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Spectral Collocation Method for The Numerical Solution Of Ordinary Differential Equations

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Abstract

Spectral collocation Methods (SCMs) are specific for differential equations. Underpinning these methods is the use of polynomial interpolants and enforcing them to satisfy the differential equation at specially chosen points. In this regard, we construct spectral method employing the row replacement strategy based on differentiation matrix. We use the row replacement strategy to solve initial value problem (IVPs), boundary value problems (BVPs), and further extend the strategy to handle the non-linear case. The result shows that the SCM enjoys rapid convergence as it compares favourably with the exact solutions.

KEYWORDS: Spectral, Collocation, Polynomial, Interpolation, Differential Equation.
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1.0 Introduction

The invention of computers have not only saved us from the delay in solving complicated mathematical problems, but they have become part of our daily routines. Computational mathematics provides a way of solving complex numerical problems by initially working on a simple problem analytically. When the analytical solution is achieved, then one can use this idea to implement such problem on a computer and compare both results. With this implementation on a simple problem, one can now add more complicated ones by including real-world factors as the case maybe. Nowadays, numerical analysts are in search of the most efficient method for solving a given problem. It is well known that interpolation can be used for polynomial (function) approximations. Ikhile [1] investigated some iterative methods having similar propagation characteristics in the determination of the zeros of a polynomial. In particular, the introduction of the effect of round-off error point arithmetic. The laudable idea of interpolation on polynomials can be extended to solve differential equations by enforcing the differential equations to have polynomial solutions [2]. This gives rise to the SCMs, in particular, the row replacement strategy, which has not only been useful for the approximation of functions but now has a great impact in the discretization for differential equations [3]. Some excellent discretization processes can be found in [4,5].

Definition 1: [6]: A polynomial is a function $f: \mathbb{C} \to \mathbb{C}$ such that, for some non-negative integer n and for some $a_k \in \mathbb{C}, 0 \leq k \leq n$, with $a_n \neq 0$,

$$f(x) = \sum_{k=0}^{n} a_k x^k \quad \forall\ x \in \mathbb{C}. \tag{1}$$

One of the pillars which numerical analysis depends upon is computation with polynomials [6]. However, we employ the row replacement approach to discretizing our differential equations. There are different types of interpolation such as polynomial, rational, Hermite, Birkhoff, etc (see [7,8]), but we concentrate on polynomial interpolation specifically. One major reason for the importance of equation (1) is that it can be used to approximate continuous functions uniformly. This implies that given any $f(x)$, defined and continuous on a closed and bounded interval $[a, b]$, there exists a $P(x)$ that is as near to the given $f(x)$ [8]. To be precise, we quote the result of Weierstrass approximation theorem.

Theorem 1 *[8] Suppose that $f(x)$ is defined and continuous on a closed interval $[a, b]$. For any $\epsilon > 0$, there exist a polynomial $P(x)$, such that,*

$$| f(x) - P(x) | < \epsilon \quad \forall\ x \in [a, b]. \tag{2}$$

2.0 Improved Lagrange Formulas

Lagrange interpolation is praised for analytic utility and beauty but deplored for numerical practice [7]. Given the set of points $x_0, \ldots, x_n$, the Lagrange basis is given by,

$$\ell_i(x) = \prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{(x - x_k)}{(x_i - x_k)}, \tag{3}$$

with interpolating polynomial,

$$P(x) = \sum_{i=0}^{n} a_i\, \ell_i(x) = f_i. \tag{4}$$

The Lagrange basis (3) has the property,

$$\ell_i(x_k) = \begin{cases} 1, & i = k \\ 0, & i \neq k \end{cases} \text{ for } i, k = 0, \ldots, n. \tag{5}$$

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The interpolating polynomial (4) has an associated system with an identity matrix given by,

$$\begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{pmatrix}. \quad (6)$$

