

Spectral Rectangular Collocation Formula: An Approach for Solving Oscillatory Initial Value Problems and/or Boundary Value Problems in Ordinary Differential Equations

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Abstract The idea of rectangularization of a $N \times N$ differentiation matrix through collocation was recently suggested to be more useful in discretization process, especially when the traditional row replacement approach fails. In this regard, we employ the state-of-the-art technique of rectangularization to discretize some oscillatory initial value problems (IVPs) and also extended the new approach to a non-linear boundary value problem (BVP). The numerical implementation was composed using some few lines of executable Python codes. Our findings are instructive and quite revealing and supported by evidence from our numerical experiments and simulations.

Keywords: spectral rectangular collocation, polynomial interpolation, oscillatory solutions, initial value problems, boundary value problems, ordinary differential equations.

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1. Introduction

The genesis of the word spectral is not absolutely clear but presumably, arises from the genuine use of Fourier sines and cosines as basis functions [1] particularly in connection with scale between two extreme points, namely the spectrum. Spectral methods should not be confused with finite element methods (FEMs) based on the fact that they are closely related. The spectral methods use basis functions which are non-zero over the whole region, while the use of basis functions which are non-zero only on small sub-regions is particular to FEMs. Also, spectral methods are known to be global methods, and seek one solution for the entire region, rather than finite difference or finite element methods which seek a solution only in a local area to the element or node N .

Spectral collocation methods (SCMs) mainly use Chebyshev properties for its computations, reason why they are sometimes referred to as Chebyshev spectral collocation or pseudospectral methods. These SCMs have been firmly established in the numerical solution of differential equations (DEs) see [2,3,4] and other references therein. SCMs are based on the representation

of a real, continuous, well-behaved function on some interval $[a, b]$ using fast and stable algorithms such as barycentric interpolation formula in [5] and finite Fourier transform in [2]. Compared with other formalizations of spectral methods such as the Galerkin approximations (see [6]), they offer convenience in the presence of variable coefficients and non-linearities [7] which make these algorithms more accurate, for a given computational power. SCMs have become increasingly popular for solving DEs due to the fact that they enjoy rapid convergence. See for example the solution of unsteady boundary layer flows that are described by systems of coupled non-linear DEs in [8]. The unknown solution of the DE is approximated by a global interpolant, such as polynomial of high degree. This global interpolant is then differentiated exactly, and the expansion coefficients are determined by requiring the equations to be satisfied at an appropriate number of collocation points [9]. Since interpolation, differentiation, and evaluation are all linear operations, the process of obtaining approximations to the values of the derivative of a function at the collocation points can be expressed as a matrix-vector multiplication [9].

Spectral discretization of DEs have been of great use in computational mathematics, engineering and other branches of science. This idea become more interesting

with the emergence of the traditional row replacement strategy see ([3,10,11,12,13]) but not quite efficient for solving DEs with boundary conditions other than -1 and 1. In this case, the choice of row to enforce the boundary conditions become *ad hoc* [7]. Due to this snag, [7] introduced an efficient means of rectangularizing the $N \times N$ differentiation matrix to enable the enforcement of the boundary conditions. In this paper, we discretize the problem posed in the sense of the work in [7]. However, the explicit form of the work in [7] can be found in [11]. Interestingly, emerging computational approach for reformulating all kinds of DEs to systems of first order equations as been established in [14].

2. Barycentric Lagrange Interpolation Formulae

The Lagrange formula is in most cases the method of choice for dealing with polynomial interpolants contrary to the general belief that it is not good for approximation because of the identity property. The point is that the Lagrange formula must be modified through the formulae of barycentric interpolation. Consider the Lagrange formula as

$$P(x) = \sum_{i=0}^N \mathcal{L}_i(x) f_i, \tag{1}$$

where

$$\mathcal{L}_i(x) = \prod_{\substack{k=0 \\ k \neq i}}^N \frac{(x - x_k)}{(x_i - x_k)}, \tag{2}$$

with property

$$\mathcal{L}_i(x_k) = \begin{cases} 1, & i = k \\ 0, & i \neq k, \end{cases} \text{ for } i, k = 0, \dots, N. \tag{3}$$

