

Numerical Solution of Ordinary Differential Equations in Fluctuationlessness Theorem Perspective

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Abstract: This paper presents a new method based on Fluctuationlessness Theorem that was proven recently for getting the numerical solutions to the Ordinary Differential Equations over appropriately defined Hilbert Spaces. Approximations to the solution are evaluated at a series of discrete points. These points are constructed as the eigenvalues of the independent variable's matrix representation restricted to an n dimensional subspace of the Hilbert Space under consideration. The approximated solution is written in the form of an n -th degree polynomial of the independent variable. The unknown coefficients are found by setting up a system of linear equations such that this solution satisfies the initial condition and the differential equation at the grid points. The numerical quality of the solution can be increased by taking greater values of n .

Key-Words: Eigenvalues, Ordinary Differential Equations, Fluctuations, Quantum Mechanics, Hilbert Spaces.

1 Introduction

An important element in the investigation of many physical systems is the mathematical modeling involving the constructions which are sufficiently correct descriptions. The handling of these formulae should not be too complicated. Differential equations arise in almost everywhere when we concern with the dynamical behavior of the system under consideration. These may be either ordinary or partial differential equations depending on the level of the multivariate in the system. Here we focus on the case of univariate, and therefore, ordinary differential equations. Despite this may be considered too simple, our main purpose is the methodology, and in a heuristic point of view it is better to start with the simplest case to construct a strong basis for a future theory. Although there is a huge knowledge accumulation about ordinary differential equations, the method we are trying to develop here seems to have a great capability of rapid numerical convergence. Despite the existence of a lot of clear and powerful methods to get the solutions, there are rather limited number of analytical approaches containing finite number of manipulations, in other words, exact solutions to the ordinary differential equations under consideration. This urged scientists to develop mostly iterative numerical solutions.[1, 2]

Fluctuations arise in every probabilistic event and

somehow describe the rather random plus or minus deviations from the means. In these cases, the individual components' behaviors can not be determined in the framework of causality. Instead, the evolution of the probability can be determined. Amongst the areas where the fluctuations gain a lot of importance, Quantum Mechanics and Non-equilibrium Statistical Mechanics, can be primarily considered. Our purpose is not to get into the details of the fluctuations and their roles in these kinds of phenomena here. Instead, we will deal with the case of fluctuationlessness in mathematical sense. We will work in an appropriately chosen Hilbert Space throughout the paper.

This paper is organized as follows: In the second section Fluctuationlessness Theorem, which is needed for this work, is explained. The third section is devoted the usage of this theorem in numerical solution for the first order linear ODEs for rather illustration. The fourth section covers the implementations presented in tables comparatively. The fifth section completes the paper via concluding remarks.

2 Fluctuationlessness Theorem

We consider the Hilbert Space \mathcal{H} on univariate functions which are analytic and therefore square integrable on a given interval as the main space and focus on its subspace \mathcal{H}_n spanned by n orthonormal func-

tions $u_1(x), u_2(x), \dots, u_n(x)$. We define the inner product of two functions $f, g \in \mathcal{H}$ as

$$(f, g) \equiv \int_a^b dx w(x) f(x) g(x), \quad (1)$$

where $w(x)$ is a given weight function. We can express a function $g(x)$ in \mathcal{H}_n as a linear combination of the functions $u_1(x), u_2(x), \dots, u_n(x)$ as

$$g(x) \equiv \sum_{i=1}^n g_i u_i(x) \quad (2)$$

where the coefficients g_i 's are real constants and depend on the structure of the function $g(x)$. This dependency can be determined by the use of the orthonormality property of the basis functions. Therefore we can calculate the inner product of u_k and $g(x)$ as follows:

$$\begin{aligned} (u_k, g) &\equiv \left(u_k, \sum_{i=1}^n g_i u_i \right) = \sum_{i=1}^n g_i (u_k, u_i) \\ &= \sum_{i=1}^n g_i \delta_{k,i} = g_k, \quad 1 \leq k \leq n \end{aligned} \quad (3)$$

Substituting this result into (2) we obtain

$$\begin{aligned} g(x) &= \sum_{i=1}^n u_i(x) (u_i, g) \\ &\equiv \sum_{i=1}^n P_i g(x) \equiv P^{(n)} g(x) \end{aligned} \quad (4)$$

Here P_i is the integral operator which projects to the subspace spanned by the basis function $u_i(x)$. The operator $P^{(n)}$ projects to the n -dimensional space spanned by the functions $u_1(x), \dots, u_n(x)$. The operator $P^{(n)}$ becomes unit operator when it acts on the subspace spanned by the basis functions $u_1(x), \dots, u_n(x)$, otherwise $P^{(n)}$ projects from \mathcal{H} to this subspace.