The system (6) reduces to,

$$\ell \boldsymbol{a} = \boldsymbol{f}. \quad (7)$$

Hence, the coefficients a_i's can be solved trivially. It is important to note that most authors work with equation (4) for small n nodes, before realizing some snags about it which make it a bad practice computationally [9]. The Lagrange matrix is an identity which is easier to solve but the system requires $O(n^2)$ additions and multiplications to be evaluated which makes it a bad choice for computations [2]. General recommendations show that one should instead use Newton's formula, which requires only $O(n)$ operations, and is independent of the evaluation point x [9]. However, we show how equation (4) can be improved for better approximation. Burret and Trefethen [9] considered spectral discretization of polynomial interpolants with special emphasis on the improved Lagrange formulas. They did this by re-writing equation (4) as,

$$P(x) = \sum_{i=0}^{n} \ell_i(x) f_i\,, \quad (8)$$

where $\ell_i(x)$ is as in (3). As in [9], the improved Lagrange formula of the first kind is given by,

$$P(x) = \mathrm{l}(x) \sum_{i=0}^{n} \frac{w_i}{(x-x_i)} f_i\,, \quad (9)$$

where the weights $w_i = \prod_{k\neq i}^{n} \frac{1}{(x_i - x_k)}$, f_i are the given functions, x_i are the collation points, x is the interpolation point, and the node polynomial $\mathrm{l}(x) = (x - x_0), \dots, (x - x_n)$. The formula (9) now requires $O(n^2)$ floating point operations to evaluate the weights w_i and does not depend on f_i. This feature allows for the evaluation of several functions, and it only requires $O(n)$ operations each provided the w_i are known while other famous formulas in particular, Newtons interpolation formula requires the computation of a new tableau for each new function. The formula (9) in addition, does not necessarily depend on the order in which the nodes are arranged, it can easily be updated recursively given new data set while the Newton's interpolation formula depends on the order, which increases the computational cost as n increases. This many orderings leads to numerical instability [9]. Burret and Trefethen [9] in their famous work proved further to obtain the second kind of the improved Lagrange formula as,

$$P(x) = \sum_{i=0}^{n} \frac{w_i}{(x-x_i)} f_i \Big/ \sum_{i=0}^{n} \frac{w_i}{(x-x_i)} \quad . \quad (10)$$

The formula (10) is still a Lagrange formula, but one with special and beautiful symmetry [9]. This method (10) like the method (9) earlier stated, are sometime referred to as the barycentric Lagrange interpolation formulas [9,10]. Both formulas enjoy the advantage of updating weight w_i in $O(n)$ operations to subsume a new set of f_i. Formulas (9,10) can all be represented in trigonometric forms (see [9]). It is interesting to note that when weights w_i have common factor in (10), they may be cancelled without any impact on $P(x)$ [11]. The numerical stability of formulas (9,10) can be found in [2,12, 13].

3.0 Spectral Collocation Methods

3.1 The Collocation Points

The composition of spectral methods, in particular, the row replacement strategy to be discussed in this paper, and the improved formulas (9,10), are mostly applied on different kinds of collocation points. Usually for periodic problems, equally spaced points are sometimes considered, and the interpolant is a trigonometric polynomial $u(x)$, while for non-periodic problems, the standard interval is $[x_0, x_n]$, where $x_0 = -1$, $x_n = 1$, and the boundary conditions $u(x_0) = u(x_n) = 0$ [11]. We state the three sets of collocation points $x_0, \dots, x_n$ in Table 1.

Table 1: Collocation Points

No	Collocation Points (x_i)	Formulas
1	Chebyshev point of the first kind	$\cos\left(\frac{\pi(2i+1)}{2n+2}\right)$
2	Chebyshev point of the second kind	$\cos\left(\frac{\pi i}{n}\right)$
3	Equispaced points	$-1 + \frac{2i}{n}$

