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A Survey of Direct Methods for Solving Variational Problems

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ABSTRACT

This study presents a comparative survey of direct methods for solving Variational Problems. This problems can be used to solve various differential equations in physics and chemistry like Rate Equation for a chemical reaction. There are procedures that any type of a differential equation is convertible to a variational problem. Therefore finding the solution of a differential equation is equivalent to solving its related variational problem. The objective of this paper is to describe the major direct methods that have been developed over the years for solving these types of problems. In this paper we focus on using orthogonal polynomials and triangular functions as basis functions. Each method needs computing operational matrices and some other parameters which are presented as well. Several numerical examples are then included to demonstrate the accuracy and applicability of the reviewed methods. Computational concerns are then discussed to provide a guideline to the preferred and the most accurate method.

Keywords: Variational problems; Direct methods; Operational matrix

INTRODUCTION

Many problems of mathematical physics and chemistry are related to the calculus of variations. Problems in control theory, minimum path of light pulse or free fall of a particle in a curved Riemannian space are afew examples.Calculus of variations mostly involves seeking the extremum of an integral involving a function of functions called functional.

$$J(y(x)) = \int_a^b F(x, y(x), y'(x))\,dx \qquad (1)$$

The variational problems are concerned with finding an extremizing function $y(x)$ for which the functional $J(y(x))$ has an extremum. The well-known Euler-Lagrange equation in the calculus of variations [1] leads to a differential equation which is generally challenging to solve.

$$F_y - \frac{d}{dx}F_{y'} = 0 \qquad (2)$$

Also the differential equation (2) could be converted to a functional like (1), so the problem of solving a differential equation like Rate Equation for a chemical reaction is equivalent to finding the extremum of an integral involving a functional.

Functional (1) in this case illustrates a simplified one, but in general the problem may include more dependent variables or higher order derivatives. In such cases the

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corres ponding equation generates several differential equations or higher ordersones [2,3], where applying a numerical direct method is recommended. The Ritz and Galerkin methods [1,2] are the most commonly used techniques in the direct methods of solving variational problems. The main approach of a direct method for solving a variational problemis to convert the problem of extremization of the functional into a problemof solving a finite number of algebraic equations.The direct methods usually have four steps [4]:

(i) Representing the candidate function in the functional as a linear combination of basis functions with coefficients to be determined.

(ii) Calculating the operational matrix and other required relations to eliminate the integral operation.

(iii) Applying the necessary condition for extremization.

(iv)Solvingan algebraic system of equations obtained from the previous steps to evaluate the coefficients.

Accuracy and efficiency of the method is dependent on the selection of the basis functions. Asuitable candidate is the orthogonal function which has received considerable attentions for approximating the solutions in the variational problems. Orthogonality provides an acceptable optimization in the computational space as discussedlater in this paper. There are three classes of orthogonal functions[5];the firstincludes sets of piecewise constant basis functions (e.g. Walsh functions and Block-Pulse), the second consists of sets of orthogonal polynomials (e.g. Laguerre and Legendre) and the third is the set of sine-cosine functions (e.g. Fourier series).In this paper we mostly focus on the second and third class. Orthogonal polynomials are defined on the general interval a ≤ x ≤ b which imposes limitations for the systems or functions that vanish outside of a short interval of time or space [6]. In addition, since most of the problems in quantum and control theory are defined in the interval (0, 1) we use shifted polynomials.

This paper is organized as follows. In section2 we first describe direct methods in solving variational problems in general. Then we review Taylor method [7], Chebyshev method [8], Legendre method [9], Laguerre method [10], Bernstein method [4] and Fourier series method[11]. In section 3, we provide three examplesand solve each using all the six methods. Finally we analyze and compare the results of the mentioned methods in section 4.

CONSTRUCTION OF DIRECT METHODS

The main approach in the direct method is to represent the candidate function as a linear combination of basis functions. The candidate function is normally the function with the highest order of derivative. For example in (1), $y'(x)$ can be expressed approximately as:

$$y'(x) \approx \sum_{i=0}^{m-1} c_i B_i = C^T B \tag{3}$$

where, vector C includes coefficients that have to be determined and vector B includes basis functions:

$$C = [c_0, c_1, ...c_{m-1}]^T, B = [B_0, B_1, ...B_{m-1}]^T \tag{4}$$

Other itemslike x and $y(x)$ could be calculated as follow:

