International Journal of Applied Engineering Research ISSN 0973-4562 Volume 17, Number 4 (2022) pp. 422-426
 https://dx.doi.org/10.37622/IJAER/17.4.2022.422-426

Calculus of Variations and Application of Rayleigh – Ritz Method in Heat and Mass Transfer Problems

P. S. Basak
Director, Gradient Wire Products Pvt Ltd

Abstract:

Calculus of variations provides a very useful mathematical tool to solve differential equations related to numerous physical problems. Utilizing variational principles, Rayleigh – Ritz method effectively converts boundary value problems into a problem of minimizing functional and effectively applied in heat and mass transfer problems. The use of a trial function to solve this method is thoroughly elaborated for an eigenvalue problem with relevant convergence. A careful choice of field equation along with boundary conditions is the key to obtaining a successful solution and adequate insight into the physics of the problem.

Keywords: Functional, BVP, Eigenvalue, Heat and mass transfer

1. INTRODUCTION:

The calculus of variations is an extremely powerful and elegant technique. Variational principles are of great scientific significance as they provide a unified approach to various mathematical and physical problems and yield fundamental exploratory ideas [1-5]. This method is concerned with changes in functionals. Functional means a quantity whose values are determined by one or several functions. A functional is a correspondence between a function in some class and the set of real numbers and is often expressed as definite integrals involving functions and their derivatives. The calculus of variations is a field of mathematical analysis that uses variations, which are small changes in functions and functional to find maxima and minima of functional. A wide range of problems can be treated in this method.

Rayleigh Ritz's method [1, 3, 5] is based on the idea of utilizing the equivalence between boundary value problem (BVP) of partial differential equations on the one hand and problems of the calculus of variations on the other hand for numerical calculation of solutions. This method involves substitution for variational problems into simpler approximating extremum problems in which a finite number of parameters need to be determined. There can be multiple fields of application of this method such as in mechanics, fluid dynamics, heat and mass transfer, semiconductors, etc [2, 5, 6]. The objective of this paper is to evolve an approximate method of solving complex heat or mass transfer equations by converting them into an eigenvalue problem.

2. BASIC OF VARIATIONAL CALCULUS: :

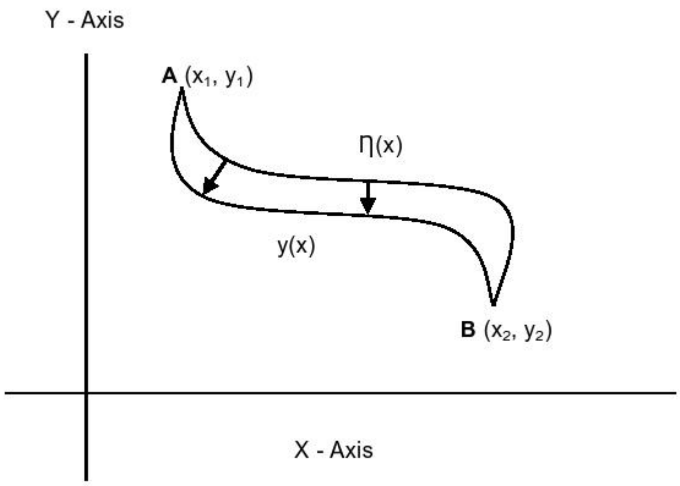

Fig.1 – y(x) is extremal and η(x) is an arbitrary function

Calculus of variations involves in solving a problem of minimum path in between points A and B such that y(x) is extremal. In order to do this, it is essential to form a functional as,

$$\phi = \int_{x_1}^{x_2} F(x, y, y')dx \qquad \ldots\ldots(1)$$

With boundary condition;

$$y(x_1) = y_1 \; \& \; y(x_2) = y_2 \qquad \ldots\ldots(2)$$

Here, ϕ is a functional because it is a function of functions.

It is now considered that y(x) is extremal which makes ϕ stationary and satisfies above boundary conditions. Another arbitrary function η(x) is introduced such that $\eta(x_1) = \eta(x_2) = 0$. This is means that η(x) is zero at the boundaries and both y(x) and η(x) have continuous derivatives. It is also defined that

$$\bar{y}(x) = y(x) + \epsilon\eta(x) \;\ldots\ldots\ldots\ldots(3)$$

$\bar{y}(x)$ therefore satisfies all boundary conditions as y(x) and $\bar{y}(x)$ represents a family of curves [3, 4].

