The Application of the Fluctuation Expansion with Extended Basis Set to Numerical Integration

COŞAR GÖZÜKIRMIZI
İstanbul Technical University
Informatics Institute
Maslak, 34469, İstanbul
TURKEY (TÜRKİYE)
cosargo@be.itu.edu.tr

METİN DEMİRALP
İstanbul Technical University
Informatics Institute
Maslak, 34469, İstanbul
TURKEY (TÜRKİYE)
demiralp@be.itu.edu.tr

Abstract: According to the fluctuationlessness theorem the matrix representation of a function can be approximated by the image of independent variable operator's matrix representation under that function. The independent variable operator's action is defined as the multiplication of the operand by the independent variable. Hence itself and therefore its matrix representation is universal, do not depend on the function. The application of this approximation to numerical integration forms a quadrature whose structure can be manipulated by changing the basis set of an n-dimensional Hilbert space. This work focuses on reflecting the effects of a complementary Hilbert space to a restricted Hilbert subspace by forming the basis set as certain linear combinations of some basis functions in order to improve the accuracy of the numerical integration based on fluctuationlessness theorem.

Key–Words: Numerical Integration, Fluctuation Expansion, Fluctuationlessness Theorem, Hilbert Spaces

1 Introduction

Fluctuation expansion is a universal tool to approximate the matrix representation of functions [1–10]. It may be used to construct a quadrature rule for numerical integration [4–7]. A quadrature is a formula expressing an integral's value as a finite linear combination of the kernel function values as follows

$$\int_a^b dx\, f(x) = \sum_{i=1}^{n} w_i f\left(x_i\right) \tag{1}$$

where growing n values are expected to increase the numerical accuracy of the integration [11–23]. A growth in n is equivalent to increasing the size of the matrix representation of the independent variable operator $\widehat{x}$. If n is increased, the formation of the quadrature rule and its application for numerical integration becomes computationally challenging. There are two approaches in literature to improve the accuracy without increasing the size of the matrix. One approach is to take the fluctuation terms in fluctuation expansion into consideration and this approach seems to be computationally inefficient at this point due to slow convergence [6–10]. The other approach is to work on the integrand in a universal manner to form several integrals converging faster when quadrature is utilized [5, 6].

In this work, steps are taken towards improving the accuracy of the utilization of fluctuationlessness theorem for numerical integration by forming the basis functions of Hilbert Space as certain linear combinations of some other orthonormal functions. By such an approach, the basis set is somehow extended to better represent the effect of the $\widehat{x}$ operator used in the calculation of the quadrature rule.

2 Fluctuation Expansion and Numerical Integration

This work focuses on the functions which are analytic and therefore square integrable in a given finite interval. Here we prefer to deal with finite intervals because the continuity implies the boundedness and therefore square integrability. We could equivalenty use semi-infinite or infinite intervals with the aid of appropriate weights, although we keep them out of the scope of this work for the simplicity of the presentation. These abovementioned functions can be considered as the elements of an infinite Hilbert space symbolized by $\mathcal{H}$ where the inner product of any two functions $f(x)$ and $g(x)$ is defined as

$$(f, g) = \int_0^1 dx\, w(x) f(x) g(x) \tag{2}$$

which induces the norm definition as follows

$$\|f\| = \sqrt{(f, f)} \tag{3}$$

where $w(x)$ is an appropriate weight function. The finite integration interval is chosen as the most widely used one, $[0,1]$ since any finite interval can be converted to this one by using an affine transform on the independent variable of the integration. $w(x)$ is assumed to be normalized to have the value of 1 for its integral over $[0,1]$.

The orthonormal basis functions can be symbolized by

$$\mathcal{U} \equiv \{u_i(x)\}_{i=1}^{\infty} \tag{4}$$

Although there is no limitation on the selection of the linearly independent basis functions to construct a basis set for $\mathcal{H}$ principally we prefer to tackle with polynomials of increasing degree. The basis functions may be formed by the orthonormalization of $x^0, x^1, \ldots, x^n, \ldots$ by appropriate methods. It is important to get the very first basis element as the constant function of 1 value after such an orthonormalization, that is, the equality

