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ORIGINAL PAPER

The fluctuationlessness approach to the numerical integration of functions with a single variable by integrating Taylor expansion with explicit remainder term

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Abstract In this paper we give the definition of the Fluctuationlessness concept and using this concept we make approximations to univariate functions by using Taylor expansion with the explicit remainder term. Then integrating this approximate expression we obtain a new quadrature-like numerical integration method. The results of numerical experiments are compared with the results obtained from the corresponding Taylor series expansion without the remainder term and errors are analyzed.

Keywords Taylor formula · Fluctuationlessness theorem · Quadrature · Numerical integration explicit remainder term · Matrix representation

1 Introduction

It is well known that many problems both in Physical Chemistry and in Quantum Chemistry require integration multivariate as well as univariate, even though problems involving multivariate integration are treated via univariate integration. Hence, seeking novel integration methods that are more efficient then the standart ones are still of undeniable importance. This work is devoted to developing such a method and

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uses the recently suggested fluctuation-free integration together with Taylor expansion and its explicit remainder term.

In the section following the introduction we state the Fluctuationlessness theorem recently conjectured and proven by M. Demiralp and a rather detailed discussion is held about this new concept which constitutes the basis of the present work. In the third section we form a new approximation scheme for functions of a single variable by restructuring the Taylor expansion with explicit remainder term and we obtain the basic structure of the new numerical integration scheme. Then in the upcoming section we form an orthonormal basis set, give the necessary formulas for calculating the coefficients of the three term recursion formula, form the Jacobi matrix and rewriting the remainder term via Fluctuationlessness theorem we obtain the final form of our new numerical integration method for univariate functions. In the fifth section we present and discuss the results of some of the numerical experiments performed. Finally we conclude the subject and suggest some prospective areas of application.

2 Fluctuationlessness theorem

The Fluctuationlessness approximation is based on a theorem which was conjectured and proven by M. Demiralp. This theorem states that the matrix representation of an algebraic operator which multiplies its argument by a scalar univariate function, is identical to the image of the independent variable's matrix representation over the same subspace via the same basis set, under that univariate function, when the fluctuation terms are ignored.

Now, to give further details about the theorem [2–5,7,6], let $\mathcal{M}_f$ stand for the matrix representation of the function f, we can write down the approximation

$$\mathcal{M}_f = \left(u,\, fu^T\right) \approx f\left(u,\, xu^T\right) \tag{2.1}$$

The function $f = f(x)$ is defined over the interval $[a, b]$ including $x = 0$ and is assumed to be analytic throughout its domain with $u_i(x)$'s being orthogonal basis functions of the Hilbert space from which our functions are chosen. We define $\mathbf{u}(x) = [u_1(x) \ldots u_n(x)]^T$. The inner product of two functions $g(x)$ and $h(x)$ under a weight function $w(x)$ is defined as follows

$$(g, h) = \int_a^b dx\, w(x) g(x) h(x) \tag{2.2}$$

Now, if we express the function $f(x)$ as

$$f(x) = \sum_{i=0}^{\infty} f_i x^i \tag{2.3}$$

and place this expression in (2.1) we obtain

$$\mathcal{M}_f = \left(\mathbf{u}, \sum_{i=0}^{\infty} f_i x^i \mathbf{u}^T\right) \tag{2.4}$$

which can than be written as

$$\mathcal{M}_f = \sum_{i=0}^{\infty} f_i \left(\mathbf{u}, x^i \mathbf{u}^T\right) \tag{2.5}$$

At this stage let us consider two operators $\mathcal{L}_1$ and $\mathcal{L}_2$ from Hilbert space, and write the inner product

$$\left(\mathbf{u}, \mathcal{L}_1 \mathcal{L}_2 \mathbf{u}^T\right) = \left(\mathbf{u}, \mathcal{L}_1 \left[P^{(n)} + \left(I - P^{(n)}\right)\right] \mathcal{L}_2 \mathbf{u}^T\right) \tag{2.6}$$