As in [5], we define the barycentric weight as

$$w_i = \frac{1}{\prod_{k \neq i} (x_i - x_k)}, \quad i = 0, \dots, N, \tag{4}$$

and the barycentric formula of the first kind as

$$P(x) = \ell(x) \sum_{i=0}^N \frac{w_i}{x - x_i} f_i. \tag{5}$$

Equation (5), like the other authors is referred to as the improved Lagrange formula of (1). The formula (5) now demands $O(N^2)$ floating point operations (flops) to evaluate the weights (4) and does not depend on data f_i . This feature allows for the evaluation of several functions, and it only requires $O(N)$ operations each provided the w_i (4) are known while Newton formula requires the computation of a new tableau for each new function. The formula (5) 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

formula depends on the order which increases the computational cost as N increases, this many ordering leads to numerical instability [5]. However, these does not imply that the Newton formula have no relevance again. There are many cases where Newton interpolation is preferable, see for example, the construction of the multi-step methods for the numerical solution of ordinary differential equations (ODEs) in [15,16,17,18,19]. In addition, the barycentric formula of the first kind (5) can be further modified into a more elegant method, which is usually used in practice (see [5]). The barycentric formula of the second kind is given by

$$P(x) = \frac{\sum_{i=0}^N \frac{w_i}{x - x_i} f_i}{\sum_{i=0}^N \frac{w_i}{x - x_i}}. \tag{6}$$

The barycentric Lagrange interpolation formula (6) is the one with special and beautiful symmetry [5]. If weights w_i (4) have common factor, they may be cancelled without any impact on $P(x)$ [20]. Methods (6) and (5) both enjoy the advantage of updating weight w_i (4) in $O(N)$ operations to subsume a new set of f_i . The trigonometric form of formulas (4), (5), and (6) can be found in [5]. Fast reduction of generalized companion matrix pairs for the barycentric Lagrange interpolants have also been consider in the excellent works in [21,22]. The formulae defined in this paper are being collocated at specifically chosen set of points x_0, \dots, x_N . As in [3], the Chebyshev point of the first kind given by

$$\cos\left(\frac{\pi(2i+1)}{2N+2}\right), \tag{7}$$

and the Chebyshev point of the second kind is given by

$$\cos\left(\frac{i\pi}{N}\right). \tag{8}$$

The interpolation based on these points (7,8) converges as $N \rightarrow \infty$. Although, (8) has been used in practice due to the fact that it takes values at the boundary. Recently, equation (7) is becoming of necessity because of the crucial role it plays in the rectangularization of the $N \times N$ matrix, see the excellent work in [7,10,23]. The stability of barycentric Lagrange interpolation formulae (5) and (6) have been investigated in [24,25,26]. Barycentric formula of the second kind (6) may diverge when interpolated globally but can still enjoy the spectral accuracy provided that the given data if outside the interval $[-1, 1]$ is scale back to the interval $[-1, 1]$. This can be achieved by using the transformation:

$$\int_b^a f(x) dx = \frac{b-a}{2} \int_{-1}^1 f\left(\frac{b-a}{2}(s+1)+a\right) ds,$$

given two maps $f: [a, b] \rightarrow \mathbb{R}$ and $\Phi: [-1, 1] \rightarrow [a, b]$. Here, $\Phi(s) = \frac{b-a}{2}(s+1) + a$. Otherwise one should use the barycentric formula of the first kind (5) instead. However, one attractive ingredient in the barycentric

to obtain the N for the discretization process of each problem in this section. We have successfully introduced this transformation for obtaining the node N in the course of the research as it can rarely be found in the literature. Consequently, this is to synergize the relationship between the step size and node during the implementation process. The implementation was carried out using *numpy*, *numpy.linalg*, *pylab* while plottings were obtained using *matplotlib.pyplot*, which are all packages on *Python*.

Example 4.1 Oscillatory DE, Source: [27]

$$u''(x) + \rho^2 u(x) = 8 \left(\cos(x) + \frac{2}{3} \cos(3x) \right), \quad (16)$$

