A New Fluctuation Expansion Based Method for the Univariate Numerical Integration Under Gaussian Weights

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Abstract: - This paper presents a new method based on quite recently proposed fluctuation expansion for the evaluation of certain operators' expectation values over Hilbert spaces. The fluctuation expansion has been constructed with the aid of a projection operator which projects to a one dimensional subspace of the Hilbert space under consideration. We, now, extend this idea to the utilization of projections to multidimensional subspace of the same Hilbert space. We take a univariate integral under a Gaussian weight (that is, bell like shaped function) and keep only zeroth order terms which contain no fluctuation functions. After some matrix algebraic manipulations we obtain an interpolation formula as a linear combination of the integral's kernel function's values at the eigenvalues of the matrix which is a upperleftmost truncation from the matrix representation of the independent variable

Key-Words: - Fluctuation Expansion, Gaussian Weight, Numerical Integration, Expectation Values, Quantum Mechanics

1 Introduction

We have recently offered a new method for the numerical evaluation of univariate integrals[1-4]. The integrand of the integral has been considered as the product of two given functions, one of which is specified as a weight function. That is,

$$\mathcal{I} \equiv \int_a^b dx W(x) f(x) \qquad (1)$$

where $W(x)$ stands for the weight function and all entities are assumed to be real valued for simplicity. Since the weight function can vanish only at a finite number of the points of the integration domain and remains positive elsewhere in the same domain by definition, we have considered its positive square root as a wave function of the quantum mechanics and have written

$$W(x) \equiv \psi(x)^2 \qquad (2)$$

where $\psi(x)$ denotes the so-called wave function. The weight function's integral over the domain has been assumed to be 1 for providing consistency to probabilistic issues since we need to use those tools for the employment of expectation or mean value concepts. That is,

$$\int_a^b dx W(x) \equiv \int_a^b dx \psi(x)^2 = 1. \qquad (3)$$

Then the integral has been interpreted as the expectation value of the function $f(x)$ with respect to the wave function mentioned above through the following formula

$$\langle f(x) \rangle \equiv \int_a^b dx W(x) \psi(x) f(x) \psi(x) \qquad (4)$$

We have assumed that $f(x)$ is continuous everywhere in a domain including the integration interval in the integration variable's complex plane and square integrable over the interval $[a, b]$ to provide the utilization of Hilbert space concepts . This enabled us to expand $f(x)$ into a Taylor series at a point, say c, in the integration interval as follows

$$f(x) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(c)(x - c)^k \qquad (5)$$

where superscript (k) stands for the k–th derivative. The next step has been the replacement of (4) with the following equation by using (5)

$$\langle f(x) \rangle = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(c) \left\langle (x - c)^k \right\rangle. \qquad (6)$$

After this point we have defined the following operators

$$
\begin{aligned}
I g(x) &\equiv g(x), \\
P_\psi g(x) &\equiv \left(\int_a^b dx \psi(x) g(x) \right) \psi(x) \qquad (7)
\end{aligned}
$$

where I and P_ψ denote the unit operator and the projection operator which projects to the subspace spanned by $\psi(x)$ in the space of square integrable functions over the interval $[\,a, b\,]$. $g(x)$ represents any function chosen from the set of functions which are square integrable over the interval $[\,a, b\,]$. To make a concrete analogy to the quantum mechanics we have assumed that this space is a Hilbert space, in other words, distance between two points, the norm of any element (vector) of the space and the angle between two vectors, are all defined and, beyond these, the space is assumed to be complete. The complementary companion of P_ψ is, of course, simply $I - P_\psi$. By keeping this fact in mind we have written the following equality

$$\left\langle (x-c)^k \right\rangle = \left\langle (x-c)\left\{\left[\, P_\psi + \left(I - P_\psi\right)\,\right](x-c)\right\}^{k-1} \right\rangle \quad (8)$$

which is required and remains valid for all positive integer k values. Its right hand side should be assumed to be 1 when k vanishes.

In the cases where the wave function $\psi(x)$ is almost sharply localized around a single point in the interval of integration (as a well-known example of sharply localized functions we can address to the delta function of Dirac) we can conjecture that P_ψ overdominates its complement, that is, behaves like or goes to, unit operator as can be shown via an analysis based on distribution theoretical tools[5]. Hence, we can rewrite (8) as the following approximation formula

$$\left\langle (x-c)^k \right\rangle \approx \left\langle (x-c)\left\{P_\psi(x-c)\right\}^{k-1} \right\rangle = \left\langle (x-c)\right\rangle^k \quad (9)$$

where the equality between the leftmost and rightmost terms holds for all nonnegative values of k. This equality can be used to construct the following approximate equality for the expectation value of $f(x)$

$$\langle f(x) \rangle \approx f\left(\langle x \rangle\right) \quad (10)$$

where the error terms contain the expectation value of x and the following entities

$$\varphi_k(c) \equiv \left\langle (x-c)\left\{\left[\, I - P_\psi\,\right](x-c)\right\}^k \right\rangle \quad (11)$$

where the integer parameter k varies between 1 (inclusive) and infinity. Amongst these functions, $\varphi_1(c)$ is directly related to the standart deviation because of its following reduced form

$$\varphi_1(c) = \left\langle x^2 \right\rangle - \left\langle x \right\rangle^2 \quad (12)$$