The following definitions being made for the operators I and $P^{(n)}$

$$\begin{aligned} Ig &= \sum_{j=1}^{\infty} (u_j, g) u_j(x) \\ P^{(n)} g &= \sum_{j=1}^{n} (u_j, g) u_j(x) \end{aligned} \tag{2.7}$$

we can rewrite (2.6) as

$$\left(\mathbf{u}, \mathcal{L}_1 \mathcal{L}_2 \mathbf{u}^T\right) = \left(\mathbf{u}, \mathcal{L}_1 P^{(n)} \mathcal{L}_2 \mathbf{u}^T\right) + \left(\mathbf{u}, \mathcal{L}_1 \left(I - P^{(n)}\right) \mathcal{L}_2 \mathbf{u}^T\right) \tag{2.8}$$

It's clear that when n goes to infinity $P^{(n)}$ tends to I, from which we deduce that $I - P^{(n)}$ tends to 0. In this situation we are left with the fluctuationlessness term only. This allows us to write the approximation

$$\begin{aligned} \left(\mathbf{u}, \mathcal{L}_1 \mathcal{L}_2 \mathbf{u}^T\right) &\approx \left(\mathbf{u}, \mathcal{L}_1 P^{(n)} \mathcal{L}_2 \mathbf{u}^T\right) \\ &= \left(\mathbf{u}, \mathcal{L}_1 \sum_{i=1}^{n} \left(u_i, \mathcal{L}_2 \mathbf{u}^T\right) u_i(x)\right) \\ &= \sum_{i=1}^{n} \left(\mathbf{u}, \mathcal{L}_1 \left(u_i, \mathcal{L}_2 \mathbf{u}^T\right) u_i(x)\right) \\ &= \sum_{i=1}^{n} (\mathbf{u}, \mathcal{L}_1 u_i) \left(u_i, \mathcal{L}_2 \mathbf{u}^T\right) \\ &= \left(\mathbf{u}, \mathcal{L}_1 \mathbf{u}^T\right) \left(\mathbf{u}, \mathcal{L}_2 \mathbf{u}^T\right) \end{aligned} \tag{2.9}$$

Therefore the approximation can be written simply as

$$\left(\mathbf{u}, \mathcal{L}_1\mathcal{L}_2\mathbf{u}^T\right) \approx \left(\mathbf{u}, \mathcal{L}_1\mathbf{u}^T\right)\left(\mathbf{u}, \mathcal{L}_2\mathbf{u}^T\right) \tag{2.10}$$

If we generalize this approximation we obtain the following approximation

$$\left(\mathbf{u}, \mathcal{L}_1 \ldots \mathcal{L}_N\mathbf{u}^T\right) \approx \left(\mathbf{u}, \mathcal{L}_1\mathbf{u}^T\right) \ldots \left(\mathbf{u}, \mathcal{L}_N\mathbf{u}^T\right) \tag{2.11}$$

When we get back to x

$$\begin{aligned} \mathcal{M}_f &= \sum_{i=0}^{\infty} f_i \left(\mathbf{u}, x^i\mathbf{u}^T\right) \\ &\approx \sum_{i=0}^{\infty} f_i \left(\mathbf{u}, x\mathbf{u}^T\right)^i \\ &= f\left(\mathbf{u}, x\mathbf{u}^T\right) \end{aligned} \tag{2.12}$$

The argument being the matrix representation of the variable x, we can write the above approximation as follows

$$\mathcal{M}_f \approx f(\mathbf{X}) \tag{2.13}$$

where $\mathbf{X}$ is an n-dimensional matrix representation of x.

3 The numerical integration scheme

We attempt to develop here a method for approximating definite integrals. To this end we shall consider the Taylor expansion of a function about a point $x = a$ together with its remainder term and integrate from $x = a$ to $x = b$. In order to be able to write a k-th degree polynomial the integrand, i.e. the function to be expanded, call it f, should be an element of the set of functions which are not only continuous on $[a, b]$ but also has k derivatives continuous on $[a, b]$. The $(k + 1)$-st derivative must also exist on $[a, b]$ so that the remainder term can be explicitly written. The Taylor theorem states that for every $x \in [a, b]$, $f(x)$ can be expressed as a sum of $P_k(x)$ and $R_k(x)$, where P_k is the (k)-th order Taylor Polynomial for f about a.