$$u_1(x) = 1 \tag{5}$$

needs to be acquired. This is necessary for the link between the fluctuationlessness theorem and the numerical integration. If one desires to extend what we are going to develop here to the most general case then the other basis functions may be chosen arbitrarily as long as they satisfy the orhonormality conditions. What we want to get here is a quadrature like formula for numerical integration. The structure of the basis set will change the node and the weight values of this formula. According to the fluctuationlessness theorem, the matrix representation of a function symbolized by $M\left(\widehat{f}\right)$ on a finite subspace of $\mathcal{H}$ can be approximated by the matrix representation of $\widehat{x}$ operator on the same finite subspace under the image of the function. In mathematical language, this approximation can be given by

$$M\left(\widehat{f}\right) \approx f\left(M\left(\widehat{x}\right)\right) \tag{6}$$

where M stands for a superoperator which maps from the space of linear bounded operators transforming between $\mathcal{H}$ and $\mathcal{H}$ to the space of $n \times n$ matrices where n is the dimension of the subspace $\mathcal{H}_n$ on which matrix representation is defined. M is called "Matrix Representation Operator". The algebraic $\widehat{x}$ operator multiplies its operand by independent variable x. The elements of $M\left(\widehat{x}\right)$ are explicitly given below

$$\mathbf{e}_i^T M\left(\widehat{x}\right)\mathbf{e}_j \equiv \left(u_i, \widehat{x}u_j\right) = \int_0^1 dx w(x) u_i(x) x u_j(x) \tag{7}$$

where $\mathbf{e}_i$ and $\mathbf{e}_j$ stand for the ith and jth standard cartesian unit vectors respectively, their only nonzero elements are 1 and located in the ith and jth positions respectively.

The approximated matrix representation in accordance with the fluctuationlessness theorem may be improved by adding the fluctuation terms to the approximation's expression as corrections. The whole equality is as follows

$$M\left(\widehat{f}\right) = f\left(M\left(\widehat{x}\right)\right) + \sum_{k=1}^{\infty} f_k \left[M\left(\widehat{x}^{\,k}\right) - M\left(\widehat{x}\right)^k\right] \tag{8}$$

where f_k coefficients can be uniquely determined, as a matter of fact, they are the Taylor series expansion coefficients of the function $f(x)$ at $x = 0$. Using the fact that the first basis function is equal to 1, the integral of the given function $f(x)$ can be expressed as

$$I \equiv \int_0^1 dx\ w(x) u_1(x) f(x) u_1(x) \tag{9}$$

The utilization of the previously given inner product definition and the application of the fluctuationlessness theorem

$$I \approx \mathbf{e}_1^T f\left(M\left(\widehat{x}\right)\right)\mathbf{e}_1 \tag{10}$$

is obtained.

The image of $M\left(\widehat{x}\right)$ under the function may be calculated by using the spectral decomposition of this matrix.

$$M\left(\widehat{x}\right) = \sum_{k=1}^{n} \xi_k \mathbf{x}_k \mathbf{x}_k^T \tag{11}$$

where ξ_k and $\mathbf{x}_k$ $(k = 1, ..., n)$ represent the real valued kth eigenvalue and its corresponding eigenvector for this matrix respectively. The validity of this decomposition comes from the symmetric nature of the matrix and is because of the hermitian character of the operator $\widehat{x}$. One can also prove that all eigenvalues here are discrete interior points of the $[0,1]$ interval [11]. All these imply that the image under the function can be shown to be

$$f\left(M\left(\widehat{x}\right)\right) = \sum_{k=1}^{n} f\left(\xi_k\right)\mathbf{x}_k \mathbf{x}_k^T \tag{12}$$

Since the numerical integral corresponds to the left uppermost element of the matrix representation of the function, the approximation can be written as follows

$$I \approx \sum_{k=1}^{n} f\left(\xi_k\right)\left(\mathbf{e}_1^T \mathbf{x}_k\right)^2 \tag{13}$$

This approximation may be considered as a quadrature because of its formula's structure. Here ξ_k values are corresponding to the nodes and $\left(\mathbf{e}_1^T \mathbf{x}_k\right)^2$ values form the weights of the quadrature.