From equation (3), we can get derivative as;

$$\bar{y}'(x) = y'(x) + \epsilon\eta'(x) \;\ldots\ldots\ldots\ldots(4)$$

Again from equation (3),

$$\frac{\partial\bar{y}}{\partial\epsilon} = \eta(x) \quad \ldots\ldots(5), (\text{as } y(x) \text{ is not a function of } \epsilon)$$

From equation (4), it may be obtained as,

$$\frac{\partial\bar{y}'}{\partial\epsilon} = \eta'(x) \quad \ldots\ldots(6)$$

Now the functional for the path $\bar{y}(x)$ can be;

$$\phi = \int_{x_1}^{x_2} F(x,\bar{y},\bar{y}')dx \quad \ldots\ldots \quad (7)$$

If y(x) is actual path and we know ϕ depends only on ϵ, it is essential to make ϕ stationary set or minimize ϕ with respect to ϵ. i.e.,

$$\left.\frac{d\phi}{d\epsilon}\right|_{\epsilon=0} = 0 \quad \ldots\ldots(8)$$

$$=> \left.\frac{d}{d\epsilon}\right|_{\epsilon=0}\left(\int_{x_1}^{x_2} F(x,\bar{y},\bar{y}')dx\right) = 0 \ldots\ldots(9)$$

By applying Leibnitz rule, $\frac{d}{d\epsilon}$ can go inside the integral. Therefore, equation (9) can be written as,

$$\int_{x_1}^{x_2} \frac{d}{d\epsilon}[F(x,\bar{y},\bar{y}')]\bigg|_{\epsilon=0} dx = 0$$

$$=> \int_{x_1}^{x_2}\left(\frac{\partial F}{\partial x}\frac{\partial x}{\partial\epsilon} + \frac{\partial F}{\partial\bar{y}}\frac{\partial\bar{y}}{\partial\epsilon} + \frac{\partial F}{\partial\bar{y}'}\frac{\partial\bar{y}'}{\partial\epsilon}\right)\bigg|_{\epsilon=0} dx = 0 \ldots\ldots(10)$$

Since x is not a function of ϵ, then $\frac{\partial x}{\partial\epsilon} = 0$

$$\therefore \int_{x_1}^{x_2}\left(\frac{\partial F}{\partial\bar{y}}\frac{\partial\bar{y}}{\partial\epsilon} + \frac{\partial F}{\partial\bar{y}'}\frac{\partial\bar{y}'}{\partial\epsilon}\right)\bigg|_{\epsilon=0} dx = 0 \quad \ldots\ldots(11)$$

We put the value of $\frac{\partial\bar{y}}{\partial\epsilon}$ and $\frac{\partial\bar{y}\prime}{\partial\epsilon}$ from equation (5) and (6) in the equation (11).

$$\therefore \int_{x_1}^{x_2}\left(\frac{\partial F}{\partial\bar{y}}\eta + \frac{\partial F}{\partial\bar{y}'}\eta'\right)\bigg|_{\epsilon=0} dx = 0 \quad \ldots\ldots(12)$$

As ϵ approaches zero, $\bar{y}(x)$ approaches to y(x) and $\bar{y}$'(x) approaches to y'(x). So, equation (12) may be written as follows;

$$\int_{x_1}^{x_2}\left(\frac{\partial F}{\partial y}\eta + \frac{\partial F}{\partial y'}\eta'\right)dx = 0 \quad \ldots\ldots \quad (13)$$

Now the second term of left hand side can be integrated by parts. Therefore the equation (13) can be written as,

$$\int_{x_1}^{x_2}\frac{\partial F}{\partial y}\eta dx + \frac{\partial F}{\partial y'}\int_{x_1}^{x_2}\eta' dx - \int_{x_1}^{x_2}\left[\frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)\int\eta' dx\right]dx \quad = 0$$

$$=> \int_{x_1}^{x_2}\frac{\partial F}{\partial y}\eta dx + \left[\frac{\partial F}{\partial y'}\eta\right]_{x_1}^{x_2} - \int_{x_1}^{x_2}\eta\frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)dx = 0 \quad \ldots\ldots(14)$$

Since, η = 0 at x_1 and x_2, equation (14) can be written as;

$$\int_{x_1}^{x_2}\frac{\partial F}{\partial y}\eta dx - \int_{x_1}^{x_2}\eta\frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)dx = 0$$

$$=> \int_{x_1}^{x_2}\left[\frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)\right]\eta dx = 0 \quad \ldots\ldots \; (15)$$

As η has been chosen as an arbitrary function; the only way equation (15) can be zero when

$$\left[\frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)\right] = 0 \quad \ldots\ldots \; (16)$$

Equation (16) is Euler – Lagrange equation. This means that y(x) must satisfy the equation (16), if it is the actual solution [1-3, 5].