$$P_k(x) = \sum_{i=0}^{k} \frac{f^{(i)}(a)}{i!}(x - a)^i \tag{3.1}$$

and $R_k(x)$ is the Remainder Term associated with $P_k(x)$. The integral form of the remainder term is,

$$R_k(x) = \frac{1}{(k)!}\int_a^x dy(x-y)^k f^{(k+1)}(y) \tag{3.2}$$

Now integrating $f(x)$ and the sum of $P_k(x)$ and $R_k(x)$ at the same time, we obtain the equality

$$\int_a^b dx f(x) = \sum_{i=0}^{k} \frac{(b-a)^{i+1}}{(i+1)!} f^{(i)}(a) + \int_a^b dx \int_a^x dy \frac{(x-y)^k}{(k)!} f^{(k+1)}(y) \tag{3.3}$$

Using integration by parts we can get rid of the double integral. Skipping intermediate steps we obtain the following general result

$$\int_a^b dx f(x) = \sum_{i=0}^{k} \frac{(b-a)^{i+1}}{(i+1)!} f^{(i)}(a) + \int_a^b dx \frac{(b-x)^{k+1}}{(k+1)!} f^{(k+1)}(x) \tag{3.4}$$

which can be rewritten as follows via an appropriate change of variable

$$\begin{aligned}\int_a^b dx f(x) = &\sum_{i=0}^{k} \frac{(b-a)^{i+1}}{(i+1)!} f^{(i)}(a) \\ &+ \frac{(b-a)^{k+2}}{(k+1)!} \int_0^1 dt (1-t)^{k+1} f^{(k+1)}((b-a)t+a)\end{aligned} \tag{3.5}$$

Defining a weight function $w_k(t)$ as

$$w_k(t) \equiv (k+1)(1-t)^k \quad k = 0, 1, 2 \tag{3.6}$$

The above integral can be written more conveniently as

$$\begin{aligned}\int_a^b dx f(x) = &\sum_{i=0}^{k} \frac{(b-a)^{i+1}}{(i+1)!} f^{(i)}(a) \\ &+ \frac{(b-a)^{k+2}}{(k+2)!} \int_0^1 dt w_{k+1}(t) f^{(k+1)}((b-a)t+a)\end{aligned} \tag{3.7}$$

It will be enlightening to see how the weight function will affect the integral at the right-hand side of this equation. For small k values the weight function gives the greatest importance to the integrand at $t = 0$ which corresponds to $f^{(k+1)}(a)$ and gives least importance to the integrand at $t = 1$ which corresponds to $f^{(k+1)}(b)$. Note that the former is the $f^{(k+1)}$ value at the point where the Taylor expansion is made

while the latter is the $f^{(k+1)}$ value at the upper limit of the integration interval. The situation for sufficiently high values on the other hand, gives greater importance to $f^{(k+1)}$ value at a. This can be easily seen by performing the following asymptotic analysis on the aforementioned integral which we shall call

$$\mathcal{I}_k \equiv \int_0^1 dt\, w_k(t) f^{(k)}\left((b-a)t+a\right) \tag{3.8}$$

which we can use in (3.7) as $\mathcal{I}_{k+1}$. To proceed further it will be convenient to define the integrand of $\mathcal{I}_k$ as

$$g(t) \equiv f^{(k)}\left((b-a)t+a\right) \tag{3.9}$$

Now, using this function the integral above can be written as

$$\mathcal{I}_k = (k+1)\int_0^1 dt\,(1-t)^k g(t) = (k+1)\int_0^1 dt\, t^k g(1-t) \tag{3.10}$$

Changing the integration variable by letting $t = z^{1/k}$ the following is obtained

$$\mathcal{I}_k = \frac{(k+1)}{k}\int_0^1 dz z^{1/k} g\left(1-z^{1/k}\right) \tag{3.11}$$

For sufficiently large k values, the approximation

$$\mathcal{I}_k \approx g(0)\int_0^1 dz \frac{(k+1)}{k} z^{1/k} \tag{3.12}$$

is valid. This implies that for sufficiently large k values the integrand will approach twice the Dirac delta function since the Delta function's support is located at one end of the interval, namely $z = 0$. Recalling that,

$$g(0) = f^{(k)}(a) \tag{3.13}$$

for sufficiently large k values, greatest importance will be given to $f^{(k)}$ value at a.