$$\begin{aligned} y(x) &= \int_0^x y'(x')\,dx' + y(0) » C^T \int_0^x B\,dx' + y(0) \\ &= C^T P B + y(0) \end{aligned} \tag{5}$$

$$x = d^T B \tag{6}$$

P is a square matrix called *Operational matrix* which needs to be calculated and d is a vector that its product to B generates x. By substituting (3), (5) and (6)in (1), the functional becomes a function of c_i:

$$J(y(x)) = J(c_0, c_1, \ldots c_{m-1}) \quad (7)$$

Thus the original extermination problem of the functional in (1) turns to the extermination of a function of a finite set of coefficients. Hence:

$$\frac{\partial J}{\partial c_i} = 0,\ i = 0,1,\ldots,m-1. \quad (8)$$

To apply boundary conditions a Lagrange multiplier technique could be employed. The first method we review is the Taylor method.

Taylor method

In the Taylor method $y'(x)$ is defined as follow:

$$y'(x) = C^T B = [c_0, c_1, \ldots c_{m-1}] \times [1, x, \ldots x^{m-1}]^T \quad (9)$$

Consequently $y(x)$ could be calculated using (5):

$$y(x) \approx C^T P B + y(0)$$

in which P is operational matrix of the Taylor method.

$$P = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1/2 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1/3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 1/(m-1) \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

We can express x in terms of B as $x = d^T B$, where:

$$d = [0,1,0,\ldots,0]^T$$

Other mostly required term in the problems is integration of the cross product of two vectors B in equation (4). Using (9) on the interval of (0, 1) we have:

$$\int_0^1 B B^T dx = \begin{bmatrix} 1 & \frac{1}{2} & \cdots & \frac{1}{m} \\ \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{m+1} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{m} & \frac{1}{m+1} & \cdots & \frac{1}{2m-1} \end{bmatrix} = D$$

In this case D is a Hilbert matrix of order m. Due to ill-conditionality of Hilbert matrix for large values of m, a modification tothis method is proposed[7, 12].In this case, in the cross product of $B B^T$, we retain only the elements equal or less than order $m-1$. Hence we have:

$$B B^T C \approx \begin{bmatrix} 1 & x & x^2 & \cdots & x^{m-1} \\ x & x^2 & \cdots & x^{m-1} & 0 \\ x^2 & \cdots & x^{m-1} & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x^{m-1} & 0 & \cdots & 0 & 0 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_{m-1} \end{bmatrix} =$$

$$\begin{bmatrix} c_0 & c_1 & c_2 & \cdots & c_{m-1} \\ 0 & c_0 & c_1 & \cdots & c_{m-2} \\ 0 & 0 & c_0 & \cdots & c_{m-3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & c_0 \end{bmatrix} \begin{bmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^{m-1} \end{bmatrix} = \hat{C} B$$

Chebyshev method

Chebyshev polynomials are defined as:

$$T_n(x) = \cos(n \arccos(x)) \quad -1 \le x \le 1$$

And shifted Chebyshev polynomials are defined as:

$$T_0(x) = 1, T_1(x) = 2x - 1,\ T_{n+1}(x) = 2(2x-1)T_n - T_{n-1} \quad 0 \le x \le 1$$

Also the following formula holds for the shifted Chebyshev polynomials:

$$4T_i(x) = \frac{1}{i+1} T'_{i+1}(x) - \frac{1}{i-1} T'_{i-1}(x),\ T_i(1) = 1, T_i(0) = (-1)^i, \quad (10)$$

$$T_i\, T_j = \frac{1}{2}(T_{i+j} - T_{|i-j|}) \qquad (11)$$

In this method $y'(x)$ is defined as follow:

$$y'(x) = C^T B = [c_0,...c_{m-1}] \times [T_0,...T_{m-1}]^T \qquad (12)$$

Hence $y(x)$ is calculated using (5) and (10):

$$y(x) \approx C^T PB + y(0) \qquad (13)$$

in which P is operational matrix of the Chebyshev method [13]:

$$P = \begin{bmatrix} 1/2 & 1/2 & 0 & 0 & 0 & \cdots & 0 \\ -1/8 & 0 & 1/8 & 0 & 0 & \cdots & 0 \\ -1/6 & -1/4 & 0 & 1/12 & 0 & \cdots & 0 \\ 1/16 & 0 & -1/8 & 0 & 1/16 & \cdots & \vdots \\ -1/30 & 0 & 0 & -1/12 & 0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & 1/(4(m-1)) \\ (-1)^m/(2m(m-2)) & 0 & 0 & \cdots & 0 & -1/(4(m-2)) & 0 \end{bmatrix}$$