The first two of these sets of points in table 1 are often used due to the fact that their points cluster near the boundary. The interpolation based on these points converges as $n \to \infty$ which can be quickly linked to theorem 1, while the last point on table 1, is not usually used in practice, reason being that the interpolation based on such point diverge rapidly as $n \to \infty$. However, equispaced points are embedded in approximation investigation because they give valuable perspective on the other two collocation points [11]. In addition, the Chebyshev points were obtained from the equally spaced points on the unit circle down to the unit interval [-1,1] [9]. Illustration is given using the popular Runge function given,

$$f(x) = \frac{1}{(1+25x^2)} \quad x \in [-1,1]. \quad (11)$$

We interpolate (globally) employing Chebyshev points by choosing a high order $n = 16$ and lower order $n = 4$ polynomial for an analytic (smooth) function (11) with their maximum error. We then compare with the equivalent equispaced points.

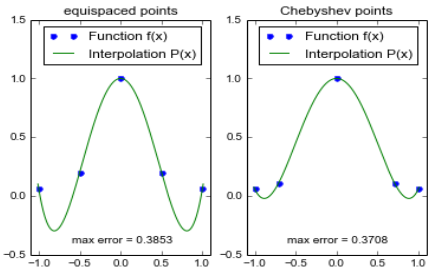

Figure 1: The interpolation of Runge function (11) at lower order $n = 4$ shows that there is a minimal difference in their errors which is not always sufficient to conclude that they are both efficient.

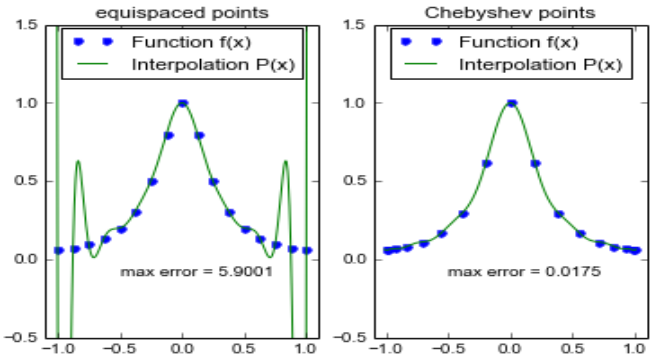

Figure 2: The interpolation of Runge function (11) at higher order $n = 16$ shows that the error though very small at the middle is very large near the boundary for equispaced point while the Chebyshev point produces a cluster near the boundaries [-1,1] which makes it preferable.

The large error at the equispaced points implies Runge phenomenon (Runge oscillations) while the oscillation can be treated by choosing to collocate using Chebyshev points (unequally spaced points) [2]. However, for an increasing n, it implies that equispaced error increases exponentially while in the Chebyshev case, the error decreases exponentially. The good thing about the global interpolation with Chebyshev points is the rapid rate of convergence i.e., exponentially fast convergence (geometric convergence) [2] usually referred to as the spectral accuracy. Another important stability criteria for interpolation is the use of the Bernstein ellipse [14].

3.2 Spectral Differentiation of Improved Lagrange Formula

In this section, we explore how polynomial interpolants can be employed to construct spectral differentiation matrix suitable for polynomial approximations using the Lagrange formula. As earlier discussed that the Lagrange formula has been criticized in literatures as a bad choice for numerical computation because of the Identity matrix associated with the formula, this ambiguity was later worked on in [9]. In the matrix version of the collocation methods, one can express the approximate solution $u(x)$ as an interpolating polynomial in Lagrange form similar to equation (4) as,

$$u(x) = \sum_{i=0}^{n} u_i \, \ell_i(x). \quad (12)$$

We respectively give the first and the second derivatives of $u(x)$ which is usually estimated at collocation points as,

$$u'(x) = \sum_{i=0}^{n} u_i \, \ell_i'(x) \quad \text{and} \quad u''(x) = \sum_{i=0}^{n} u_i \, \ell_i''(x), \quad (13)$$

where $u_i = u(x_i)$. Further derivation put forward in [9] resulted into,

$$\ell_i'(x_j) = \frac{w_i/w_j}{x_j - x_i} \quad \text{and} \quad \ell_i''(x_j) = -2\frac{\frac{w_i}{w_j}}{x_j - x_i}\left(\sum_{k\neq j} \frac{\frac{w_k}{w_j}}{x_j - x_i} - \frac{1}{x_j - x_i}\right). \quad (14)$$