4 Approximation via fluctuationlessness

In order to apply the Fluctuationlessness theorem an orthonormal set of functions $\{u_i(t)\}$ are to be formed. The fact that the integral of the weight function is 1 implies

that $u_1(t) \equiv 1$. Using such a basis set and utilizing the Fluctuationlessness Theorem the following approximation can be made

$$\int_0^1 dt w_{k+1}(t) f^{(k+1)}((b-a)t+a) \approx \mathbf{e}_1^T f^{(k+1)}\left((b-a)\mathbf{T}^{(n)} + a\mathbf{I}_n\right)\mathbf{e}_1 \quad (4.1)$$

where $\mathbf{e}_1$ is the n-dimensional unit vector whose first component is one and the rest of the components zero. $\mathbf{T}^{(n)}$ stands for the $(n \times n)$ matrix representation of the operator $\hat{t}$ (which in fact multiplies its operand with the argument itself) and $\mathbf{I}_n$ represents the n-dimensional unit matrix. The components of $\mathbf{T}^{(n)}$ can either be evaluated by calculating the integral $T_{i,j}^{(n)} = \int_0^1 dt w_{k+1}(t) u_i(t) t u_j(t)$ or by utilizing a recursive formula. Now combining (4.1) with (3.7) we can write the approximation

$$\int_a^b dx f(x) \approx \sum_{i=0}^{k} \frac{(b-a)^{i+1}}{(i+1)!} f^{(i)}(a) + \frac{(b-a)^{k+2}}{(k+2)!} \mathbf{e}_1^T f^{(k+1)}((b-a)\mathbf{T}^{(n)} + a\mathbf{I}_n)\mathbf{e}_1 \quad (4.2)$$

If we define the following two parameter function family

$$\phi_{k,n}(a,b) = \sum_{i=0}^{k} \frac{(b-a)^{i+1}}{(i+1)!} f^{(i)}(a) + \frac{(b-a)^{k+2}}{(k+2)!} \mathbf{e}_1^T f^{(k+1)}((b-a)\mathbf{T}^{(n)} + a\mathbf{I}_n)\mathbf{e}_1 \quad (4.3)$$

we can write (4.2) as follows

$$\int_a^b dx f(x) \approx \phi_{k,n}(a,b) \quad k = 0, 1, \ldots \quad \text{and} \quad n = 1, 2, \ldots \quad (4.4)$$

The approximants in (4.3) contain matrix algebraic entities. To be able to deal with scalar entities we consider the eigenpairs of $\mathbf{T}^{(n)}$ which satisfy the equality

$$\mathbf{T}^{(n)}\mathbf{t}_i = \tau_i \mathbf{t}_i, \quad i = 1, 2, \ldots, n \quad (4.5)$$

where none of the eigenvalues are multiple and the eigenvectors are normalized in the Frobenius sense. The spectral decomposition of $\mathbf{T}^{(n)}$ is as follows

$$\mathbf{T}^{(n)} = \sum_{i=1}^{n} \tau_i \mathbf{t}_i \mathbf{t}_i^T \quad (4.6)$$

which means

$$f^{(k+1)}((b-a)\mathbf{T}^{(n)} + a\mathbf{I}_n) = \sum_{i=1}^{n} f^{(k+1)}((b-a)\tau_i + a)\mathbf{t}_i\mathbf{t}_i^T \tag{4.7}$$

and therefore

$$\begin{aligned}\phi_{k,n}(a,b) = &\sum_{i=0}^{k} \frac{(b-a)^{i+1}}{(i+1)!} f^{(i)}(a) \\ &+ \frac{(b-a)^{k+2}}{(k+2)!} \sum_{i=1}^{n} f^{(k+1)}((b-a)\tau_i + a)(\mathbf{e}_1^T\mathbf{t}_i)^2\end{aligned} \tag{4.8}$$

which is the scalar format representation of the above mentioned approximants and constitutes an approximation formula for the univariate integral under consideration. The approximants $\phi_{k,n}$ form a two index scalar family.