Now we define a new operator, \hat{x} which multiplies its operand by x and its domain is \mathcal{H} . The action of this operator on a function from \mathcal{H}_n can be expressed as follows.

$$\hat{x}g(x) = \sum_{j=1}^n g_j \hat{x}u_j(x) = \hat{x}P^{(n)}g(x) \quad (5)$$

As we can see from this equation, although the function $P^{(n)}g(x)$ is in the space spanned by the basis functions $u_1(x), \dots, u_n(x)$, the function formed by multiplying this function with x may not be in this space. In those cases, \hat{x} operator will cause a space

extension. To avoid from this situation, we will work with $P^{(n)}\hat{x}$ instead of $P^{(n)}\hat{x}$. In this case we obtain

$$\begin{aligned} P^{(n)}\hat{x}g(x) &= \sum_{j=1}^n g_j P^{(n)}\hat{x}u_j(x) \\ &= P^{(n)}\hat{x}P^{(n)}g(x) \end{aligned} \quad (6)$$

If we denote the operator which is the restriction of \hat{x} from \mathcal{H}_n to \mathcal{H}_n by \hat{x}_{res} and define as,

$$\hat{x}_{res} \equiv P^{(n)}\hat{x}P^{(n)} \quad (7)$$

then we can construct its matrix representation by following standard procedures.

We define a function $h(x)$ via

$$h(x) \equiv P^{(n)}\hat{x}P^{(n)} = \sum_{j=1}^n g_j P^{(n)}\hat{x}P^{(n)}u_j(x) \quad (8)$$

and see that $h(x)$ is in the space spanned by the functions $u_1(x), u_2(x), \dots, u_n(x)$. Therefore we can write

$$h(x) = \sum_{k=1}^n h_k u_k(x) \quad (9)$$

and

$$\sum_{k=1}^n h_k u_k(x) = \sum_{j=1}^n g_j P^{(n)}\hat{x}P^{(n)}u_j(x) \quad (10)$$

which implies

$$h_i = \sum_{j=1}^n \left(u_i, P^{(n)}\hat{x}P^{(n)}u_j \right) g_j, \quad 1 \leq i \leq n \quad (11)$$

It is better to express the above relation in terms of cartesian vectors. We define

$$\mathbf{g} = [g_1 \dots g_n]^T, \quad \mathbf{h} = [h_1 \dots h_n]^T, \quad (12)$$

$$X_{i,j}^{(n)} = \left(u_i, P^{(n)}\hat{x}P^{(n)}u_j \right), \quad 1 \leq i, j \leq n \quad (13)$$

So equation (11) can be rewritten in a compact form by these matrices and vectors as follows:

$$\mathbf{h} = \mathbf{X}^{(n)} \mathbf{g} \quad (14)$$

Here the matrix $\mathbf{X}^{(n)}$ is the matrix representation of the operator \hat{x}_{res} from \mathcal{H}_n to \mathcal{H}_n . This matrix maps from the n -dimensional cartesian space \mathcal{K}_n to the same space.