3 Fluctuation Expansion and Gauss Quadrature

The matrix representation of the $\widehat{x}$ operator is closely related to the Jacobi matrix used in the construction of Gauss quadrature in recent modern perspectives. It is possible to show that under unit weight and with a basis set formed by the orthonormalization of $x^0, x^1, \ldots, x^n$ over the $[\,0,1\,]$ interval, the quadrature formed by the fluctuationlessness theorem is Gauss quadrature (this remains valid also for some other intervals and some type of weight functions). For that purpose, it is necessary to investigate the three consecutive term recursion of the basis set whose elements are denoted by $u_1(x)$,...,$u_n(x)$,... The $\widehat{x}$ operator increments the degree of its polynomial operand by 1. Therefore,

$$xu_n(x) = \sum_{i=1}^{n+1} c_i u_i(x) \tag{14}$$

If an inner product is performed to both sides of this equality,

$$c_j = (u_j, xu_n)\,, \quad j = 1, \ldots, n+1 \tag{15}$$

is observed using the orthogonality of the basis set. Since $\widehat{x}$ is a Hermitian operator, this equality can also be written as

$$c_j = (u_n, xu_j)\,, \quad j = 1, \ldots, n+1 \tag{16}$$

u_n is an $(n-1)$ degree polynomial. xu_j is a $(j-1)$ degree polynomial multiplied by its independent variable, therefore a j degree polynomial. Since a polynomial is orthogonal to all polynomials of smaller degree,

$$c_j = (u_n, xu_j) = 0, \quad j = 1, \ldots, n-2 \tag{17}$$

Therefore the contributions up to $j = n-1$ are all 0. This implies that the multiplication of a polynomial by its independent variable can be expressed by a linear combination of itself, the orthonormal polynomial of one smaller degree and the orthonormal polynomial of one greater degree. Using the above expression, the coefficients of this linear combination are found as

$$\begin{aligned} c_{n+1} &= \; (u_{n+1}, xu_n) &\equiv \alpha_n \\ c_{n-1} &= \; (u_n, xu_{n-1}) &\equiv \alpha_{n-1} \\ c_n &= \; (u_n, xu_n) &\equiv \beta_n \end{aligned} \tag{18}$$

Using α and β parameters to form a compact expression, the recursion becomes

$$\begin{aligned} xu_j(x) \;&=\; \alpha_j u_{j+1}(x) + \beta_j u_j(x) + \alpha_{j-1} u_{j-1}(x) \\ &\qquad \alpha_0 = 0, \;\; j = 1, 2, \ldots \end{aligned} \tag{19}$$

Utilizing the recursion to form the matrix representation of $\widehat{x}$ operator, it can be observed that

$$M\left(\widehat{x}\right) = \begin{bmatrix} \beta_1 & \alpha_1 & & & \\ \alpha_1 & \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha_{n-2} & \beta_{n-1} & \alpha_{n-1} \\ & & & \alpha_{n-1} & \beta_n \end{bmatrix} \tag{20}$$

In Gauss quadrature, the weights of a quadrature are given by

$$w_i = \int_a^b dx\; w(x) L_i(x) \tag{21}$$

where L_i is the Lagrange polynomial. A Lagrange polynomial may be expressed in terms of a Lagrange polynomial of one smaller degree by

$$L_i(x) = (x - x_i)\, \overline{L}_i(x) + 1 \tag{22}$$

Multiplying both sides of this expression by $L_i(x)$ and integrating,

$$\begin{aligned} & \int_a^b dx\; w(x) L_i(x)^2 \\ = \; & \int_a^b dx\; w(x) L_i(x) \left(x - x_i\right) \overline{L}_i(x) \\ + \; & \int_a^b dx\; w(x) L_i(x) \end{aligned} \tag{23}$$

The rightmost term is the definition of the weights of the quadrature w_i. The first term at the right of this equation vanishes since $(x - x_i)\, L_i(x)$ is proportional to $u_{n+1}(x)$ which is orthogonal to any polynomial whose degree is less than n and since $\overline{L}_i(x)$'s degree is $(n-2)$. Therefore an integral expression is obtained for the weights of the quadrature. Since the kernel of the integral is positive, the weights of the quadrature are also positive as expected in quadrature approximations. The first n equations in three consecutive term recursion given above can be written as a vector equation whose vector unknown contains $u_1(x)$,...,$u_n(x)$ as its elements while its matrix coefficient is the matrix representation of $\widehat{x}$ operator minus x times n dimensional unit matrix and the right hand side vector's only nonzero element is located at the bottommost location and is proportional to $u_{n+1}(x)$. In order to annihilate the right hand side and make the vector equation an eigenvalue problem $u_{n+1}(x)$ should vanish. That is, it should be the characteristic polynomial of the matrix. Therefore the nodes are the eigenvalues of this matrix.