We can also express x in terms of B as $x = d^T B$, where $d = [1/2, 1/2, 0, ..., 0]^T$. To calculate integration of the cross product of two vectors B in equation (12) we use (11):

$$\int_0^1 B\,B^T\, dx = \begin{bmatrix} 1 & 0 & -\frac{1}{3} & \cdots & \frac{(-1)^m - 1}{2m(m-2)} \\ 0 & \frac{1}{3} & 0 & \cdots & 0 \\ -\frac{1}{3} & 0 & \frac{7}{15} & \cdots & \frac{(m^2-2m+4)((-1)^m-1)}{2(m-4)(m-2)m(m+2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{(-1)^m - 1}{2m(m-2)} & 0 & \frac{(m^2-2m+4)((-1)^m-1)}{2(m-4)(m-2)m(m+2)} & \cdots & \frac{2m^2-4m+1}{(2m-1)(2m-3)} \end{bmatrix} = D$$

a review of this method could be found in [8].

Legendre method

Legendre polynomials are solutions to Legendre's differential equation:

$$\frac{d}{dx}[(1-x^2)\frac{d}{dx}P_n(x)] + n(n+1)P_n(x) = 0$$

and shifted Legendre polynomials are defined using the recursive relation:

$$P_0(\mathrm{x}) = 1, P_1(\mathrm{x}) = 2\mathrm{x} - 1, (\mathrm{n}+1)P_{\mathrm{n}+1}(\mathrm{x}) = (2\mathrm{n}+1)(2\mathrm{x}-1)P_{\mathrm{n}}(\mathrm{x}) - \mathrm{n}P_{\mathrm{n}-1}(\mathrm{x}) \quad 0 \le \mathrm{x} \le 1$$

The shifted Legendre polynomials are orthogonal in the interval (0,1):

$$\int_0^1 P_i(x)P_j(x)\,dx = \begin{cases} 0 & i \ne j \\ 1/(2i+1) & i = j \end{cases} \qquad (14)$$

The following formula also holds:

$$P_i(x) = \frac{1}{2(2i+1)}(P'_{i+1}(x) - P'_{i-1}(x)),$$
$$P_i(0) = (-1)^i, P_i(1) = 1 \quad (15)$$

In this method $y'(x)$ is defined as:

$$y'(x) = C^T B = [c_0, c_1, c_2, ...c_{m-1}] \times [P_0, P_1, P_2, ...P_{m-1}]^T \quad (16)$$

Thus $y(x)$ is calculated using (5) and (15) as follow:

$$y(x) \approx C^T PB + y(0)$$

in which P is the operational matrix of the Legendre method [13]:

$$P = \frac{1}{2}\begin{bmatrix} 1 & 1 & 0 & 0 & \cdots & 0 \\ -\frac{1}{3} & 0 & \frac{1}{3} & 0 & \cdots & 0 \\ 0 & -\frac{1}{5} & 0 & \frac{1}{5} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ & & & -\frac{1}{2m-3} & 0 & \frac{1}{2m-3} \\ 0 & 0 & 0 & \cdots & -\frac{1}{2m-1} & 0 \end{bmatrix}$$

We also express x in terms of B as $x = d^T B$, in which:

$$d = [1/2, 1/2, 0, ..., 0]^T$$

To calculate integration of the cross product of the two vectors B in equation (16) we use formula (14):

$$\int_0^1 B B^T dx = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & \frac{1}{3} & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{2m-1} \end{bmatrix} = D \quad (17)$$

Laguerre method

Laguerre polynomials are solutions to Laguerre's differential equation:

$$xL''_n(x) + (1-x)L'_n + nL_n = 0$$

Also Laguerre polynomials could becalculated using the following recursive formula:

$$L_0(x) = 1, L_1(x) = -x + 1, (n+1)L_{n+1}(x) = (2n+1-x)L_n(x) - nL_{n-1}(x) \quad 0 \le x \le \infty$$

The following formula holds for the Laguerre polynomials:

$$iL_{i-1}(x) = iL'_{i-1}(x) - L'_i(x), \; L_i(0) = 1 \quad (18)$$

In this method $y'(x)$ is defined as:

$$y'(x) = C^T B = [c_0, c_1, c_2, ...c_{m-1}] \times [L_0, L_1, L_2, ...L_{m-1}]^T \quad (19)$$

then $y(x)$ is calculated using the formula (5) and (18) as follow:

$$y(x) \approx C^T PB + y(0)$$

in which P is operational matrix of the Laguerre method [13]:

$$P = \begin{bmatrix} 1 & -1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & -1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{bmatrix}$$

x can also be expressed in terms of B as $x = d^T B$, where:

$$d = [1, -1, 0, ..., 0]^T$$

Due to the lack of orthogonality in the interval (0,1), calculating integration of the cross product of the two vectors B in equation (19)is more complex comparing to other polynomials.