The wave function depends on not only space coordinates but also on time in quantum dynamics where the evolution of the system in time is at the focus. Hence, in the case of the quantum dynamical problems, the integral $\mathcal{I}$ of (1) becomes a parametric integral since its kernel and therefore its weight function depends on time parameter. This is reflected as a time dependence in the wave function. Hence, φ_k entities above also become time dependent. This results in time dependent, or in quantum dynamical terminology, temporally fluctuating function. Hence, despite the nonexistence of time dependence here, we call these entities fluctuation functions. In φ_k, k characterizes the number of the apperances of the operator $\left[\, I - P_\psi\,\right]$ which is responsible for the fluctuation (or deviation for the limited case here) in the error term of (10) and the argument c, which gives function structure to φs, denotes the focus of the expansion. Therefore, we explicitly call $\varphi_k(c)$ "k-th Order Fluctuation Function at the Point c". Although we have assumed that k does not vanish we can extend the definition of $\varphi_k(c)$ to cover $k = 0$ where the fluctuation function becomes the difference between the expectation value of x and c. The only way to make this fluctuation zero is to take $c = \langle x \rangle$. All these mean that (10) is a zeroth order fluctuation expansion around the point where x takes its expectation value. We do not intend to give full details of the complete analysis presented in our recent works since we are intending to use only zeroth order fluctuation expansion, that is, the expression obtained by ignoring the first and higher order terms (the terms containing at least first power of $\left[\, I - P_\psi\,\right]$) in the fluctuation expansion of the expectation value of the function $f(x)$. We use the zeroth order approximation under a new projection operator which projects to a subspace spanned by not only a single function but a set of orthogonal functions. We also make specifications about the integral limits and the weight function here.

Paper is organized as follows. The second section presents the formulation of the new method proposed here. Third section is about the calculation of certain universal constants. Fourth section contains certain numerical comparisons. Fifth section finalizes the paper by giving concluding remarks.

2 Formulation of the Method

Let us specify the interval as $(-\infty, \infty)$ and the weight function in (1) as follows

$$W(x, t, u) = \frac{1}{\sqrt{\pi}t}e^{-\frac{(x-u)^2}{t^2}} \quad (13)$$

where t is a positive parameter and u stands for a real parameter. (13) defines the wave function as follows

$$\psi(x, t, u) = \frac{1}{\pi^{\frac{1}{4}}\sqrt{t}}e^{-\frac{(x-u)^2}{2t^2}} \qquad (14)$$

We can now rewrite (1) as

$$\mathcal{I}(t, u) = \int_{\infty}^{\infty} dx\psi(x, t, u)f(x)\psi(x, t, u) \qquad (15)$$

then consider the Hilbert space spanned by the functions which are square integrable under the weight function $W(x)$. The nonnegative integer powers of x form a basis set for this space since any function in this Hilbert space can be expressed as a linear combination of these functions as long as it is continous everywhere except infinity. Gram-Schmidt orthonormalization of this set produces the basis set whose elements are given through the following equality

$$\phi_n(x, t, u) \equiv A_n(t)e^{-\frac{(x-u)^2}{2t^2}}H_{n-1}\left(\frac{(x-u)}{t}\right) \qquad (16)$$

where the positive integer n starts from 1 and runs up to infinity and the symbol H_{n-1} stands for the Hermite polynomials[6]. The normalization constant A_n is explicitly given as follows

$$A_n(t) \equiv \frac{1}{\pi^{\frac{1}{4}}2^{\frac{n-1}{2}}\sqrt{(n-1)!}\sqrt{t}} \qquad (17)$$

Let us define the following projection operator

$$\mathcal{P}_n g(x) \equiv \sum_{k=1}^{n}\left(\int_{-\infty}^{\infty}dx\phi_k(x, t, u)g(x)\right)\phi_k(x, t, u) \qquad (18)$$

where $g(x)$ is any function chosen from the Hilbert space spanned by $\phi_k(x, t, u)$, $(k = 1, 2, ...)$ and n stands for a positive integer. This operator apparently truncates the representation of any given function in the Hilbert space mentioned above to a finite linear combination of the orthonormal basis functions defined above. In other words, it projects any given function in the Hilbert space spanned by $\phi_k(x, t, u)$, $(k = 1, 2, ...)$ functions to the subspace spanned by first n basis functions, that is, $\phi_k(x, t, u)$, $(1 \le k \le n)$. This multidimensionality of the subspace onto which the projection operator transforms is the basic extension of the fluctuation expansion here.