Now we can write the following equation for the operator \hat{x} .

$$\begin{aligned} \hat{x} &\equiv \left(P^{(n)} + [\hat{I} - P^{(n)}] \right) \hat{x} \left(P^{(n)} + [\hat{I} - P^{(n)}] \right) \\ &= P^{(n)}\hat{x}P^{(n)} + [\hat{I} - P^{(n)}] \hat{x}P^{(n)} \\ &\quad + P^{(n)}\hat{x}[\hat{I} - P^{(n)}] + [\hat{I} - P^{(n)}] \hat{x}[\hat{I} - P^{(n)}] \end{aligned} \quad (15)$$

We call \hat{x}_{fluc} for the part

$$\begin{aligned} \hat{x}_{fluc} &\equiv [\hat{I} - P^{(n)}] \hat{x} P^{(n)} + P^{(n)} \hat{x} [\hat{I} - P^{(n)}] \\ &+ [\hat{I} - P^{(n)}] \hat{x} [\hat{I} - P^{(n)}] \end{aligned} \quad (16)$$

and the operator \hat{x} now can be written as the sum of \hat{x}_{res} and \hat{x}_{fluc} .

The operator $[\hat{I} - P^{(n)}]$ approaches to $\hat{0}$ operator as n goes to infinity. The matrix representation of this operator in the space spanned by the basis functions $u_1(x), \dots, u_n(x)$ is the $\mathbf{0}$ matrix. However, its infinite matrix representation in \mathcal{H} differs from infinite zero matrix, although its norm gets smaller as n increases. This nonzero behavior can be interpreted as the interactions between \mathcal{H}_n and its complementary companion over \hat{x} . The indices of the basis functions appearing in the operator $[\hat{I} - P^{(n)}]$ are greater than n . The orthonormality of the basis functions brings the oscillations in the variation of these basis functions. As a matter of fact, u_n has exactly n zeros in the orthogonality domain. This means oscillations between positive and negative values. The frequency of these oscillations increases as n grows and this results in great cancelations amongst the output terms from the action of $[\hat{I} - P^{(n)}]$ on any function in \mathcal{H} . In other words, the image of any function from \mathcal{H} under this operator fluctuates around zero and somehow measures the fluctuations around zero. Hence we call this entity "Fluctuation Operator of n -th Order".

The discussions above can be applied on the square of \hat{x} also. In this case the matrix representation of \hat{x}_{fluc}^2 operator in \mathcal{H}_n is not equal to zero matrix and the matrix representation of $P^{(n)} \hat{x} [\hat{I} - P^{(n)}] \hat{x} P^{(n)}$ operator in this space is equal to the subtraction of the square of the matrix representation of $P^{(n)} \hat{x} P^{(n)}$ from $P^{(n)} \hat{x}^2 P^{(n)}$, hence it is a positive definite entity. This term describes the dominant contribution coming from the fluctuations. Therefore we call $P^{(n)} \hat{x} [\hat{I} - P^{(n)}] \hat{x} P^{(n)}$ "Independent Variable's First Order Fluctuation Operator".

The approximations by ignoring the terms which contain the Fluctuation operator is called as **Fluctuationlessness Approximation**. Therefore we can express the \hat{x} operator as

$$\hat{x} \approx \hat{x}_{res} \equiv P^{(n)} \hat{x} P^{(n)} \quad (17)$$

in the fluctuationlessness limit. An algebraic multiplication by a function type operator \hat{f} is defined via an analytical function $f(x)$ on the interval $[a, b]$ as follows:

$$\hat{f} \equiv f(\hat{x}) \quad (18)$$

Hence \hat{f} is an algebraic operator in terms of \hat{x} and its fluctuationlessness approximation can be given as

$$\hat{f} \approx f(\hat{x}_{res}) \equiv f(P^{(n)} \hat{x} P^{(n)}) \quad (19)$$

The matrix representation which is the counterpart of this approximation is written as follows

$$\mathbf{M}_f^{(n)} \approx f(\mathbf{X}^{(n)}) \quad (20)$$

where $\mathbf{M}_f^{(n)}$ stands for the matrix representation of the operator \hat{f} 's restricted form mapping from \mathcal{H}_n to \mathcal{H}_n . [3, 4, 5]

3 Application of the Fluctuationlessness Theorem on Numerical Solution of ODEs

We consider the following first order linear nonhomogeneous ordinary differential equation with an initial condition, for illustrative purposes.

$$\begin{aligned} f'(x) + a_0(x) f(x) &= q(x), \\ f(0) &= f_0 \end{aligned} \quad (21)$$