A recursive formula for calculating this product is proposed in [10].

$$\int_0^1 B\,B^T\,dx = \begin{bmatrix} 1 & 1/2 & 1/6 & -1/24 & -19/120 & \dots \\ 1/2 & 1/3 & 5/24 & 7/60 & 37/720 & \dots \\ 1/6 & 5/24 & 13/60 & 73/360 & 883/5040 & \dots \\ -1/24 & 7/60 & 73/360 & 299/1260 & 9533/40320 & \dots \\ -19/120 & 37/720 & 883/5040 & 9533/40320 & 46007/181440 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} = D$$

Bernstein method

In this method, Bernstein polynomials are used as basis functions, i.e.

$$y'(x) = C^T B = [c_0, c_1, c_2, \dots c_{m-1}] \times [B_0, B_1, B_2, \dots B_{m-1}]^T \quad (20)$$

For a fixed m, B_i is defined as:

$$B_i(x) = \binom{m}{i} x^i (1-x)^{m-i}$$

To calculate $y(x)$, we use (5):

$$y(x) \approx C^T PB + y(0)$$

in which P is the operational matrix of integration. This matrix is calculated using the procedure discussed below [14, 15]. The following relation holds between operational matrices of Bernstein polynomials (P_B) and Legendre polynomials (P_L)

$$P_B = MP_L N$$

in which M and N are $m \times m$ basis conversion matrices with the following elements:

$$\mu_{\kappa,j} = \frac{2j+1}{\mu+j+1}\binom{\mu}{\kappa}\sum_{\iota=0}^{j}(-1)^{\iota+j}\frac{\binom{j}{\iota}\binom{j}{\iota}}{\binom{\mu+j}{\kappa+\iota}},$$

$$\kappa, j = 0,1,\dots,\mu-1.$$

$$n_{k,j} = \frac{1}{\binom{m}{j}}\sum_{i=r}^{min\{j,k\}}(-1)^{k+i}\binom{k}{i}\binom{k}{i}\binom{m-k}{j-i},$$

$$r = max\{0, j+k-m\}.$$

Also the following relation holdsbetween these matrices:

$$[B_0, B_1, B_2, \dots B_{m-1}]^T = M\,[P_0, P_1, P_2, \dots P_{m-1}]^T \quad (21)$$

To express x in terms of B we can write $x = d^T B$, where:

$$d = [0, 1/(m-1), 2/(m-1), \dots 1]^T$$

In addition, we use (20) and (21)to calculate integration of the cross product of vectors B :

$$\int_0^1 B\,B^T\,dx = \int_0^1 (M\,[P_0, P_1, P_2, \dots P_{m-1}]^T)([P_0, P_1, P_2, \dots P_{m-1}]M^T)\,dx = MD_P M = D$$

in which D_P is the integration of the cross product of the Legendre polynomials calculated in (17). An implementation of Bernstein direct method to solve variational problems could be found in [4].

Fourier series method

In this method, the candidate function defined on the interval $[0, L]$, is expanded into a Fourier series, i.e. linear combination of the functions $\cos(2k\pi x/L)$ and $\sin(2k'\pi x/L)$; hence $y'(x)$ is defined as follow:

$$y'(x) = C^T B = [c_0, c_1, c_2, \dots c_{m-1}] \times [1, cos\frac{2\pi x}{L}, \dots, cos\frac{2n\pi x}{L}, sin\frac{2\pi x}{L}, \dots sin\frac{2n\pi x}{L}]^T \quad (22)$$