We can now proceed by using this operator as a first approximation to unit operator. Since we can write

$$(x - c)^m = \mathcal{I}\{(x - c)\mathcal{I}\}^m \qquad (19)$$

we can get the following approximation by staying at the zeroth order truncation of a fluctuation expansion via $\mathcal{P}_n$

$$(x - c)^m \approx \mathcal{P}_n\{(x - c)\mathcal{P}_n\}^m \qquad (20)$$

where n and m stand for a positive and a nonnegative integer respectively. Since a careful glance at the definition of the wave function shows that

$$\psi(x, t, u) = \phi_1(x, t, u) \qquad (21)$$

we can write

$$\langle(x - c)^m\rangle \approx \left\langle\{(x - c)\mathcal{P}_n\}^{m-1}(x - c)\right\rangle \qquad (22)$$

where we have used the fact that the action of $\mathcal{P}_n$ on $\phi_1(x, t, u)$ is again $\phi_1(x, t, u)$ because it is same as the unit operator on the space spanned by $\phi_1(x, t, u)$. If we define an $(n \times n)$ type matrix $\mathbf{X}_n(t, u)$ whose elements are given through the following equalities

$$X_{jk}^{(n)}(t, u) \equiv \int_{-\infty}^{\infty}dx\phi_j(x, t, u)x\phi_k(x, t, u) \qquad (23)$$

where j and k are positive integers varying between 1 and n inclusive, then, we can rewrite (22) as the following quadratic form

$$\langle(x - c)^m\rangle \approx \mathbf{e}_1^{(n)T}(\mathbf{X}_n(t, u) - c\mathbf{I}_n)^m\mathbf{e}_1^{(n)} \qquad (24)$$

where $\mathbf{I}_n$ and $\mathbf{e}_1^{(n)}$ represent n dimensional unit matrix and the first cartesian unit vector, whose only nonzero element is 1 and located at the first position, in n–th dimensional Euclid space. Equation (24) enables us to write

$$\langle f(x - c)\rangle \approx \sum_{m=0}^{\infty}\frac{1}{m!}f^{(m)}(c)\mathbf{e}_1^{(n)T}(\mathbf{X}_n(t, u) - c\mathbf{I}_n)^m\mathbf{e}_1^{(n)} \qquad (25)$$

and therefore

$$\langle f(x - c)\rangle \approx \mathbf{e}_1^{(n)T}f(\mathbf{X}_n(t, u))\mathbf{e}_1^{(n)} \qquad (26)$$

as long as $f(x)$ converges everywhere except perhaps infinity in the complex plane of x.

Now, for further simplification, we can deal with the structure of the matrix $\mathbf{X}_n(t, u)$ and write

$$\int_{-\infty}^{\infty}dx\phi_j(x, t, u)\left(\frac{x - u}{t}\right)\phi_k(x, t, u)$$

$$= \frac{\pi^{-\frac{1}{2}}2^{1-\frac{j+k}{2}}}{\sqrt{(j-1)!(k-1)!}}\int_{-\infty}^{\infty}d\xi e^{-\xi^2}H_{j-1}(\xi)\xi H_{k-1}(\xi) \qquad (27)$$

where the integers j and k start from 1 and run up to and including n. The right hand side of this equlity does not depend on t and u as can be noticed immediately. This independence urges us to define an $(n \times n)$ type matrix $\mathbf{\Xi}_n$ whose elements are defined through the following equality

$$\Xi_{jk} \equiv \int_{-\infty}^{\infty} dx \phi_j(x,t,u) \left(\frac{x-u}{t} \right) \phi_k(x,t,u) \quad (28)$$

where j and k stand for positive integers less than or equal to n. We can now express $\mathbf{X}_n(t,u)$ in terms of $\mathbf{\Xi}_n$ after a careful look at the structures of those matrices as given below

$$\mathbf{X}_n(t,u) = u\mathbf{I}_n + t\mathbf{\Xi}_n \quad (29)$$

which enables us to rewrite (26) as

$$\langle f(x-c) \rangle \approx \mathbf{e}_1^{(n)^T} f\left(u\mathbf{I}_n + t\mathbf{\Xi}_n \right) \mathbf{e}_1^{(n)} \quad (30)$$

and therefore as

$$\mathcal{I}(t,u) \approx \mathbf{e}_1^{(n)^T} f\left(u\mathbf{I}_n + t\mathbf{\Xi}_n \right) \mathbf{e}_1^{(n)} \quad (31)$$