In research areas related to Gauss quadrature the matrix representation of $\widehat{x}$ matrix is also known as Jacobi matrix. The only difference is that the Gauss quadrature by convention uses the orthonormal polynomials in $[-1,1]$ (it can also be extended to some other intervals and weight functions but always remains limited to the polynomials) interval, whereas in this work, $[0,1]$ interval is utilized. One other important restriction in Gauss quadrature is that the use of polynomials with one by one increasing degrees is compulsory. However, the present method is not limited by these restrictions; nonpolynomial functions and arbitrarily degree changing polynomial basis functions can be comfortably used as well.

Considering the formulation for the nodes and the weights of Gauss quadrature, it is observed that increasing the size of the Hilbert subspace results in an equal increase in the number of nodes of the quadrature. Instead of increasing the number of nodes in the quadrature, forming a basis set to better approximate the effect of the $\widehat{x}$ operator is expected to construct more efficient quadratures.

4 The Extended Basis Set

The basis set of the n-dimensional Hilbert space may be constructed as certain linear combinations in order to better approximate the effect of the operators defined in infinite Hilbert space. For that end, the nth basis function may be replaced by a linear combination of the nth and $(n+1)$th basis functions. By doing so, a basis function from $(\mathcal{H}-\mathcal{H}_n)$, the complementary space of the subspace $\mathcal{H}_n$, is reflected to $\mathcal{H}_n$. In a more general case, the new nth basis function symbolized by $u_n^*(x)$ will be

$$u_n^*(x) \equiv g_1 u_n(x) + \cdots + g_{k+1} u_{n+k}(x) \qquad (24)$$

where the g coefficients should be chosen in such a way that the orthonormality is preserved. Since a polynomial is orthogonal to all polynomials of smaller degree, the introduction of $u_n^*(x)$ does not violate the orthogonality condition. For the normalization of the basis function, the necessary and sufficient condition is

$$\sqrt{g_1^2 + \cdots + g_{k+1}^2} = 1 \qquad (25)$$

For determining the g values, the objective is chosen as to annihilate many fluctuation terms as much as possible. The use of fluctuation expansion for numerical integration gives

$$\begin{aligned} I &= \mathbf{e}_1^T f\left(M\left(\widehat{x}\right)\right)\mathbf{e}_1 \\ &+ \sum_{k=0}^{\infty} f_k \mathbf{e}_1^T \left(M\left(\widehat{x}^{\,k}\right) - M\left(\widehat{x}\right)^k\right)\mathbf{e}_1 \end{aligned} \qquad (26)$$

The fluctuations are represented by the infinite sum and are named as the contributions of the integral fluctuations. The integral fluctuation corresponding to the ith term of the series is the ith order integral fluctuation. They are given by

$$R_k = \mathbf{e}_1^T \left(M\left(\widehat{x}^{\,k}\right) - M\left(\widehat{x}\right)^k\right)\mathbf{e}_1\,, \quad k \geq 0 \qquad (27)$$

If all integral fluctuations are 0, then the numerical integration is exact. Experiments have shown that using $n=2$ and substituting the second basis function with a linear combination of the second and the third basis function, the integral fluctuations can be suppressed. Leaving g_1 and g_2 arbitrary, it is observed that the first two integral fluctuations vanish. For annihilating the third order integral fluctuation, the necessary condition was observed to be taking $g_1=1$ and $g_2=0$. This behavior is due to the definition of the integral fluctuations. There the Jacobi matrix is multiplied by itself as many times as the order of fluctuation. The rightmost column and the bottommost line will have an effect on the left uppermost element signifying the effect on the numerical integral. Therefore an increase in n will delay this effect and this is observable by only the investigation of matrix multiplication. Annihilating the $(2n-1)$th order integral fluctuation leaves g_2 as 0 and therefore creates the basis set of Gauss quadrature. Instead, leaving this integral fluctuation nonzero and annihilating the $2n$th fluctuation is possible. It was observed that such an approach also decreases the absolute value of the higher integral fluctuations. The linear combination coefficients were chosen as to annihilate $2n$th order integral fluctuation. The other equation to solve for g_1 and g_2 is obtained from the normalization condition. The integral fluctuations for $n=2$ is obtained as given in Table 1.

Order	Regular B. Set	Extended B. Set
0	0	0
1	0	0
2	0	0.007455721
3	0	0
4	0.005555555	-0.006089339
5	0.013888888	-0.007843812
6	0.022486772	-0.006301896
7	0.030092592	-0.002896843
8	0.036265432	0.001327769
9	0.040972222	0.005730764
10	0.044355592	0.009951743

Table 1: The comparison of the first ten integral fluctuations for the regular and extended basis sets constructed from the orthonormal polynomials mentioned above.