For $k \neq j$ and $n \leq 1$, thus, Lagrange interpolation formula which computes the spectral matrices $D_{ji}^{(1)}$ and $D_{ji}^{(2)}$ is explicitly written as,

$$D_{ji}^{(1)} = \begin{cases} \frac{w_i/w_j}{x_j - x_i}, & i \neq i \\ -\sum_{\substack{k=0 \\ k\neq j}}^{n} D_{jk}^{(1)}, & j = i \end{cases} \quad \text{and} \quad D_{ji}^{(2)} = \begin{cases} 2D_{ji}^{(1)}\left(D_{jj}^{(1)} - \frac{1}{x_j - x_i}\right), & i \neq i \\ -\sum_{\substack{k=0 \\ k\neq j}}^{n} D_{jk}^{(2)}, & j = i. \end{cases} \quad (15)$$

The spectral differentiation matrices obtained implies that if u is a vector of function values associated with the collocation point (x_i), then $D^{(1)}\,u$ is the vector obtained by interpolating function u, then differentiating the interpolant at the collocation points. Also, the same for the case of $D^{(2)}\,u$. The formula is valid even in the case of rational interpolation (see [5]).

4.0 Numerical Experiment

In this section, we examine the power of spectral differentiation matrix on a simple function and compare with the derivative of the function. As it is well known that numerous numerical methods are capable of solving differential equation [15-20], but we discuss herein the implementation procedure for our SCM using the row replacement strategy in the case of the first and second order differential equations. The implementation was carried out using Python v3 via Jupyter notebook.

Example 1 Consider a given function and its derivative given in [21]

$$u(x) = 8x^4 + 3x^3 + 2x^2 - x + 1 \text{ and } u'(x) = 32x^3 + 9x^2 + 4x - 1. \quad (16)$$

Table 2: Implementing u(x) using spectral differentiation matrix for N = 4 Chebyshev points

Error $\lvert \boldsymbol{u}'(\boldsymbol{x}) - \boldsymbol{D}\,\boldsymbol{u}(\boldsymbol{x})\rvert$	0.00000000e+00	3.55271368e-15	2.44249065e-15	3.55271368e-15	1.42108547e-14

$$D_4^{(1)}(x) = \begin{pmatrix} -5.5000\text{e}+00 & 6.8284\text{e}+00 & -2.0000\text{e}+00 & 1.1716\text{e}+00 & -5.0000\text{e}-01 \\ -1.7071\text{e}+00 & 7.0711\text{e}-01 & 1.4142\text{e}+00 & -7.0711\text{e}-01 & 2.9289\text{e}-01 \\ 5.0000\text{e}-01 & -1.4142\text{e}+00 & -8.8818\text{e}-16 & 1.4142\text{e}+00 & -5.0000\text{e}-01 \\ -2.9289\text{e}-01 & 7.0711\text{e}-01 & -1.4142\text{e}+00 & -7.0711\text{e}-01 & 1.7071\text{e}+00 \\ 5.0000\text{e}-01 & -1.1716\text{e}+00 & 2.0000\text{e}+00 & -6.8284\text{e}+00 & 5.5000\text{e}+00 \end{pmatrix},$$

where $D_4^{(1)}(x)$ is the first spectral differentiation matrix obtained from (15).