A Rayleigh Quotient constructed over $\mathbf{T}^{(n)}$ by means of arbitrary vectors stays always between 0 and 1. Thus the eigenvalues of this matrix are located between 0 and 1. The eigenvalue of $\mathbf{T}^{(1)}$ is $1/(k+3)$ which is also the mean value of t under $w_{k+1}(t)$ and approaches 0 as k goes to infinity. The fact that $n = 2$ produces two eigenvalues which are closer to zero than 1 and that this situation holds for higher values of k implies that the values $(b-a)\tau_i + a$ are closer to a than b. Hence the evaluation of spectral decomposition terms in (4.6) should be easier than the evaluation of the definite integral of $f(x)$ at $x = a$, because each of these terms can be approximated by truncated Taylor series with higher quality than the corresponding Taylor series truncation for $f(x)$ at $x = a$.

5 On the basis set

In the previous section, we already talked about the necessity of choosing a set of orthogonal basis functions. To this end a sequence of polynomials can be chosen so that they form an orthogonal basis set with respect to a measure, say μ, if and only if the following conditions hold:

i) The degree of the i-th polynomial is i where i is a non-negative integer,
ii) For i-th and j-th degree polynomials p_i and p_j

$$\int p_i p_j d\mu = C_i \delta_{ij}, \quad C_i \neq 0$$

The above integral being a formal expression, the integration limits have been ignored above.

The case where the constant C_i is equal to zero for some specific i, belongs to the cases of degenerate orthogonality. Then we say that the chosen set of orthogonal polynomials is not regular or that the aforementioned measure μ is not regular.

Orthogonal polynomials are known to satisfy three term recurrence relations [1] which make them particularly useful especially in the context of the present work. It can be shown that sequences of monic polynomials satisfy the relation

$$p_{i+1}(x) = (x - \gamma_i)\, p_i(x) - \eta_i^2\, p_{i-1}(x) \tag{5.1}$$

where γ_i's and η_i^2's stand for coefficients of three term recurrence relation and p_i stands for any sequence of orthogonal polynomials. The situation of C_i being non-zero is equivalent to η_i being non-zero. The case where there is some η_i equal to zero corresponds to non-regular sequences of orthogonal polynomials. It is well known that, γ_i's and η_i's are not only the means for constructing the relevant orthogonal polynomials, but are also necessary for the calculation of the zeros of these polynomials. These coefficients are also undeniably important in the construction of the related quadrature rules, and needless to say the second summation appearing in Eq. (4.8) has the structure of a quadrature.

The basis polynomials used in this work are expressable in terms of Jacobi polynomials $P_{m-1}^{(k,0)}$ as

$$u_m(t) \equiv \frac{\sqrt{2m+k}}{\sqrt{k+2}}\, P_{m-1}^{(k+1,0)}(2t-1), \quad m = 1, 2, \ldots \tag{5.2}$$

$u_m(t)$'s form an orthonormal basis set under the weight function given by (3.6) over the integration interval [0, 1]. Obviously the factor appearing in front of the Jacobi polynomials also fulfills the normalization requirement. Using the three term recursion for the Jacobi polynomials $P_m^{(k,0)}(t)$, the following three term recursion between $u_m(t)$ functions can be obtained after certain intermediate algebraic steps.

$$\alpha_m u_{m+1}(t) = (t - \beta_m) u_m(t) - \alpha_{m-1} u_{m-1}(t), \quad m = 1, 2, 3, \ldots \tag{5.3}$$

where

$$\alpha_m \equiv \frac{m(m+k+1)}{2m+k+1} \frac{1}{\sqrt{2m+k}} \frac{1}{\sqrt{2m+k+2}}, \quad m = 1, 2, 3, \ldots \tag{5.4}$$

$$\beta_m \equiv \frac{2m(m-1) + (k+1)(2m-1)}{(2m+k+1)(2m+k-1)}, \quad m = 1, 2, 3, \ldots \tag{5.5}$$