The drawback due to the $(2n-2)$ integral fluctuation is compensated by the higher order terms. Note that the integral fluctuations have the Taylor expansion coefficients as multiplier. Therefore, the extension of the basis set better reflects the effects of the higher derivatives of the function on the integral with the exception of $2n-2$ derivative. Since the value of the derivatives of the function is closely related to the smoothness of the function, it is possible to conjecture that as the steepness of the function in the interval increases, the advantage of the quadrature formed by the extended basis set will be more apparent.

5 The Algorithm

The algorithm for the formation and use of the quadrature with extended basis set comprises the following steps.

1) Numerical integration problem with the interval $[0, 1]$ and unit weight is considered. The polynomials $x^0, x^1, \ldots, x^n$ are orthogonalized by Cholesky decomposition and normalized. For that purpose, the Gram matrix with the definition

$$\mathbf{G} = \left(\mathbf{u}, \mathbf{u}^T\right) \tag{28}$$

where $\mathbf{u}$ is a vector with the elements

$$\mathbf{u} \equiv \begin{bmatrix} x^0 \\ \vdots \\ x^n \end{bmatrix} \tag{29}$$

is formed. The orthogonalization is performed by first considering the Cholesky decomposition of the Gram matrix as

$$\mathbf{G} = \mathbf{L}\mathbf{L}^T \tag{30}$$

After the decomposition $\mathbf{L}^{-1}\mathbf{u}$ is calculated and the elements of the resulting vector are the orthogonal polynomials.

This method is preferred in the algorithm since MuPAD programming language has predefined procedures which simplify the programming effort [24].

2) The u_n basis function is replaced by the linear combination of u_n and u_{n+1} with the form

$$u_n^*(x) \equiv g_1 u_n(x) + g_2 u_{n+1}(x) \tag{31}$$

3) The integral fluctuations are determined for both the original basis set and the extended basis set.

4) The $(2n-1)$ order integral fluctuation is set equal to zero and the resulting equation is simultaneously solved with the equality arising from the normalization of the basis function.

5) The $M(\widehat{x})$ matrix for the extended basis set is formed by the insertion of the linear combination coefficients.

6) The eigenpairs of $M(\widehat{x})$ are calculated for the original basis set (Gauss quadrature) and the extended basis set case to determine the nodes and the weights of the two quadratures.

7) The quadratures are utilized to numerically integrate any given function.

8) The Maclaurin expansion term with $(2n-2)$th derivative is subtracted from the function to be integrated. The quadrature is applied to this new function and the integral of the Maclaurin term is calculated analytically and added to the integral by the quadrature. The reason for such an approach is that it is known that the quadrature formed from the extended basis set only increases this integral fluctuation. Therefore, the Maclaurin term exclusion may be expected to form a quadrature that outperforms Gauss quadrature for all functions. It was observed that it was not the case.

9) The relative error is calculated and visualized for all cases.

6 Numerical Results

First, the application of the fluctuation expansion with extended basis set to numerical integration of polynomials is investigated. The polynomial $(1+\alpha x)^{20}$ is chosen for that purpose. The graph of the integral values in the domain $[0, 1]$ for different Hilbert space dimensions is given in figure 1. This is a plot of the integral values for different α. α parameter changes the steepness of the polynomial and as α increases the use of the extended basis set is expected to be more profitable. As exemplified by this integration, the in-

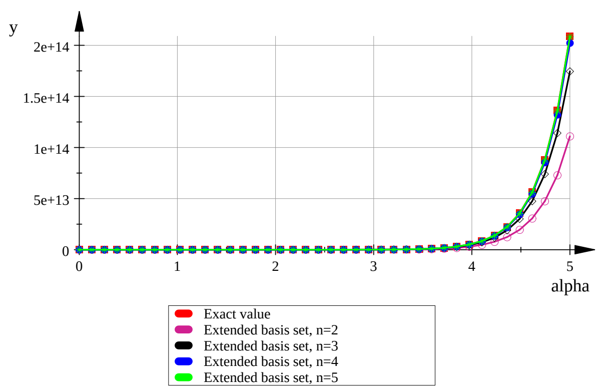

Figure 1: The plot of the integral values against the α parameter for $(1+\alpha x)^{20}$.

crease in the number of nodes increases the accuracy of the numerical integration. It is also important to compare the results of the integration with extended basis set to the results without the extended basis set, or namely the Gauss quadrature with the same number of nodes. The plot of the integral values of $(1+\alpha x)^{20}$ in the domain $[\,0,1\,]$ for the two different quadratures is given in figure 2. Five nodes are utilized in both of the quadratures.