The elements of Fourier series functions are orthogonal in the interval $[0,L]$:

$$\int_0^L cos(\frac{2k\pi x}{L})cos(\frac{2k'\pi x}{L})\,dx = \int_0^L sin(\frac{2k\pi x}{L})sin(\frac{2k'\pi x}{L})\,dx = \begin{cases} 0 & k \neq k' \\ L/2 & k = k' \end{cases} \quad (23)$$

$$\int_0^L \cos(\frac{2k\pi x}{L})\sin(\frac{2k'\pi x}{L})\,dx = 0 \quad (24)$$

Consequently, $y(x)$ could be calculated using (5) as follow:

$$y(x) \approx C^T PB + y(0)$$

in which P is the operational matrix of the Fourier method [13]:

$$P = \left[\begin{array}{c|cccc|cccc} 1/2 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \hline 0 & 0 & 0 & \cdots & 0 & 1/(2\pi) & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1/(4\pi) & \cdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 1/(2n\pi) \\ \hline 1/(2\pi) & -1/(2\pi) & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 1/(4\pi) & 0 & -1/(4\pi) & \cdots & \vdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 & \vdots & \vdots & \ddots & \vdots \\ 1/(2n\pi) & 0 & \cdots & 0 & -1/(2n\pi) & 0 & 0 & \cdots & 0 \end{array}\right]$$

To express x in terms of B, we can write $x = d^T B$, where:

$$d = [\frac{1}{2},0,...,0,\frac{-\sin(2\pi x)}{\pi},...,\frac{-\sin(2n\pi x)}{n\pi}]^T$$

Also integration of the cross product of vectors B in (22) is calculated using (23) and (24):

$$\int_0^1 B\,B^T\,dx = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & \frac{1}{2} & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{2} \end{bmatrix} = D$$

This method is proposed in [11].

The interested reader would be referred to other methods, like Haar wavelet method [16], Walsh functions [17, 18], wavelets [6, 19] and block pulse methods [5, 20 and21].

NUMERICAL EXAMPLES

In this section we apply the above mentioned six methods (Taylor, Chebyshev, Legendre, Laguerre, Bernstein and Fourier) on three examples. According to the construction of the examples, some more calculations may be required in each method. All numerical experiments presented in this section are computed in double precision, using Mat lab 2012 on a PC with a 3GHz processor and 4GB of memory.

Example 1: Consider the problem of finding the minimum of the following integral with given boundary conditions:

$$J(y(x)) = \int_0^1 (y'^2 + xy' + y^2)\,dx, \quad y(0) = 0, y(1) = \frac{1}{4} \quad (25)$$

The exact solution of (25) could be found using (2):

$$y(x) = \frac{e^{1-x} - 2e^{2-x} + 2e^{x} - e^{x+1} - 2 + 2e^{2}}{4(e^{2}-1)}$$

In all the methods, we define vector V as $V = \int_0^1 B\,dx$, according to the definition of B in (4). In Taylor, Chebyshev, Legendre, Laguerre, Bernstein and Fourier methods, V is calculated sequentially as:

$V = (1, \frac{1}{2}, \frac{1}{3}, ..., \frac{1}{m})$,

$V = (1, 0, -\frac{1}{3}, 0, ..., -\frac{(-1)^m - 1}{2(m)(m-2)})$,

$V = (1,0,0,...0)$,

$V = (1, \frac{1}{2}, \frac{1}{6}, -\frac{1}{24}, -\frac{19}{120}, ...)$,

$V = (\frac{1}{m+1}, ..., \frac{1}{m+1})$, $V = (1,0,0,...0)$. In this example, using (3), (5) and (6) J turns to:

$$J = C^T DC + C^T Dd + C^T PDP^T C$$

We apply boundary conditions of (25) using Lagrange multiplier λ as follow:

$$\hat{J} = J + \lambda(C^T V - \frac{1}{4})$$

To extremize $\hat{J}$ using (8) we have:

$$\frac{\delta \hat{J}}{\delta C} = 2DC + Dd + 2PDP^T C + \lambda V = 0,$$

$$\frac{\delta \tilde{J}}{\delta \lambda} = C^T V - \frac{1}{4} = 0$$

Using two recent equations, the Lagrange multiplier and consequently vector C are calculated. The results are listed in table 1 for m=3 and Table 2 for m=5. The answers that are closer to the exact solution are in bold font.

