (x, y) \in C. \tag{44}$$

Substituting (42) into (41) and using (43) and Parseval's equation [12] we get the following estimate

$$\| \delta u \|_{L_2} \leq \left\{ \frac{I}{(\lambda_{nm}^4)_{\min}} \right\}^{1/2}. \tag{45}$$

In (45) we used $(\lambda_{nm}^4)_{\min}$ to denote the smallest eigenvalue of the spectral problem (43), (44) and

$$\| \delta u \|_{L_2} = \int_{-b}^{b} \int_{-a}^{a} (\delta u)^2 \, dx \, dy. \tag{46}$$

For the specific case when $a = b = 1$ and $k = 0.2$, approximate solution (39) gives, when substituted in (2) $I = 0.006515$. Also $(\lambda_{nm}^2)_{\min} = 2\pi^2$ so that (45) becomes

$$\| \delta u \|_{L_2} \leq 0.004089. \tag{47}$$

4. CONCLUSIONS

A method, based on the least square residual, for finding approximate solutions of heat conduction problems, has been presented in this paper. It resembles Kantorovich's method since differential equations are obtained for finding adjustable parameters. In Kantorovic's method these differential equations are the necessary conditions for the minimum of the variational integral, while in the method presented here they are a necessary and sufficient condition for the minimum of the square residual. Therefore the value of the integral of the square residual (2) is minimum on the approximate solution determined by the present method, when compared with other approximate solutions of the same type. The differential equation for determining the adjustable parameter by the present method is always of the higher order than the corresponding equations in other methods. In the analyzed problems the natural boundary conditions have the same structure as the differential equations for finding the adjustable functions by other methods [in example (A) Galerkin, in example (B) local potential and in example (D) Galerkin method]. The non-linear heat conduction problem of this method reduces to the corresponding non-linear two point boundary value problem.

In comparison with other methods the results obtained here are in good agreement.

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LA METHODE DES MOINDRES CARRES: APPROCHE DE KANTOROVICH

Résumé—On présente une version de la méthode des moindres carrés dans laquelle les paramètres ajustables sont fonctions d'une variable indépendante. La minimisation du résidu des moindres carrés est faite dans le sens du calcul variationnel. La procédure est appliquée à quelques problèmes de conduction thermique. Dans un exemple, on obtient une estimation de l'erreur dans la solution approchée.

DIE METHODE DER KLEINSTEN QUADRATE: VORGEHEN NACH KANTOROVICH

Zusammenfassung — Es wird eine Version der Methode der kleinsten Fehlerquadrate beschrieben, bei der die anzupassenden Parameter einer Versuchslösung Funktionen einer unabhängigen Variablen sind. Die Minimierung der Fehlerquadratsumme wird im Simme der Variationsrechnung durchgeführt. Das Verfahren wird auf einige Wärmeleitungsprobleme angewendet. Für ein Beispiel wird eine Fehlerabschätzung der Näherungslösung angegeben.

МЕТОД НАИМЕНЬШИХ КВАДРАТОВ — ПОДХОД КАНТОРОВИЧА

Аннотация — Предложен вариант метода наименьших квадратов в случае, когда подгоночные параметры в пробном решении являются функциями независимого переменного. Минимизация невязки осуществляется средствами вариационного исчисления. Метод проверен на нескольких задачах теплопроводности. В одном из примеров получена оценка погрешности приближенного решения.