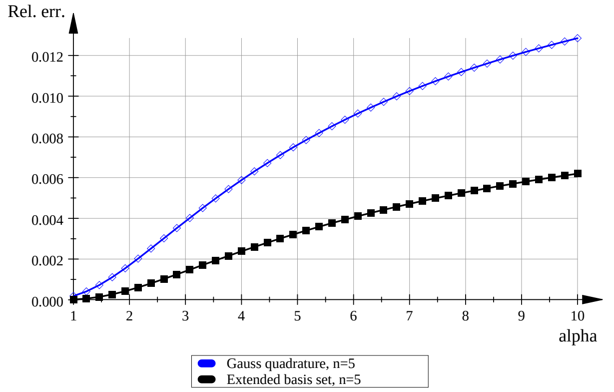

Figure 2: The plot of relative error against the α parameter for the numerical integration of $(1+\alpha x)^{20}$.

The relative error is calculated by

$$\epsilon = \frac{I_{exact} - I_{approx.}}{I_{exact}} \tag{32}$$

The results for the exponential function $e^{\alpha x}$ also show the high numerical precision provided by the extended basis set. The relative error formed by the three different methods are provided in figures 3, 4, 5 and 6. These methods are

- The application of the fluctuation expansion for numerical integration without the extended basis set, or namely the Gauss quadrature,
- The application of the fluctuation expansion for numerical integration with the extended basis set,
- The application of the fluctuation expansion for numerical integration with the extended basis set and Maclaurin term exclusion.

It is observed that the effect of the Maclaurin term exclusion is rather small. Yet, the extended basis set outperforms Gauss quadrature for this example.

As the size of the Hilbert space increases, the extended basis set still forms more accurate results as given in figures 5 and 6. The quadrature formed by the extended basis set is expected to approach Gauss quadrature as the number of basis functions imposed on the basis function of the finite Hilbert space with the highest index is held constant.

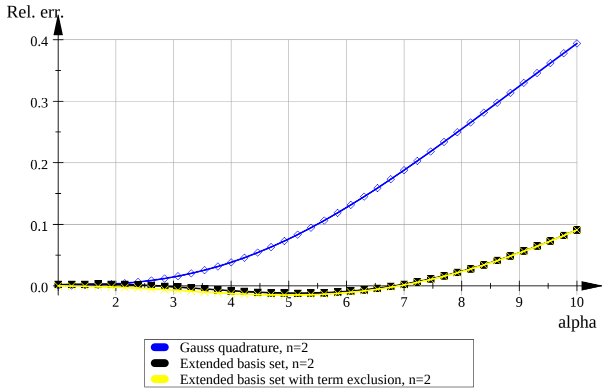

Figure 3: The plot of relative error against the α parameter for the numerical integration of $e^{\alpha x}$ for α in $[\,1,10\,]$ where $n=2$.

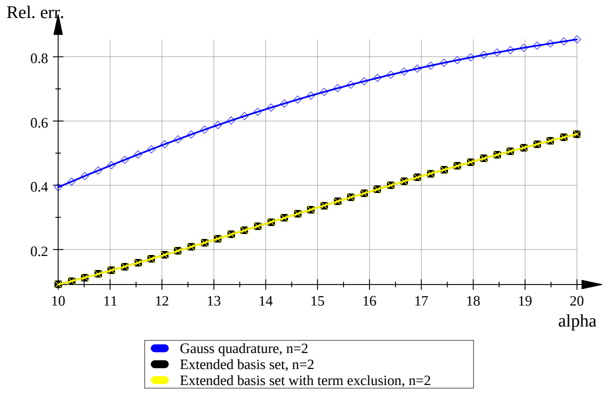

Figure 4: The plot of relative error against the α parameter for the numerical integration of $e^{\alpha x}$ for α in $[\,10,20\,]$ where $n=2$.