We will search for the solution in the interval of $[0, 1]$. We take the space of the square integrable functions as the Hilbert Space, \mathcal{H} . We define the inner product of two functions g_1, g_2 in this space as

$$(g_1, g_2) \equiv \int_0^1 dx w(x) g_1(x) g_2(x), \quad (22)$$

where $w(x)$ is a weight function normalized as follows:

$$\int_0^1 dx w(x) = 1 \quad (23)$$

We define an orthonormal set of functions as

$$\{u_i(x)\}_{i=1}^{\infty}$$

Each function in this set is generated from the independent set $\{1, x, x^2, \dots, x^n, \dots\}$, successively. We take the first element as

$$u_1(x) = 1. \quad (24)$$

Instead of using the independent variable x , we will use the algebraic multiplication operator \hat{x} which multiplies its operand by the independent variable x , throughout the work. The spectrum of this operator is the closed interval $[0, 1]$. Therefore it has a continuous spectrum and there is no multiplicity in any eigenvalues. For the functions $a_0(x)$, $f(x)$ and $q(x)$

we will respectively use \widehat{a}_0 , \widehat{f} and \widehat{q} which multiply their operands by $a_0(x)$, $f(x)$ and $q(x)$, respectively. Their spectrums are the continuous intervals of $[a_0(x)_{\min}, a_0(x)_{\max}]$, $[f(x)_{\min}, f(x)_{\max}]$ and $[q(x)_{\min}, q(x)_{\max}]$, respectively. They may have multiple eigenvalues depending on the structure of the functions. The operator \widehat{f}' is used for the derivative of $f(x)$ which multiplies its operand by $f'(x)$. The ordinary differential equation in (21) can be expressed in terms of the images of u_1 under all these operators mentioned above as follows:

$$(\widehat{f}' + \widehat{a}_0\widehat{f})u_1(x) = \widehat{q}u_1 \quad (25)$$

We can express the equation (25) in corresponding cartesian space by changing each operator by its matrix representation and the function $u_1(x)$ by the unit cartesian vector \mathbf{e}_1 whose only nonzero element is located at the first position and has the value of 1. In other words, let \mathbf{M}_g denote the matrix representation of the operator \widehat{g} . We can write the following equation:

$$[\mathbf{M}_{f'} + \mathbf{M}_{a_0}\mathbf{M}_f]\mathbf{e}_1 = \mathbf{M}_q\mathbf{e}_1, \quad (26)$$

Here the vectors and the matrices are of infinite dimension. In order to work on finite dimensional entities we will use an n -dimensional subspace \mathcal{H}_n of \mathcal{H} spanned by the functions $u_1(x), u_2(x), \dots, u_n(x)$ instead of the space \mathcal{H} . Therefore we need to reduce the dimension by using $n \times n$ upperleftmost part of the related matrices. Hence, we can rewrite (26) as

$$[\mathbf{M}_{f'}^{(n)} + \mathbf{M}_{a_0}^{(n)}\mathbf{M}_f^{(n)}]\mathbf{e}_1^{(n)} = \mathbf{M}_q^{(n)}\mathbf{e}_1^{(n)} \quad (27)$$

If we denote the matrix representation of the operator \widehat{x} on the subspace \mathcal{H}_n as $\mathbf{X}^{(n)}$ as we did before, then we can write the following approximated expressions by using the Fluctuationlessness Theorem.

$$\begin{aligned} \mathbf{M}_{f'}^{(n)} &\approx f'(\mathbf{X}^{(n)}) \\ \mathbf{M}_{a_0}^{(n)} &\approx a_0(\mathbf{X}^{(n)}) \\ \mathbf{M}_f^{(n)} &\approx f(\mathbf{X}^{(n)}) \\ \mathbf{M}_q^{(n)} &\approx q(\mathbf{X}^{(n)}) \end{aligned} \quad (28)$$

The matrix $\mathbf{X}^{(n)}$ is symmetric and its spectral representation can be written as follows.

$$\mathbf{X}^{(n)} = \sum_{i=1}^n \xi_i \mathbf{x}_i \mathbf{x}_i^T, \quad (29)$$

Here \mathbf{x}_i is the eigenvector with a unit norm of the i -th eigenvalue ξ_i . Substituting (28) in (27) we obtain the

following result.