3. RAYLEIGH – RITZ METHOD:

This method has been developed using calculus of variations principle to solve differential equation. It is a direct numerical method of approximating eigenvalue, originated in the context of solving physical boundary value problems.

A second order differential equation of following form is considered.

$$\frac{d}{dx}(py') - qy - f = 0 \quad \ldots\ldots \; (17)$$

If Y(x) is the solution of equation (17), then functional ϕ would be [1];

$$\phi = \int_{x_1}^{x_2}[pY'^2 + qY^2 + 2fY]dx \quad \ldots\ldots \quad (18)$$

Then, functional ϕ should be minimum for Y(x) to be the solution for equation (17). For the heat transfer problems, the following field equation may be written as;

$$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2} \quad \ldots\ldots \; (19)$$

Where, T, t, x and k are temperature, time, distance and heat transfer coefficient. The method of separation of variables often leads to transform partial differential equations to ordinary differential equations which usually form an eigenvalue problem such as;

$$T = A(t)Y(x) \quad \ldots\ldots \quad (20)$$

$$\text{and hence,}\frac{1}{k}\frac{A'(t)}{A(t)} = \frac{Y''(x)}{Y(x)} = -\lambda \quad \ldots\ldots\ldots \quad (21)$$

Thus the following differential equation (22) can be derived under boundary conditions (23);

$$Y'' + \lambda Y = 0 \quad \ldots\ldots \quad (22)$$

$$\mathrm{Y = 0, at\ x = -1\ and\ Y = 0\ at\ x = 1, where\ -1 \le x \le 1} \quad .... \ (23)$$

This problem may be replaced by problem of minimization of functional by following method. First y(x) is considered to be actual solution of differential equation (22). Then it may be written as;

$$\int_{-1}^{1} \left(\frac{d^2y}{dx^2} + \lambda y \right) \eta dx = 0 \quad ......(24)$$

Here, η is an arbitrary function of x which vanishes at x = -1 and at x = 1. Integration by parts is applied to the first term of left hand side of equation (24).

$$=> \left[\eta \frac{dy}{dx} \right]_{-1}^{1} - \int_{-1}^{1} \left(\eta' \frac{dy}{dx} \right) dx + \lambda \int_{-1}^{1} \eta y dx = 0 \quad ......(25)$$

The first term of equation (25) will be zero as η vanishes at x = -1 and at x = 1. Therefore the equation (25) can be written as;

$$=> -\int_{-1}^{1} \left(\frac{d\eta}{dx} \frac{dy}{dx} \right) dx + \lambda \int_{-1}^{1} \eta y dx = 0 \quad ......(26)$$

$$=> \int_{-1}^{1} \left(\frac{d\eta}{dx} \frac{dy}{dx} \right) dx - \lambda \int_{-1}^{1} \eta y dx = 0 \quad ....(27)$$

Now, if the arbitrary function η(x) approaches y(x) then the functional can be expressed as;

$$\phi = \int_{-1}^{1} \left(\frac{dy}{dx} \right)^2 dx - \lambda \int_{-1}^{1} y^2 dx$$

$$=> \phi = \int_{-1}^{1} \left[\left(\frac{dy}{dx} \right)^2 - \lambda y^2 \right] dx$$

$$\therefore \phi = \int_{-1}^{1} \left[y'^2 - \lambda y^2 \right] dx \quad ..... \ (28),$$

under the samecondition.