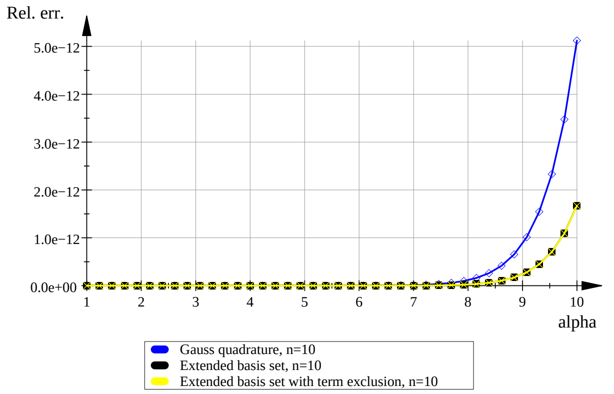

Figure 5: The plot of relative error against the α parameter for the numerical integration of $e^{\alpha x}$ for α in $[\,1,10\,]$ where $n=10$.

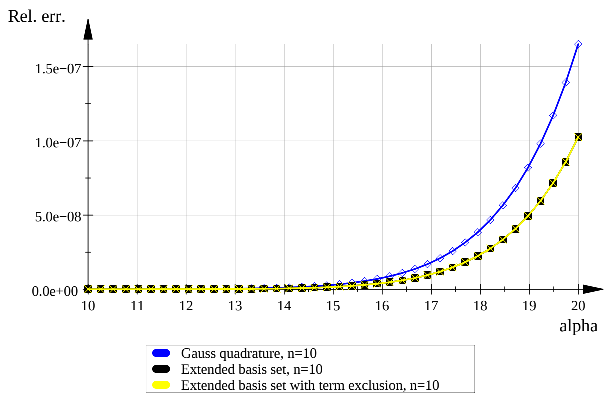

Figure 6: The plot of relative error against the α parameter for the numerical integration of $e^{\alpha x}$ for α in $[10, 20]$ where $n = 10$.

Also, it is possible to perform Taylor term exclusion at any point in the integration interval or even at points outside the interval. Such an approach is observed to be effective if the function contains a singularity outside the integration interval and the Taylor expansion is formed at a point distant to the singularity.

7 Conclusion

In this work, the utilization of the fluctuation expansion with extended basis set for numerical integration is investigated. The results may be itemized as given below.

- It is observed that the nodes and the weights of the Gauss quadrature is related to the eigenpairs of the matrix representation of the $\widehat{x}$ operator. The inner product of the Hilbert space for fluctuation investigations is determined by the interval and the weight of the considered integration. New quadrature rules may be formed by this method with the restriction that the first basis function must be chosen as $u_1(x) \equiv 1$.

- The determination of the integral fluctuations is independent of the function. The integral fluctuations appear as important tools to investigate the error of the quadratures. Note that the error of certain numerical integrations has the integral fluctuations multiplied by the value of the derivatives of the function at certain points. If all the integral fluctuations vanish, the numerical integration is exact. However, if that is not the case, each contribution by the integral fluctuation may add up or somewhat balance each other. Therefore a powerful quadrature rule does not imply that the numerical integration will give a more accurate result compared to any other quadrature rule for any function.

- Changes in the basis set of the Hilbert space changes the nodes and the weights of the quadrature. Such new quadratures may be used to form better quadrature rules in accordance with the given certain characteristics of the numerical integration problem under consideration.

- If the basis set for Gauss quadrature is used with the exception that the nth basis function is replaced by a linear combination of nth and $(n+1)$th basis function, a new quadrature may be formed. If the coefficients of the linear combination are chosen to annihilate the lowest order nonzero integral fluctuation, Gauss quadrature is formed. If the coefficients are chosen to annihilate the second lowest order nonzero integral fluctuation, the higher order integral fluctuations were observed to have smaller moduli. Due to the definition of the fluctuation expansion, such quadratures are effective in the integration of non-smooth functions. Such linear combinations are also tried at other basis functions taking into account the orthonormality and linear independence of the basis functions. Using a linear combination at the smaller degree basis functions, it was observed that the accuracy was not as well as replacing the nth basis function. The reason is that such an approach involves many more nonzero fluctuations.

- The method may be adapted to different integration intervals, weights and basis sets. Also, the number of functions used in the linear combination may be increased. However such an approach would necessitate the solution of a nonlinear polynomial equation set with high precision.

- For future work, it is important to generalize the method to the multiple integration of multivariate functions.

References:

[1] **Demiralp, M.**, 2005. A fluctuation expansion method for the evaluation of a function's expectation value, *Int. Conf. on Numerical Analysis and Applied Mathematics, Wiley, Rhodes, Greece*, **4A**, 141–145.