$$\sum_{i=1}^n [f'(\xi_i) + a_0(\xi_i)f(\xi_i) - q(\xi_i)] (\mathbf{x}_i^T \mathbf{e}_1^{(n)}) \mathbf{x}_i = 0 \quad (30)$$

Since the eigenvectors are linearly independent the coefficients of \mathbf{x}_i should vanish. So we can write the following equations:

$$f'(\xi_i) + a_0(\xi_i)f(\xi_i) - q(\xi_i) = 0 \quad 1 \leq i \leq n \quad (31)$$

We propose the following structure for the approximated solution of the differential equation.

$$p(x) \equiv \sum_{i=0}^n f_i x^i \quad (32)$$

To find the unknown constants f_i , ($1 \leq i \leq n$) in (32) we construct a set of vectors and matrices as follows:

$$\mathbf{f}^T \equiv [f_1 \quad \dots \quad f_n]$$

$$\mathbf{a}^T \equiv [a_0(\xi_1) \quad \dots \quad a_0(\xi_n)]$$

$$\mathbf{q}^T \equiv [q(\xi_1) \quad \dots \quad q(\xi_n)]$$

$$\mathbf{V} = \begin{bmatrix} 1 & \xi_1 & \dots & \xi_1^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \xi_n & \dots & \xi_n^{n-1} \end{bmatrix}$$

$$\mathbf{K}_1 \equiv \begin{bmatrix} a_0(\xi_1)\xi_1 & 0 & \dots & 0 \\ 0 & a_0(\xi_2)\xi_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_0(\xi_n)\xi_n \end{bmatrix}$$

$$\mathbf{K}_2 \equiv \begin{bmatrix} 1 & 0 & 0 & \vdots \\ 0 & 2 & 0 & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & n \end{bmatrix}$$

Since all the eigenvalues are distinct, then \mathbf{V} is invertible. Therefore \mathbf{f} can be found uniquely as

$$\mathbf{f} = (\mathbf{K}_1\mathbf{V} + \mathbf{V}\mathbf{K}_2)^{-1}(\mathbf{q} - \mathbf{a}) \quad (33)$$

4 Implementation

In this section we will give some numerical examples. For the implementations some linear first order differential equations are selected, their exact and numerical solutions are presented in tables comparatively. The mesh points we used for calculations are chosen in the interval $[0, 1]$ as the eigenvalues of the representation matrix $\mathbf{X}^{(n)}$ which has the general term formed by the inner product of the functions $u_i(x)$ and $xu_j(x)$, where the indices i and j are between 1 and n included. We used Mathematica 5.2 for calculations. We obtain the results on 5 grid points for the solutions of the differential equations. We work on the space that is spanned by the orthonormal vectors

$$\begin{aligned} u_1(x) &= 1 \\ u_2(x) &= \sqrt{3}(2x - 1) \\ u_3(x) &= \sqrt{5}(6x^2 - 6x + 1) \\ u_4(x) &= \sqrt{7}(20x^3 - 30x^2 + 12x - 1) \\ u_5(x) &= 210x^4 - 420x^3 + 270x^2 - 60x + 3 \end{aligned} \quad (34)$$

The representation matrix obtained by the inner product of the vectors in (34) is a symmetric, positive definite, 3-banded matrix. The eigenvalues of this matrix are 0.0469, 0.2300, 0.5000, 0.7692 and 0.9531. We will consider the initial value problems throughout the work.

Our first equation is a homogenous linear first order ODE with constant coefficients given as:

$$y'(x) - y(x) = 0, \quad y(0) = 1 \quad (35)$$

The analytical solution for this equation is $y(x) = e^x$. Using the methods we developed in the third section, we obtained the following results for the numerical and analytical solutions.

i	Analytical	Numerical
1	1.0480277	1.0480289
2	1.2595636	1.2595603
3	1.6487212	1.6487229
4	2.1581139	2.1581123
5	2.5937116	2.5937127

From this table we can see that the approximated and the exact functions are almost equal to each other, the numerical solution is accurate up to 6 digits.