Table1. Estimated and exact values of *y(x)* for *m=3* in example 1

x	Taylor	Chebyshev	Legendre	Laguerre	Bernstein	Fourier	Exact
0.0	0.000000	0.000000	0.000000	0.000000	0.000000	-0.035312	0.000000
0.1	0.052772	0.041272	0.041816	**0.041980**	0.035487	-0.006940	0.041950
0.2	0.094870	0.078514	**0.079239**	0.079722	0.070553	0.026887	0.079317
0.3	0.127984	0.111882	**0.112516**	0.113401	0.104482	0.062799	0.112473
0.4	0.153800	0.141530	**0.141892**	0.143190	0.136559	0.096627	0.141750
0.5	0.174008	**0.167613**	**0.167613**	0.169263	0.166066	0.125000	0.167442
0.6	0.190295	0.190288	**0.189925**	0.191796	0.192288	0.146627	0.189806
0.7	0.204349	0.209708	**0.209074**	0.210961	0.214508	0.162799	0.209065
0.8	0.217859	0.226030	**0.225305**	0.226934	0.232011	0.176887	0.225413
0.9	0.232513	0.239409	**0.238865**	0.239889	0.244080	0.193059	0.239012
1.0	0.250000	0.250000	0.250000	0.250000	0.250000	0.214687	0.250000
J	0.200800	0.197606	**0.197595**	0.197618	0.198920	0.192884	0.197593

Table 2. Estimated and exact values of *y(x)* for *m=5* in example 1

x	Taylor	Chebyshev	Legendre	Laguerre	Bernstein	Fourier	Exact
0.0	0.000000	0.000000	0.000000	0.000000	0.000000	-0.034893	0.000000
0.1	0.043757	0.041258	**0.041950**	0.042684	**0.041950**	-0.003490	0.041950
0.2	0.080721	0.078672	**0.079317**	0.082206	**0.079317**	0.035201	0.079317
0.3	0.113806	0.112083	**0.112473**	0.118092	**0.112473**	0.070983	0.112473
0.4	0.144206	0.141589	**0.141750**	0.149970	**0.141750**	0.099738	0.141750
0.5	0.171913	0.167445	**0.167442**	0.177576	**0.167442**	0.125000	0.167442
0.6	0.196225	0.189973	**0.189806**	0.200754	**0.189806**	0.149738	0.189806
0.7	0.216261	0.209458	**0.209066**	0.219458	**0.209066**	0.170983	0.209065
0.8	0.231474	0.226058	**0.225413**	0.233757	**0.225413**	0.185201	0.225413
0.9	0.242166	0.239703	**0.239012**	0.243836	**0.239012**	0.196509	0.239012
1.0	0.250000	0.250000	0.250000	0.250000	0.250000	0.215106	0.250000
J	0.197965	0.197609	**0.197593**	0.198298	**0.197593**	0.191090	0.197593

Example 2: Consider the problem of finding the minimum of the following integral with given boundary conditions:

$$J(y(x)) = \int_0^1 (y^2 - y'^2)\,dx, \quad y(0) = 0, y(1) = 1$$

(26)

The exact solution of (26) could be found using (2):

$$y(x) = \frac{\sin x}{\sin 1}$$

In this example J is calculated as:

$$J = C^T PDP^T C - C^T DC$$

To apply boundary conditions, we use Lagrange multiplier λ as follow:

$$\widehat{J} = J + \lambda(C^T V - 1)$$

Then, the following equations are derived:

$$\frac{\delta \widehat{J}}{\delta C} = 2PDP^T C - 2DC + \lambda V = 0$$

$$\frac{\delta \tilde{J}}{\delta \lambda} = C^T V - 1 = 0$$

The results of applying all the methods are listed in table 4 for m=3 andtable 5 for m=5.

Table 3. Estimated and exact values of *y(x)* for *m=3* in example 2

x	Taylor	Chebyshev	Legendre	Laguerre	Bernstein	Fourier	Exact
0.0	0.000000	0.000000	0.000000	0.000000	0.000000	-0.054826	0.000000
0.1	0.175495	0.121225	**0.118898**	0.126243	0.148966	0.050408	0.118641
0.2	0.303140	0.239411	**0.236308**	0.244846	0.278883	0.164115	0.236097
0.3	0.394586	0.353929	**0.351214**	0.356486	0.392814	0.281057	0.351194
0.4	0.461487	0.464150	**0.462598**	0.461843	0.493821	0.394764	0.462782
0.5	0.515495	0.569444	**0.569444**	0.561593	0.584968	0.500000	0.569746
0.6	0.568264	0.669183	**0.670734**	0.656416	0.669318	0.594764	0.671018
0.7	0.631446	0.762737	**0.765451**	0.746990	0.749933	0.681057	0.765585
0.8	0.716694	0.849477	**0.852580**	0.833993	0.829876	0.764115	0.852502
0.9	0.835661	0.928774	**0.931101**	0.918103	0.912211	0.850408	0.930901
1.0	1.000000	1.000000	1.000000	1.000000	1.000000	0.945173	1.000000
J	-0.873964	-0.642307	**-0.642095**	-0.646322	-0.665903	-0.707786	-0.642092