It is worth noting that we have already pointed out to the fact that $u_1(t) = 1$ and for the sake of convenience in utilizing the recursive relation given in (5.3), u_0 is to be taken as zero. Now using the recursion the whole orthonormal basis set $\{u_m(t)\}_{m=1}^{\infty}$ can be constructed and hence at least theoretically speaking the matrix $\mathbf{T}$ whose components are given by $(u_\ell, t u_m)$ can be constructed. Although since the operator $\hat{t}$ is defined on an infinite Hilbert space, $\mathbf{T}$ is infinite dimensional; in practice, as was already mentioned its finite n-dimensional truncation $\mathbf{T}^{(n)}$ will be used, which really means that only the first n of the u_m's will be needed. A quick glance at the three term recursion will ensure that the matrix $\mathbf{T}^{(n)}$ will be not only tridiagonal but also symmetric. An alternative way to construct the matrix $\mathbf{T}^{(n)}$ can be achieved by using (5.3)

and multiplying it from the left by u_ℓ and forming the inner product. This, together with orthogonality of the basis functions gives the following

$$T^{(n)}_{\ell,m} = \alpha_\ell \delta_{\ell,m-1} + \beta_\ell \delta_{\ell,m} + \alpha_{\ell-1}\delta_{\ell,m+1}, \quad 1 \le \ell, m \le n \tag{5.6}$$

Namely,

$$\mathbf{T}^{(n)} = \begin{bmatrix} \beta_1 & \alpha_1 & 0 & \dots & 0 \\ \alpha_1 & \beta_2 & \alpha_2 & \dots & 0 \\ 0 & \alpha_2 & \beta_3 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \alpha_{n-1} \\ 0 & \dots & 0 & \alpha_{n-1} & \beta_n \end{bmatrix} \tag{5.7}$$

Having obtained the components of $\mathbf{T}^{(n)}$ its eigenvalues and eigenvectors can now be easily calculated. These entities can be used in approximating the definit integral defined by (3.8).

6 Numerical results

In this section we compare results for the definit integral taken on $[a, b]$, with the exact values and with the values obtained by simply integrating the truncated Taylor series at the same interval. All our calculations were done with Mathematica 6.02 and the working precision was held at 22 digits while the results reported are rounded to 12 digits.

Two sets of tables are given below. In the first three examples integrals of functions that are analytic all over the plane are considered. Our aim is to show that the method proposed here works sufficiently well for the targeted group of integrands. The last three examples are summarized in the rest of the tables where we compare the results obtained from the present method, with the exact values and the results obtained from the integration of the Taylor polynomials of the functions which are analytic over the interval of integration but which have one or more branch cuts outside the relevant interval. Although calculations were performed for the aforementioned six integrands for possible variations in n and k; not all of them are given here in order to avoid an unnecessarily lengthy section. It is well known that Taylor expansion can only be a good choice within the convergence interval. However as is observed from the tables, the correction arising from the Fluctuationlessness term overcomes this difficulty, even for points relatively far from a, which is also the point where the expansion is made.

In Table 1 exact values of the integral $\int_0^b dx sin(x)$ are compared for $b = 1, 2, 3, 4, 5$ with the results obtained from integrating the fifth Taylor polynomial expanded about $a = 0$. The results of the proposed method are also given for the same a and b values where n is taken to be 10. The integrand chosen here does have oscillatory nature and helps us check and see how well the method works in such cases. The results are correct up to 12 digits and although the oscillations are not so wild as to seriously

Table 1 Comparison of integral values of $f(x) = sin(x)$ with the values obtained from the integration of Taylor approximation and present work results ($k = 5, n = 10, a = 0$)

b	Exact values	Present method	Taylor polynomial
1.00	0.45969769413	0.45969769413	0.45972222222
2.00	1.41614683655	1.41614683655	1.42222222222
3.00	1.98999249660	1.98999249660	2.13750000000
4.00	1.65364362086	1.65364362086	3.02222222222
5.00	0.71633781454	0.71633781454	8.15972222222

Table 2 Comparison of integral values of $f(x) = BesselJ(2, x)$ with the values obtained from the integration of Taylor approximation and present work results ($k = 5, n = 10, a = 0$)

b	Exact values	Present method	Taylor polynomial
1.00	0.03962923860	0.03962923860	0.03958333333
2.00	0.27232067768	0.27232067768	0.26666666667
3.00	0.70944933496	0.70944933496	0.61875000000
4.00	1.15682081551	1.15682081551	0.53333333333
5.00	1.37047019297	1.37047019297	−1.30208333333

Table 3 Comparison of integral values of $f(x) = 1/\Gamma(x)$ with the values obtained from the integration of Taylor approximation and present work results ($k = 5, n = 10, a = 1$)

b	Exact values	Present method	Taylor polynomial
2.00	1.08514266436	1.08514266436	1.08575591637
3.00	1.83699237285	1.83699237285	1.85315054320
4.00	2.14882693985	2.14882693985	1.81076625361
5.00	2.24084570255	2.24084570255	−2.76238802756
6.00	2.26189261126	2.26189261175	−27.4792705172

affect the results, they are quite impressive to say the least. It is also worth stating that $sin(x)$ is quite smooth and analytic over the plane.