[2] **Demiralp, M.**, 2005. Determination of quantum expectation values via fluctuation expansion, *Lecture Series on Computer and Computational Sciences, Selected Papers from Int. Conf.*

of Computational Methods in Science and Engineering, **4A**, 146–149.

[3] **Baykara, N.A. and Demiralp, M.**, 2005. Fluctuation expansion in the quantum optimal control of one dimensional perturbed harmonic oscillator, *Lecture Series on Computer and Computational Sciences, Selected Papers from Int. Conf. of Computational Methods in Science and Engineering*, 56–59.

[4] **Kalay, B. and Demiralp, M.**, 2008. Smoothening the integrands to increase the quality of fluctuationlessness approximation in numerical integration, *Proceedings of the 1st WSEAS Int. Conf. on Multivariate Analysis and its Application in Science and Engineering*, 204–208.

[5] **Üsküplü, S. and Demiralp, M.**, 2008. Univariate integration via space extension based no fluctuation approximation, *International Conference on Numerical Analysis and Applied Mathematics*, 566–569.

[6] **Kalay, B.**, 2007. Fluctuationlessness approximation and integration folding as method for numerical integration, M.Sc. Thesis, İstanbul Teknik Univ. (in Turkish).

[7] **Gözükırmızı, C. and Demiralp, M.**, 2008. Introductory steps for the design of an algorithm for finding the higher order fluctuation terms via symbolic simplifications, *Proceedings of the 1st WSEAS Int. Conf. on Multivariate Analysis and its Application in Science and Engineering*, 189–192.

[8] **Demiralp, M.**, 2008. Finite subspace matrix representation of the multiplication operator's resolvent in terms of fluctuation matrices, *International Conference on Numerical Analysis and Applied Mathematics*, 159–162.

[9] **Demiralp, M.**, 2008. Approximation of the independent variable's resolvent via Hilbert Space folding on its constant subspace, *ICCMSE 2008 (In print)*.

[10] **Gözükırmızı, C. and Demiralp, M.**, 2008. Evaluation of fluctuation coefficients for three consecutive term recursive basis functions, *International Conference on Numerical Analysis and Applied Mathematics*, 231–234.

[11] **Stoer, J. and Bulirsch, R.**, 2002. Introduction to numerical analysis, Springer-Verlag, New York.

[12] **Hildebrand, F. B.**, 1987. Introduction to numerical analysis, Dover, New York.

[13] **Gautschi, W.**, 1983. How and how not to check Gaussian quadrature formulae, *BIT Numerical Mathematics*, **23**, 209–216.

[14] **Gauss, C.F.**, 1886. Methodus nova integralium valores per approximationem inveniendi, Gesellschaft Wissenschaft, Göttingen.

[15] **Golub, G.H. and Welsch, J.H.**, 1969. Calculation of Gauss quadrature rules, *Mathematics of Computation*, **23**, 221–230.

[16] **Ma, J.**, **Rokhlin, V. and Wandzura, S.**, 1996. Generalized Gaussian quadrature rules for systems of arbitrary functions, *SIAM Journal on Numerical Analysis*, **33**, 971–996.

[17] **Maucher, R.**, 1996. A symbolic computation procedure for the generation of Gauss quadrature rules with a user-defined weight function, *Communications in Numerical Methods in Engineering*, **12**, 141–145.

[18] **Laurie, D.P.**, 2001. Computation of Gauss-type quadrature formulas, *Journal of Computational and Applied Mathematics*, **127**, 201–217.

[19] **Trefethen, L.N.**, 2008. Is Gauss quadrature better than Clenshaw-Curtis, *Siam Review*, **50**, 67–87.

[20] **Laurie, D.P.**, 1996. Anti-Gaussian quadrature formulae, *Mathematics of Computation*, **65**, 739 –747.

[21] **Patterson, T.N.L.**, 1992. Modified optimal quadrature extensions, *Numerische-Mathematik*, **64**, 511–520.

[22] **Milovanović, G.V. and Cvetković, A.S.**, 2005. Orthogonal polynomials and Gaussian quadrature rules related to oscillatory weight functions, *Journal of Computational and Applied Mathematics*, **179**, 263–287.

[23] **Gautschi, W.**, 1970. On the construction of Gaussian quadrature rules from modified moments, *Mathematics of Computation*, **24**, 245–260.

[24] **Creutzig, C. and Oevel, W.**, 2004. MuPAD Tutorial, Second Edition, Springer, New York.