Table 4. Estimated and exact values of *y(x)* for *m=5* in example 2

x	Taylor	Chebyshev	Legendre	Laguerre	Bernstein	Fourier	Exact
0.0	0.000000	0.000000	0.000000	0.000000	0.000000	-0.055574	0.000000
0.1	0.116789	0.121591	**0.118641**	0.114127	**0.118641**	0.054441	0.118641
0.2	0.225898	0.239004	**0.236098**	0.222183	**0.236098**	0.175952	0.236097
0.3	0.333887	0.353100	**0.351195**	0.326187	**0.351195**	0.293126	0.351194
0.4	0.442094	0.463658	**0.462782**	0.427618	**0.462782**	0.399401	0.462782
0.5	0.548564	0.569760	**0.569746**	0.527433	**0.569746**	0.500000	0.569746
0.6	0.649987	0.670167	**0.671017**	0.626070	**0.671017**	0.599401	0.671018
0.7	0.743636	0.763695	**0.765585**	0.723457	**0.765585**	0.693126	0.765585
0.8	0.829298	0.849598	**0.852502**	0.819027	**0.852502**	0.775952	0.852502
0.9	0.911211	0.927946	**0.930901**	0.911720	**0.930901**	0.854441	0.930901
1.0	1.000000	1.000000	1.000000	1.000000	1.000000	0.944425	1.000000
J	-0.647887	-0.642358	**-0.642092**	-0.651837	**-0.642092**	-0.705697	-0.642092

Example 3: Consider the problem of finding the minimum of the following integral with given boundary conditions:

$$J(y(x)) = \int_0^1 \left(\frac{1}{2}y''^2 - 4xy\right) dx, \qquad (27)$$

$$y(0) = 0, y'(0) = 0, y(1) = \frac{1}{2}, y'(1) = \frac{2}{3}$$

The exact solution of (27) could be found using (2):

$$y(x) = \frac{1}{30}x^5 - \frac{13}{30}x^3 + \frac{27}{30}x^2$$

In this example we suppose:

$$y''(x) = C^T B$$

Using similar procedure in (5), we obtain:

$$y'(x) \approx C^T PB + y'(0) = C^T PB$$

$$y(x) \approx C^T P^2 B + y(0) = C^T P^2 B$$

Then,the functional (27) turns to:

$$J = \frac{1}{2}C^T DC - 4C^T P^2 Dd$$

Next, the boundary conditions are applied:

$$\hat{J} = J + \lambda_1(C^T V - \frac{2}{3}) + \lambda_2(C^T PV - \frac{1}{2})$$

Accordingto (8) we have:

$$\frac{\delta \hat{J}}{\delta C} = DC - 4P^2 Dd + \lambda_1 V + \lambda_2 PV = 0$$

$$\frac{\delta \hat{J}}{\delta \lambda_1} = C^T V - \frac{2}{3} = 0, \ \frac{\delta \hat{J}}{\delta \lambda_2} = C^T PV - \frac{1}{2} = 0,$$

Tables 5 and 6 provides results of applying the mentioned methods for m=3 and m=5.

Table 5. Estimated and exact values of *y(x)* for *m=3* in example 3

x	Taylor	Chebyshev	Legendre	Laguerre	Bernstein	Fourier	Exact
0.0	0.000000	0.000000	0.000000	0.000000	0.000000	-0.002566	0.000000
0.1	0.013640	0.008421	**0.008675**	-0.065328	0.008072	-0.014334	0.008567
0.2	0.050916	0.032000	**0.032800**	-0.232583	0.029317	-0.012687	0.032544
0.3	0.106640	0.068296	**0.069675**	-0.462328	0.059925	0.005565	0.069381
0.4	0.176000	0.115000	**0.116800**	-0.720000	0.096955	0.039818	0.116608
0.5	0.254557	0.169921	**0.171875**	-0.975911	0.138328	0.085899	0.171875
0.6	0.338250	0.231000	**0.232800**	-1.205250	0.182834	0.137667	0.232992
0.7	0.423390	0.296296	**0.297675**	-1.388078	0.230125	0.189353	0.297969
0.8	0.506666	0.364000	**0.364800**	-1.509333	0.280722	0.237767	0.365056
0.9	0.585140	0.432421	**0.432675**	-1.558828	0.336009	0.283515	0.432783
1.0	0.656250	**0.500000**	**0.500000**	-1.531250	0.398238	0.330766	0.500000
J	0.061805	-0.180164	**-0.180555**	25.145138	-0.148710	0.148724	-0.180634