After dealing with a rather straightforward example, analytic over its integration domain, we give two more examples where the integrands are chosen from Special Functions. They are also both analytic over their integration domain. This is done so as to test the method on a couple of analytic functions that are not that straightforward as $sin(x)$.

In Table 2 Bessel function of the first type is taken into consideration for the integration domain $[0, b]$ where $b = 1, 2, 3, 4, 5$. The results obtained from integrating the fifth Taylor polynomial expanded about $a = 0$ are better then the corresponding ones in Table 1. Nevertheless the results obtained using the Fluctuationlessness correction with $n = 10$ gives approximations that agree with the exact values up to 12 digits.

In Table 3 the integrand chosen is $1/\Gamma(x)$ rather than $\Gamma(x)$ so that points that are not analytic are avoided even though they are outside the integration domain $[1, b]$ where $b = 2, 3, 4, 5, 6$. Once again results obtained from integrating the fifth Taylor polynomial are quite bad. On the other hand Fluctuationlessness correction with $n = 10$ gives approximations that agree with exact values up to 12 digits in almost all cases except for $b = 6$ where the agreement is 10 digits.

The next six tables portray the results arising from integrands with a branch point outside the integration interval, but quite close to the point where the Taylor expansion is made. Clearly such examples are worth trying. The first of the next three exam-

Table 4 Comparison of integral values of $f(x) = ln(x)$ with the values obtained from the integration of Taylor approximation and present work results ($k = 5, n = 15, a = 1$)

b	Exact values	Present method	Taylor polynomial
2.00	0.38629436112	0.38629436112	0.40000000000
3.00	1.29583686600	1.29583686600	2.53333333333
4.00	2.54517744448	2.54517744473	18.9000000000
5.00	4.04718956217	4.04718964695	104.000000000
6.00	5.75055681537	5.75056237356	408.333333333

Table 5 Comparison of integral values of $f(x) = ln(x)$ with the values obtained from the present work results ($k = 0, n = 15, a = 1$)

b	Exact values	Present method
2.00	0.38629436112	0.38629436112
3.00	1.29583686600	1.29583686600
4.00	2.54517744448	2.54517744448
5.00	4.04718956217	4.04718956217
6.00	5.75055681537	5.75055681534

Table 6 Comparison of integral values of $f(x) = 1/x$ with the values obtained from the integration of Taylor approximation and present work results ($k = 5, n = 20, a = 1$)

b	Exact values	Present method	Taylor polynomial
2.00	0.69314718056	0.69314718056	0.61666666666
3.00	1.09861228867	1.09861228867	−5.60000000000
4.00	1.38629436112	1.38629436112	−85.6500000000
5.00	1.60943791243	1.60943791204	−524.533333333
6.00	1.79175946923	1.79175940744	−2101.25000000

ples is $\int_a^b dxln(x)$ where the Taylor expansion is made about $a = 1$. In Table 4, for $b = 2, 3, 4, 5, 6$ exact values are compared with results obtained from the integration of the fifth Taylor polynomial. As it can be observed from the table, values obtained from the integration of the Taylor polynomial are catastrophic, while the values obtained after the correction made by the Fluctuationlessness application are quite well for smaller b values, and not so bad for higher b values. Then we attempt to achieve a better precision and in Table 5 calculate the values of the same function for the same integration intervals with the only difference being the use of $k = 0$, which in fact means that we are using the zeroth order Taylor expansion. Thus Taylor values having become meaningless, we discard the third column from the table. Here we obtain 12 digits of precision for all b values used and thus this tells us that whenever a nearby branch point exists using the zeroth order Taylor expansion provides us with better results taking into consideration that higher order Taylor terms do not cope well with that kind of problematic situation.