Hence, the solution of the problem of boundary value differential equation can be transformed to minimization of functional ϕ of equation (28)

Interestingly, a generalized method [5] may be easily developed for second order differential equation of following form;

$$a(x)Y'' + b(x)Y' + c(x)Y = f(x) \quad ...... \quad (29)$$

then the functional will be;

$$\phi = \int_{x_1}^{x_2} [F(x, y, y'']dx$$

$$\phi = \int_{x_1}^{x_2} \left[P(x)Y'^2 + Q(x)Y^2 + R(x)Y \right] dx \quad ...... \quad (30)$$

The function F is established in such a way that it should satisfy Euler – Lagrange equation (16). For the functional ϕ it is possible to find P(x), Q(x) and R(x) such as;

$$P(x) = e^{\int \frac{b(x)}{a(x)} dx} \quad .....(31A)$$

$$Q(x) = -\frac{c(x)}{a(x)} P(x) \quad .... \ (31B)$$

$$R(x) = \frac{2f(x)}{a(x)} P(x) \quad ...... \ (31C)$$

In this method, a trial function is assumed ω(x) which should be continuous in the range and satisfy essential boundary conditions. A trial function can be a polynomial as;

$$\omega(x) = a_1\psi_1(x) + a_2\psi_2(x) + \dots + a_n\psi_n(x) \quad .... \ (32)$$

Here, a_1, a_2, ..., a_n are unknown coefficients and ψ_1, ψ_2, ..., ψ_n are assumed functions. It is to be noted that the assumed functions ψ_i should satisfy the essential boundary conditions and be continuous in the range of x. With this trial function, the functional ϕ is calculated. In order to get nearly exact solution, it is necessary to differentiate ϕ with respect to coefficients of trial function such as a_1, a_2, ..., a_n and forced to zero. i.e.,

$$\frac{d\phi}{da_1} = \frac{d\phi}{da_2} = \dots = \frac{d\phi}{da_n} = 0 \quad ......(33)$$

This treatment would result in adjusting a_1, a_2, ..., a_n itself in such a way that ω(x) gives almost exact solution. It should be noted that one must take sufficiently large number of coefficients of ω(x) so that the solution converges and approaches to very near to the actual solution [6].

4. RESULTS & DISCUSSIONS:

Solving the equation (22) under the boundary conditions (23) by Rayleigh – Ritz method, a trial function with one term is first considered as;

$$\omega(x) = a_1(1 - x^2) \quad ....(34)$$

The results of approximate solution of eigenvalue with one and two terms are compared with exact solution and illustrated in the following table 1.

Table 1: Comparison of λ obtained from Rayleigh Ritz method with exact solution.

Method	Functions	Value of λ
Rayleigh Ritz with one term	$(1 - x^2)$	2.50
Rayleigh Ritz with two terms	$(1 - x^2), x^2(1 - x^2)$	2.46740
Exact solution	$\{(n - 1/2)\pi)\}^2$, n=1, 2, 3, ...	2.46744

The evaluation of λ with other trial functions satisfying the essential boundary conditions is also carried out. It is interesting to point out that calculation with other trial

International Journal of Applied Engineering Research ISSN 0973-4562 Volume 17, Number 4 (2022) pp. 422-426
© Research India Publications. https://dx.doi.org/10.37622/IJAER/17.4.2022.422-426

functions leads to identical the value of λ. However, the rate of convergence differs with the choice of trial function. It is evident from the figure 2 that trial function with $(1-x^2)^{i+1}, i = 1, 2, ...$ has rate of convergence reasonably slow, whereas, functions with $x^{2i-2}(1-x^2), i = 1, 2, ...$ converges within 2 terms. The speed of convergence for some specific functional is available in the literature [1, 2]. However, these estimates are so complicated that they are impractical in the concrete situation [5]. For this reason, it is easier to calculate $y_n(x)$ and $y_{n+1}(x)$ and compare the results. If the values of two successive terms coincide within the limits of desired accuracy (usually less than 0.01%) then the solution of the variational problem is taken as $y_n(x)$ and the corresponding value of λ is accepted. Otherwise, this process is repeated till the values agree within the desired accuracy.