$$u(0) = 1, u'(0) = 0,$$

where $\rho = 5$ and $H = \frac{\pi}{10}$. The exact solution is

$$u(x) = \frac{1}{3} (\cos(x) + \cos(3x) + \cos(5x)).$$

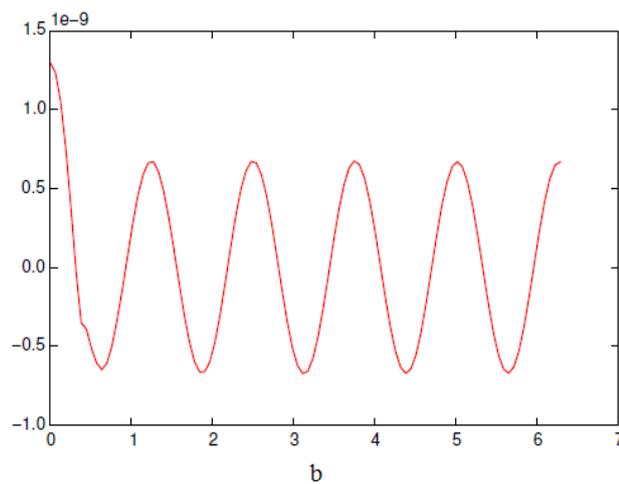
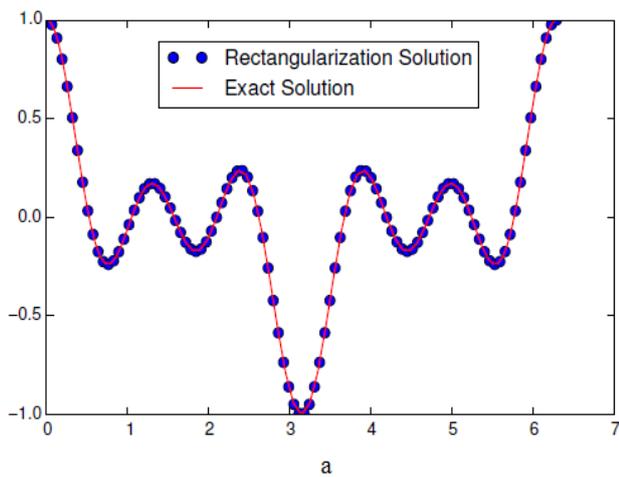


Figure 3. The exact and rectangularization solutions (a) of the problem (16) with the error at $N = 100$ (b)

Example 4.2 Complex DE, Source: [30]

$$u'' + u = 0.001e^{ix}, u(0) = 1, \quad (17)$$

$$u'(0) = 0.9995i, i^2 = -1.$$

The DE (17) represents motion on a perturbed circular orbit in complex plane in which the point $u(x)$ spirals slowly outward such its distance from the origin at any given time x is

$$\Omega(x) = \sqrt{(\text{Re}(u(x)))^2 + (\text{Im}(u(x)))^2}. \quad (18)$$

The theoretical solution is given by $u(x) = \cos x + 0.0005x \sin x + i(\sin x - 0.0005x \cos x)$. We analyze problem (17) using our rectangular discretization approach in the interval $[0,40]$ which corresponds to 20 orbits of the point $u(x)$ at $H = \frac{\pi}{2^q}$.

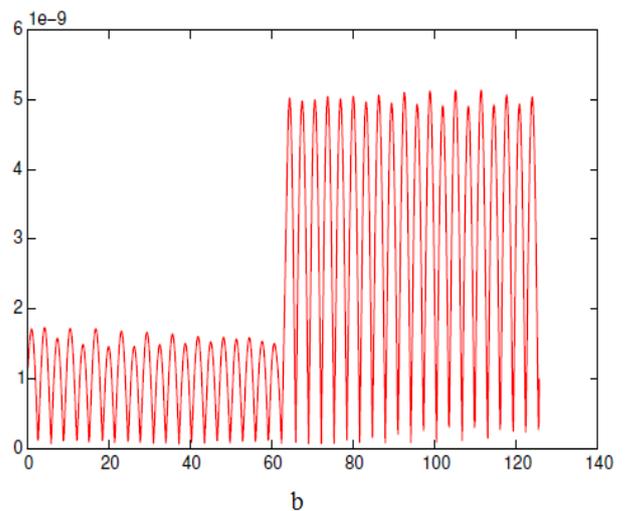
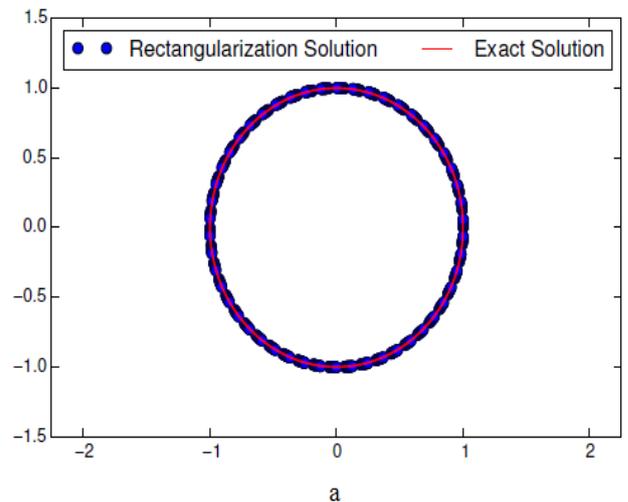