4.1 Implementation Procedure for First Order ODE

Consider the first order linear ODE,

$$a(x)\frac{du}{dx} + b(x)u = f(x), \quad (17)$$

$$u(-1) = c. \quad (18)$$

The linear scalar problem (17) and its initial condition (18) can be discretized in the collocation method as,

$$A\boldsymbol{u} = (\text{diag}(a)D_{n+1} + \text{diag}(b))\,\boldsymbol{u} = \boldsymbol{f}, \quad (19)$$

$$B\boldsymbol{u} = (1\,0\,0\,\ldots\,0)\boldsymbol{u} = c. \quad (20)$$

Vectors obtained through the discretization at $n+1$ Chebyshev points are in boldface. Explicitly, the vectors are $x = (x_1, \dots, x_{n+1})^T$, $b = (b_1(x), \dots, b_{n+1}(x))^T$. Also, we use $n+1$ rather than n points for vector $\boldsymbol{u}$ in order to collocate the differential equation (19) at n points. The row replacement strategy i.e., enforcing the boundary condition process is achieved by solving the $(n+1) \times (n+1)$ system,

$$\begin{pmatrix} B \\ Q\ A \end{pmatrix} \boldsymbol{u} = \begin{pmatrix} c \\ Q\ f(x) \end{pmatrix}, \tag{21}$$

where,

$$\mathrm{Q} = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}. \tag{22}$$

This implies that Q is a $n \times (n+1)$ matrix that erases the first row of any right multiplier. It is obviously natural to pick this row, which corresponds to the differential equation system at the left boundary, in order to replace it with a side condition based on the known function value at the same location [22]. One should bear in mind that the simplifying replacement of $u(-1)$ by c should be done before computation, this reduces the system to a square one of size $n+1$. Hence, system (21) can be solved.

Example 2: We consider the IVP [21],

$$u'(x) + \alpha\, u(x) = 0, \tag{23}$$

with initial value condition $u(-1) = 1$ and $\alpha = 0.5$. The exact solution of (23) is given by $u(x) = e^{-0.5(x+1)}$. The computation was carried out at points $n = 10$.

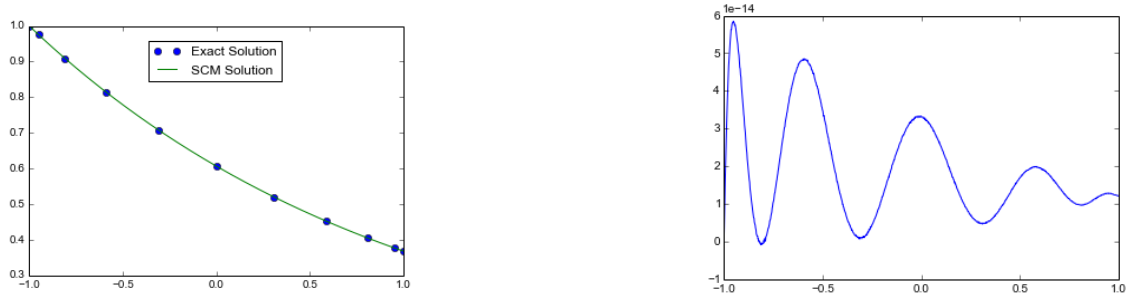

Figure 3: The SCM solution and exact solution of problem (23) (left), and the error between the solutions (right)

4.2 Implementation Procedure for Second Order ODE

For higher order DEs, we also consider a linear problem of order m and a linear functional,

$$a_m(x)u^m + \cdots + a_1(x)u'(x) + a_0(x)u(x) = f(x), \tag{24}$$

$$r(u, \dots, u^{m-1}) = c_i, \quad i = 1, \dots, m. \tag{25}$$

For the case $m = 2$, with one condition at each boundary, we employ the row replacement strategy. In particular, we give a clear picture of the second order ODE case,

$$u''(x) = f \ , \ u(\pm 1) = 0. \tag{26}$$

This can be discretized by setting $r_i = u''(x_i)$, and rewriting (26) as $r_i = u''(x_i) = D^2 u_i = f_i$, $1 \le i \le n-1$. More explicitly in system form as,

$$\begin{pmatrix} \\ D_n^2 \\ \\ \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_{n-1} \\ u_n \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_{n-1} \\ f_n \end{pmatrix}. \tag{27}$$

The matrix D_n^2 maps a vector **u** to a vector **f**. In order to impose the boundary conditions, we replace f_0 and f_n by 0, first and last row of D_n^2 by -1 and 1 respectively. Hence, the resolving the system (27) can be solved by obtaining the coefficients for the vector **u**.