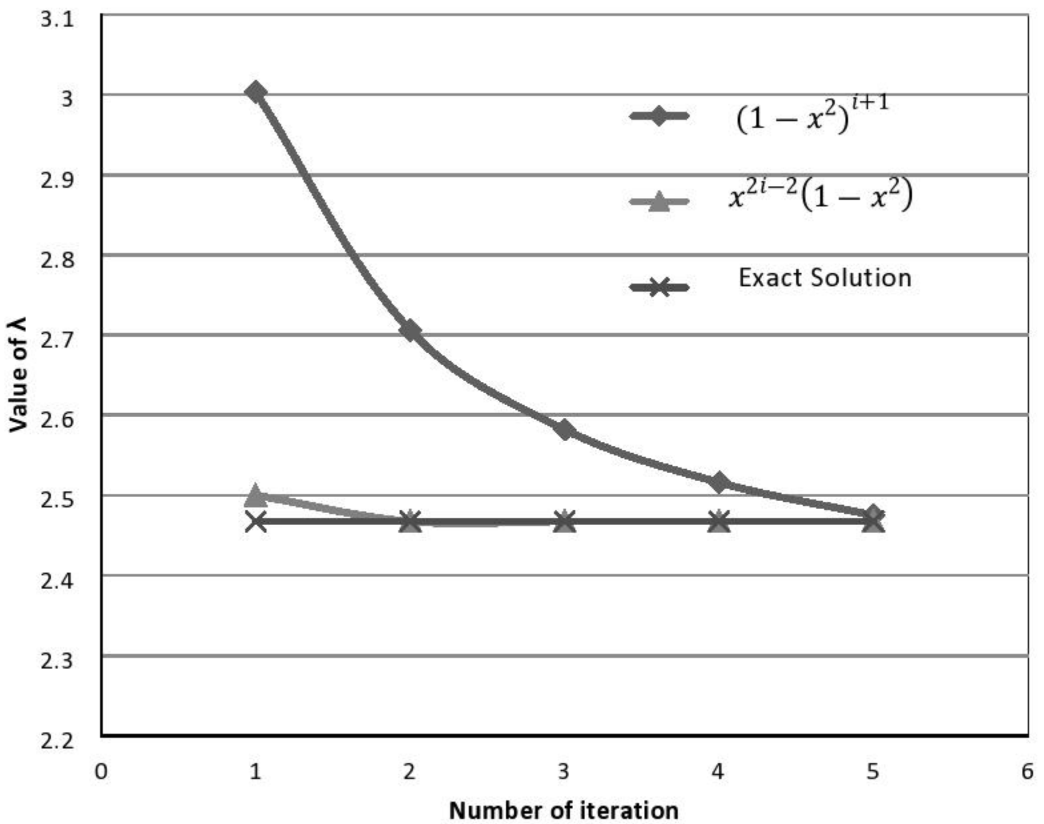

Fig. 2 – Dependence of Convergence on nature of trial function

It is evident from table 1 that with only two terms the solution is approaching near exact solution with less than 0.01% error. This shows the power of this method and its diverse range of applications. It is to be noted that in many occasions, it is not possible to derive the exact solution due to the complexity of the problem and this method can be the only reliable solution to those problems.

5. SUMMARY:

There can be several applications of the Rayleigh Ritz's method in the metallurgical engineering and materials science area. Applications in the field of heat and mass transfer, extractive processing, etc may be the potential areas where this method can be used. This method is extremely useful when the field equation along with boundary conditions makes the problem very complex and an exact solution is not possible. It is important to point out that the selection of a proper field equation with careful choice of boundary conditions is the key to the successful solution. Extreme care should be taken in the physics of the problem at the time of choosing field equation and boundary conditions which will lead to near accurate results and give an insight into the phenomenon. It is shown that the test of convergence can be carried out by calculating two successive terms. If the values coincide within the limits of accuracy, then the solution can be taken. This method is mathematically not rigorous and can be sufficiently reliable.

Discretization of this method can also be used in the advanced stage which involves the division of the range into 10 or 20 equal parts and solving the equation to obtain further accurate results. This is the basis of finite element method.

REFERENCES

[1] Kantorovich L. V. and Krylov V. I., 1964, Approximated Methods of Higher Analysis, Interscience Publishing, New York.

[2] Finlayson B. A., 1972, The Method of Weighted Residuals and Variational Principles, Academic Press, New York.

[3] Kot M., 2014, Chapter 4: Basic Generalization – A First Course in Calculus of Variations, American Mathematical Society. ISBN: 978-1-4704-1495-5.

[4] Storaski T., Nakasona Y. and Yoshimoto S., 2018, Chapter 1: Fundamentals of Finite Element Method, Engineering Analysis with ANSYS Software, Elsevier Publishing. ISBN: 978-0-0810-2164-4.

[5] Gupta A. S., 1997, Calculus of Variations with Applications, PHI Publishing, New Delhi. ISBN: 978-81-203-1120-6

[6] Basak P. S., Gupta A. S. and Pabi S. K., 1991, Solute distribution during steady state cellular growth, Metallurgical Trans., Vol. 22A,1991, p.3035. DOI:10.1007/BF02650264