Now, we consider the following first order homogenous ODE with constant coefficients.

$$y'(x) + 2y(x) = 0, \quad y(0) = 1 \quad (36)$$

The analytical solution for this equation is

$$y(x) = e^{-2x}.$$

In the following table we present the analytical and numerical solutions we obtained.

i	Analytical	Numerical
1	0.910446	0.910462
2	0.630318	0.630296
3	0.367879	0.367904
4	0.214710	0.214686
5	0.148647	0.148665

We can observe from this table that, the numerical solution is correct up to 4 digits. If we compare this solution with the previous solution, although the problems and the solutions are similar, the accuracy shows a slight difference. This is because of the behavior of the exponential function. As the absolute value of the power of exponential functions increases, the smoothness of the graph decreases. Therefore the numerical solution moves away from the exact solution depending on the power of $\exp(x)$.

Now we will work with the following first order linear ODE with variable coefficients presented below:

$$y'(x) + xy(x) = 0, \quad y(0) = 1 \quad (37)$$

The exact solution for this problem is

$$y(x) = e^{-x^2/2}.$$

We can see the results for the exact and approximated solutions in the following table.

i	Analytical	Numerical
1	0.998900	0.998896
2	0.973725	0.973730
3	0.882497	0.882493
4	0.743891	0.743893
5	0.634962	0.634961

We observe from this table that the accuracy is of order 5. Therefore we had a good approximation for this problem.

Continuing with the first order linear ODEs with variable coefficients, we will obtain a numerical solution for the following problem.

$$y'(x) + \sin(x)y(x) = 0, \quad y(0) = 2 \quad (38)$$

Here the analytical solution is $y(x) = 2e^{\cos x - 1}$. The table below shows the results for the analytical and

numerical solutions to the equation (38).

i	Analytical	Numerical
1	1.997801058	1.9977937
2	1.947679782	1.9476848
3	1.769557902	1.7695603
4	1.509216170	1.5092068
5	1.312999357	1.3130095

It can be seen from this table that the numerical solution of the problem in (38) has a 4-digit accuracy.

Now we will focus on the nonhomogeneous linear first order ODEs. The following is an initial value problem with constant coefficients and the right hand side of the equation is a constant.

$$y'(x) + 4y(x) = 20, \quad y(0) = 2 \quad (39)$$

The exact solution for this equation can be given as

$$y(x) = 5 - 3e^{-4x}.$$

We present the numerical and analytical results in the following table.

i	Analytical	Numerical
1	2.51326	2.51203
2	3.80810	3.80978
3	4.59399	4.59215
4	4.86170	4.86356
5	4.93371	4.93216

We observe from this table that the numerical solution to the problem (38) is 2-digit accurate. Since the exact solution contains 4-th power of the exponential function, the numerical solution showed a slight difference.

Our last example is with constant coefficients but the right hand side is a function of x .

$$y'(x) - 4y(x) = \cos x, \quad y(0) = 1 \quad (40)$$

The analytical solution for this equation is

$$y(x) = \frac{1}{17} (21e^{4x} - 4 \cos x + \sin x).$$

The numerical and analytical results can be seen in the following table.

i	Analytical	Numerical
1	1.25798	1.29379
2	2.89361	2.85366
3	8.94937	8.99647
4	26.6677	26.6461
5	55.8175	55.8789

This numerical solution is a 1-digit accuracy to the problem (40). This accuracy is less than the results we obtained for the other problems. This may be caused again by the high power of the exponential function in the solution, which diminishes the smoothness of the function.

5 Conclusion

In this work a new method has been developed for an approximation of the numerical solution to the linear ODEs by using Fluctuationlessness Theorem. Only initial value problems were considered in this stage and the solution was achieved in the interval of $[0, 1]$. The results are considerably satisfactory. However the structure of the functions in the solution affected the order of approximation. If the coefficients in the approximated solution are compared with the Maclaurin coefficients of the exact solution, the quality of the approximation can be noticed. This method is an introductory form for the moment, but it will be applied to higher order initial and boundary value problems. Also the convergence will be tested for an arbitrary interval $[a, b]$. It is aimed to solve nonlinear ODEs and even PDEs numerically by Fluctuationlessness Theorem for the future applications.

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