Example 3: Consider the second order BVP [14],

$$u''(x) = e^{4x}, \quad u(-1) = 0, \quad u(1) = 0. \tag{28}$$

The exact solution is given by $u(x) = (e^{4x} - x\sinh(4) - \cosh(4))/16$. The numerical solution was obtained via N =15 points.

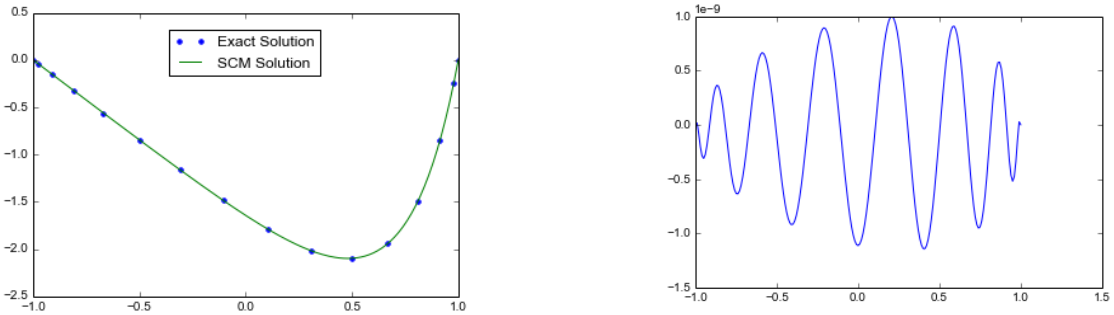

Figure 4: The SCM solution and exact solution of problem (28) (left), and the error between the solutions (right)

Example 4 Application to non-linear Case: Consider [21],

$$u'(x) = 2u^2, \quad u(-1) = 1. \tag{29}$$

The exact solution is given by $u(x) = -\frac{1}{2x+1}$. The numerical solution was obtained via $N = 25$ points.

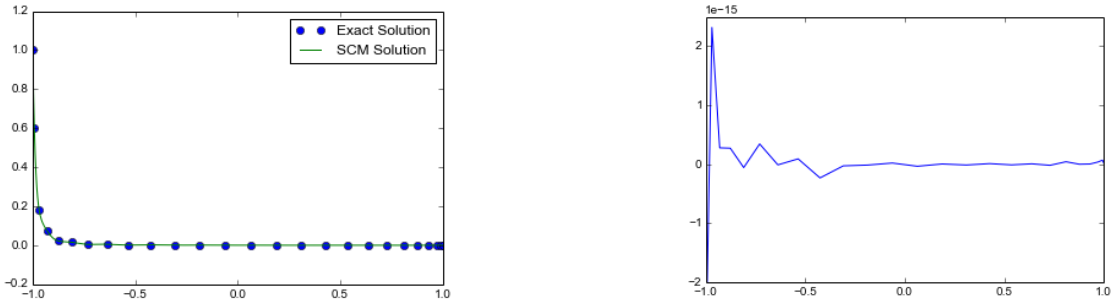

Figure 5: The SCM solution and exact solution of problem (29) (left), and the error between the solutions (right)

5. Conclusion

We have discussed about the Lagrange formula, in particular, the improved Lagrange formulas of the first kind and second which can be evaluated at a specifically chosen points. The improved Lagrange formulas have been used for the construction of spectral method based on discretization of polynomials, forcing DEs into polynomial through the row replacement strategy. Our results show that the SCM enjoys rapid convergence as compared with the exact solutions of the differential equations (see Figures 3, 4, and 5). It is our hope that the algorithm of emerging numerical codes for the DEs will be dominated by the use of SCMs. Emphasis are now being placed on spectral methods when approximating, for which we have introduced a concept of discretizing IVP, BVP and a non-linear case because they enjoy spectral convergence unlike other conventional approaches.

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