Figure 4. The exact and rectangularization solutions (a) of the problem (17) with the error at $N = 80$ (b)

Table 1. RDM solution to problem (17), $\Omega(x_f)=1.0019719765344917$, $x_f = 40\pi$

| q | N | Exact Solution $\Omega(x_f)$ | Rectangularization solution $\Omega(x_p)$ | Error $ \Omega(x_f) - \Omega(x_p) $ |
|-----|-----|------------------------------|---|-------------------------------------|
| 1 | 80 | 1.0019719765344917 | 1.0019719839296723 | 7.395180690039638e-09 |
| 2 | 160 | 1.0019719765344917 | 1.0019719775239968 | 9.895051444885894e-10 |

Table 2. The rectangularization approach as compared with existing results

| q | [28] | [29] | [30] | Rectangularization solution $\Omega(x_p)$ |
|--------------------|--------------|--------------|--------------|---|
| 1 | 0.9656450 | NA | 1.0095800 | 1.0019719 |
| 2 | 0.993734 | 1.004118 | 1.0096427 | 1.0019719 |
| Best error (q = 9) | 1.429765e-04 | 1.766276e-03 | 1.112223e-04 | 9.895051e-10 |

5. Spectral Rectangularization Approach for Non-linear DE

The spectral rectangularization by collocation method for non-linear DEs is another area of exploit. In this non-linear case, the scalar boundary value problem (BVP) brings no significant complications for the approach. We consider an m th order non-linear BVP

$$h^m(u) = f(x), \quad -1 < x < 1, \tag{19}$$

$$g_i(u^{m-1}) = c_i, \quad i = 1, \dots, m, \tag{20}$$

where h is the non-linear differential operator and g_i is the non-linear differential functional. To achieve this task, we employ the Newton-iterative scheme for polynomial approximation as illustrated in [31]. At $m = 1$ in (19), we have the vector form as

$$\mathbf{h}(\mathbf{u}) - \mathbf{f} = 0. \tag{21}$$

On perturbing the solution u , say $\mathbf{u} + \delta$ and expanding $\mathbf{h}(\mathbf{u} + \delta)$ in Taylor's series about $\delta = 0$, we have

$$\mathbf{h}(\mathbf{u} + \delta) - \mathbf{f} = 0, \tag{22}$$

$$\mathbf{h}(\mathbf{u}) + \mathbf{h}'(\mathbf{u})\delta + O(h^2) = \mathbf{f}, \tag{23}$$

$$\mathbf{h}'(\mathbf{u})\delta = \mathbf{f} - \mathbf{h}(\mathbf{u}). \tag{24}$$

We multiply the re-sampling matrix $P_{N,-m}$ by (24).

$$P_{N,-m}\mathbf{h}'(\mathbf{u})\delta = P_{N,-m}[\mathbf{f} - \mathbf{h}(\mathbf{u})], \tag{25}$$

where \mathbf{h}' is a N square matrix. Now, for the case of the system

$$\begin{cases} u' + Yu^n = 0 \\ u(0) = u_0, \quad x > 0, \quad n \in \mathbb{N}. \end{cases} \tag{26}$$

We can express $h(u) = u' + Yu^n$ and $f = 0$, and further express

$$\mathbf{h}(\mathbf{u}) = D_{N+m}\mathbf{u} + \Upsilon(\mathbf{u} \circ \mathbf{u} \circ \dots \circ \mathbf{u}), \tag{27}$$

where \circ is the Hadamard point-wise or element-wise product. We then differentiate $\mathbf{h}(\mathbf{u})$

$$\mathbf{h}'(\mathbf{u}) = D_{N+m} + \Upsilon(\mathbf{u}^{n-1} + (n-1)\mathbf{u}^{n-1} + nO(\mathbf{u}^q)), \tag{28}$$

$$= D_{N+m} + \Upsilon(\mathbf{u}^{n-1} + (n-1)\mathbf{u}^{n-1}), \tag{29}$$

$$= D_{N+m} + \Upsilon((n-1+1)\mathbf{u}^{n-1}), \tag{30}$$

$$= D_{N+m} + n\Upsilon\mathbf{u}^{n-1}, \tag{31}$$

$$= D_{N+m} + n\Upsilon(\text{diag}(\mathbf{u})^{n-1}). \tag{32}$$

We are interested in the element in the main diagonal that is the reason why we apply $\text{diag}()$. We then substitute our result into equation (24) to have