The second such example we report here is the integral $\int_a^b dxx^{-1}$ where the Taylor expansion is made about $a = 1$ once again. In Table 6, for $b = 2, 3, 4, 5, 6$ exact values are compared with results obtained from the integration of the fifth Taylor polynomial. The values obtained from the integration of the Taylor polynomial are even more catas-

Table 7 Comparison of integral values of $f(x) = 1/x$ with the values obtained from the present work results ($k = 0, n = 20, a = 1$)

b	Exact values	Present method
2.00	0.69314718056	0.69314718056
3.00	1.09861228867	1.09861228867
4.00	1.38629436112	1.38629436112
5.00	1.60943791243	1.60943791243
6.00	1.79175946923	1.79175946923

Table 8 Comparison of integral values of $f(x) = 1/(1 + 25x^2)$ with the values obtained from the integration of Taylor approximation and present work results ($k = 5, n = 25, a = 0$)

b	Exact values	Present method	Taylor polynomial
0.20	0.15707963258	0.15707963268	0.17333333333
0.40	0.22142974348	0.22142974356	1.14666666667
0.60	0.24980915442	0.24980915448	8.52000000000
0.80	0.26516353269	0.26516353654	37.4933333333
1.00	0.27468015339	0.27467941394	117.666666667

Table 9 Comparison of integral values of $f(x) = 1/(1 + 25x^2)$ with the values obtained from the present work results ($k = 0, n = 25, a = 0$)

b	Exact values	Present method
0.20	0.15707963258	0.15707963268
0.40	0.22142974348	0.22142974356
0.60	0.24980915442	0.24980915448
0.80	0.26516353269	0.26516353273
1.00	0.27468015339	0.27468015339

prophic in this case and here too the Fluctuationlessness correction does quite well for this case. And as observed from Table 6 a choice of $b = 6$ gives a value of -2101.25 in comparison to the correct answer of 1.79. Even in such a disastereous case the suggested scheme seems to correct this number up to an accuracy of eight digits when n is taken to be 20. In Table 7 however once again we do a zeroth order Taylor expansion followed by Fluctuationlessness approximation by choosing $n = 20$. This time results are accurate up to 12 digits. Since Taylor values are meaningless the third column is discarded from Table 7. The third example chosen and analyzed in Tables 8 and 9 is the classical example of Runge, namely the integral $\int_a^b dx/(1 + 25x^2)$. The Taylor expansion was made about $a = 0$ and b values chosen were 0.2, 0.4, 0.6, 0.8 and 1.0. Although there is no singularity appearing anywhere in the integration interval, nevertheless in the complex plane singularities occur at $x = \pm 0.2i$. Results are given in Table 8 for $k = 5$ and $n = 25$. The observations clearly portray very similar results to those of Tables 4 and 6. Even as b takes the value of 1.0 Taylor results are way off the exact values and the present method seems to do reasonably well correcting the Taylor values up to the nineth digit. However once again choosing $k = 0$, i.e. a zeroth order Taylor expansion corrected with the present method by taking $n = 25$ gives results accurate to 12 digits.

7 Conclusion

The results obtained are quite promising, but it is important to notice that when our integration interval stays nearby a branch point, even if it does not contain this branch point, the results are badly affected from this, and how badly it is affected seems to depend on the distance to the branch point. The method works perfectly well as a new numerical quadrature-like method for integrations over intervals being sufficiently distant from the branch points of the function in question. For the functions which are not analytic outside our approximation interval, we have two choices for curing the ill-conditioning created by this situation: Either we can choose the point about which we make the series expansion as far as possible from the branch-cut, or we use much higher n values in creating our Jacobi matrix. For functions which are not analytic inside the approximation interval the method is not appropriate to use.

An important discussion may be held on the choice of n. A tolerance value can be determined and while we increase n by steps of 5, we check for the difference between last two consecutive terms. If the absolute value of this difference is less than the tolerance we stop and take this n, otherwise we try for the upcoming n value.

Another and perhaps most important point to be emphasized is the universality of the method. The truncated matrices of any dimension and the corresponding eigenpairs are only calculated once and after being archived can be used whenever they are needed, which makes the cost of calculations quite low.

As future work various basis functions other than polynomials are intended to be used with the method.

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