Table 6. Estimated and exact values of *y(x)* for *m=5* in example 3

x	Taylor	Chebyshev	Legendre	Laguerre	Bernstein	Fourier	Exact
0.0	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.023009	0.008150	**0.008567**	2.319386	**0.008567**	-0.021229	0.008567
0.2	0.068649	0.031534	**0.032544**	5.448594	**0.032544**	-0.026732	0.032544
0.3	0.115709	0.068006	**0.069381**	6.131684	**0.069381**	-0.015587	0.069381
0.4	0.157560	0.115074	**0.116608**	3.731172	**0.116608**	0.007390	0.116608
0.5	0.197312	0.170259	**0.171875**	-0.644708	**0.171875**	0.037696	0.171875
0.6	0.242991	0.231325	**0.232992**	-5.014755	**0.232992**	0.073910	0.232992
0.7	0.302763	0.296374	**0.297969**	-7.397553	**0.297969**	0.114680	0.297969
0.8	0.380195	0.363812	**0.365056**	-6.684239	**0.365056**	0.155986	0.365056
0.9	0.469547	0.432180	**0.432783**	-3.511272	**0.432783**	0.194224	0.432783
1.0	0.551103	0.499856	**0.500000**	-1.133214	**0.500000**	0.231793	0.500000
J	1.008580	-0.179982	**-0.180634**	3.78015e+4	**-0.180634**	0.226489	-0.180634

DISCUSSION

In this section we compare the results fromdifferent aspects and propose the most suitable methods. Generally, the most important factorforany numerical method is its precision. Defining $E = [\sum (y_{exact} - y)^2]^{1/2}$ for $x = 0, 0.1, 0.2, ..., 1$ leads to the results stated in table 7 which is the average of 2-norm error of each method for $m = 3$ and $m = 5$. The table shows that the Legendre method is the most accurate method and the Chebyshev and Bernstein methods come next.

Another item for comparingthe methods is the stability in calculations. To investigatethis aspect of the methods, we have calculated the condition numbers of the operational and cross product matrices. Table 8 demonstrates 2-norm condition numberof matrix D and table 9 shows 2-norm condition number of matrix P.Large values correspond to less stability in calculations [22]. The Fourier method has a smalland fixed value, i.e. increasing the values of m will not affect stability of the method. In contrary,large values in Taylor and Laguerre methods means instability of them. This fact is clearly observed in example 3.

Table 7. Average 2-norm error of the mentioned methods

	Taylor	Chebyshev	Legendre	Laguerre	Bernstein	Fourier
Example 1	0.021651	0.001557	0.000176	0.013591	0.008893	0.142327
Example 2	0.158968	0.006894	0.000309	0.065820	0.041192	0.229742
Example 3	0.213991	0.003950	0.000317	9.916558	0.094291	0.425528
Average	0.131537	0.004134	0.000267	3.331989	0.048125	0.265866

Table 8. 2-norm condition number of matrix *D*

	Taylor	Chebyshev	Legendre	Laguerre	Bernstein	Fourier
m=3	Inf	17.955027	12.869192	4.048917	8.155323	3.491829
m=5	Inf	26.295272	32.578352	6.742044	98.238061	6.789601

Table 9. 2-norm condition number of matrix *P*

	Taylor	Chebyshev	Legendre	Laguerre	Bernstein	Fourier
m=3	524.0567	3.785859	5.000000	3432.798	8.155323	2.000000
m=5	47660.72	6.242669	9.000000	1.42e+09	126.0000	2.000000

CONCLUSION

Anoverview of direct numerical methods for solving variational problems is discussed. The purpose of a direct method is to reduce a nonlinear problem like differential equations which appear in physical chemistry to a problem of solving a system of algebraic equations. To achieve this, operational matrix of integration and cross product of basis functions are constructed for several algorithms. According to the provided examples, Legendre method is the preferred method and Chebyshev and Bernstein methods are the second choices. Fourier method is suggested only for large number of basis functions, and Taylor and Laguerre methods are not suitable for problems considering high precision.

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