$$\begin{aligned} &(D_{N+m} + n\Upsilon(\text{diag}(\mathbf{u})^{n-1}))\delta \\ &= 0 - D_{N+m}\mathbf{u} + \Upsilon(\mathbf{u} \circ \mathbf{u} \circ \dots \circ \mathbf{u}), \end{aligned} \tag{33}$$

where the Jacobian matrix $J = D_{N+m} + n\Upsilon(\text{diag}(\mathbf{u})^{n-1})$ and $\delta = x_{n+i} - x_n$. More clearly,

$$\mathbf{h}'(\mathbf{u})\delta(\mathbf{x}) = \mathbf{f}(\mathbf{x}) + \mathbf{h}(\mathbf{u}). \tag{34}$$

Hence, we can solve the system (34).

Example 5.1 Consider a non-linear problem. Source: [32]

$$u' = u^2 + 1, \quad u(0) = 1, \quad x \in [0, 1], \quad H = 0.07, \quad N = 20. \tag{35}$$

Table 3. The rectangularization solution to the non-linear problem (35) as compared with other results

| Authors | [32] | [33] | [34] | Rectangularization solution |
|------------|-----------|---------|----------|-----------------------------|
| Best Error | 2.420e-07 | 2.0e-06 | 1.337e-6 | 5.10702591328e-15 |

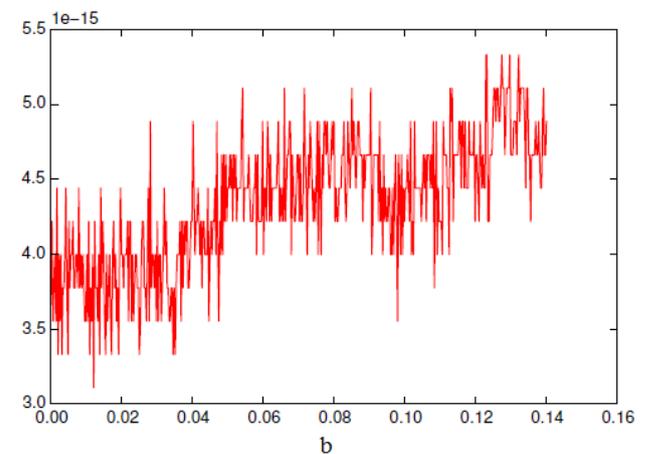
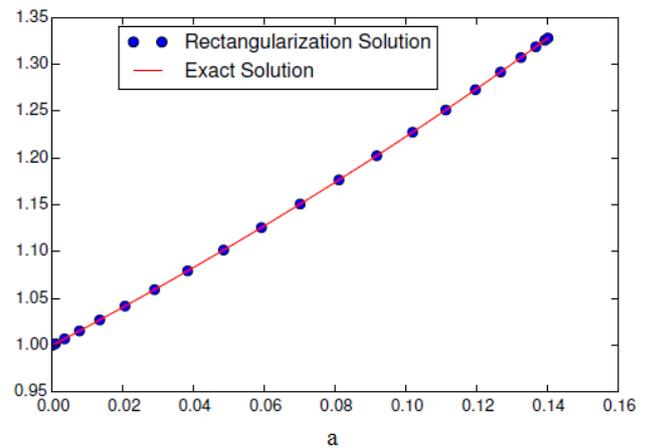


Figure 5. The exact and rectangularization solutions to non-linear problem (35) (a) and the error (b)

6. Conclusion

We have properly formulated and implemented our spectral method based on the state-of-the-art rectangularization approach for the solution of oscillatory IVPs and non-linear BVP in DEs. This approach requires the discretization of polynomials, forcing DEs into polynomial through the introduction of the re-sampling matrix $P_{N,-m}$ which re-samples the differentiated polynomials into a lower-degree subspace. The solutions of the DEs are then represented as finite vectors of their values at certain points. Each such vector implicitly defines a global interpolant, and operations on the DEs are replaced by the same operations applied to the corresponding interpolants.

Emphasis are now being placed on spectral methods when approximating for which we have introduced the concept of transforming the N into H using the relation (15) before discretizing the IVPs and BVP through rectangularization. In doing this, we observe spectral convergence unlike other conventional approaches. Our results of striking accuracy with efficient use of computer resources outperform the existing results (see Table 1, Table 2, Table 3). In particular, result as in Figure 3, Figure 4, Figure 5 shows the spectral accuracy and efficiency of the new rectangularization approach. It is our hope that the algorithm of emerging numerical codes for the discretization of DEs will be dominated by the used of the rectangularization approach just as it has already started in [7].

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