To proceed towards the ultimate form of our approximation formula we need to explicitly express the kernel matrix of the quadratic form above. To this end we can use the Cayley – Hamilton Theorem and write (a_k parameters are unknown yet)

$$f\left(u\mathbf{I}_n + t\mathbf{\Xi}_n \right) = \sum_{k=1}^{n-1} a_k \mathbf{\Xi}_n^{k-1} \quad (32)$$

If we postmultiply both sides of this equation by the j–th eigenvector of $\mathbf{\Xi}_n$ and denote its corresponding eigenvalue by $\xi_{j,n}$ then we can write

$$f\left(u + t\xi_{j,n} \right) = \sum_{k=1}^{n} a_k \xi_{j,n}^{k-1}, \qquad 1 \le j \le n \quad (33)$$

which can be put into the following matrix form

$$\mathbf{V}_n \mathbf{a}_n = \mathbf{f}_n \quad (34)$$

where

$$\mathbf{a}_n^T \equiv [\, a_1 \dots a_n \,] \quad (35)$$
$$\mathbf{f}_n^T \equiv [\, f(u + \xi_{1,n}) \dots f(u + \xi_{n,n}) \,] \quad (36)$$

and

$$\mathbf{V}_n \equiv \begin{bmatrix} 1 & \xi_{1,n} & \xi_{1,n}^2 & \cdots & \xi_{1,n}^{n-1} \\ 1 & \xi_{2,n} & \xi_{2,n}^2 & \cdots & \xi_{2,n}^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \xi_{n,n} & \xi_{n,n}^2 & \cdots & \xi_{n,n}^{n-1} \end{bmatrix} \quad (37)$$

Now, (31) and (32) lead us to write

$$\mathcal{I}(t,u) = \mathbf{q}_n^T \mathbf{a}_n \quad (38)$$

where

$$\mathbf{q}_n \equiv [\, q_{1,n} \dots q_{n,n} \,] \quad (39)$$

and

$$q_{k,n} \equiv \mathbf{e}_1^{(n)^T} \mathbf{\Xi}_n^{k-1} \mathbf{e}_1^{(n)}, \qquad 1 \le k \le n \quad (40)$$

Equation (38) can be combined with (34) to get the following equation as long as $\mathbf{V}_n$ is invertible.

$$\mathcal{I}(t,u) = \mathbf{q}_n^T \mathbf{V}_n^{-1} \mathbf{f}_n \quad (41)$$

If we define

$$\mathbf{w}_n^T = \mathbf{q}_n^T \mathbf{V}_n^{-1} \quad (42)$$

where the elements of the vector $\mathbf{w}_n$ are denoted by $w_{1,n}$, ..., $w_{n,n}$ respectively then we can get the ultimate form of our approximation formula as follows

$$\mathcal{I}(t,u) \approx \sum_{k=1}^{n} w_{k,n} f(u + t\xi_{k,n}) \quad (43)$$

We call $w_{1,n}$, ..., $w_{n,n}$ values "weights" and $\xi_{1,n}$, ..., $\xi_{n,n}$ values "nodes" within an analogy to the Gauss quadratures.

3 Evaluation of Universal Constants

To finalize our method what we need is the evaluation of weights and nodes. Since these entities are directly related to $\mathbf{\Xi}_n$ which is free of $f(x)$ the weights and nodes are universal. Hence, once they are evaluated for a specific n value they can be used in (43) for any $f(x)$ under some constraints like to be continuos. This section is therefore devoted to the evaluations of these universal constants. To this end we can start with the following recursion between consecutive Hermite polynomials

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \quad (44)$$

which is valid for all nonnegative integer values of n by assuming $H_{-1}(x)$ identically zero. If we keep in mind the facts

$$\int_{-\infty}^{\infty} d\xi e^{-x^2} H_j(x) H_k(x) = \delta_{j,k} 2^j j! \sqrt{\pi} \quad (45)$$

and

$$\delta_{j,k} a_{j,k} = a_{j,j} = a_{k,k} \quad (46)$$

where $\delta_{j,k}$ and $a_{j,k}$ stand for the Kroenecker's symbol and any two-indexed-entity respectively then we can arrive at the following equality

$$\Xi_{j,k} = \sqrt{\frac{k}{2}}\delta_{j,k+1} + \sqrt{\frac{k-1}{2}}\delta_{j,k-1} \quad (47)$$

where j and k take integer values between 1 and n inclusive. Ξ_n is apparently a symmetric matrix and, beyond this, its only nonzero diagonals are the upper and lower adjacent neighbors of the main diagonal. The elements of these diagonals are $1/\sqrt{2}$, 1, $\sqrt{3/2}$, ..., $\sqrt{(n-1)/2}$ in downward ordering. By using these values it is possible to numerically evaluate the eigenvalues of Ξ_n. These eigenvalues which are nodes in fact permit us to determine $\mathbf{V}_n$ and therefore all weights. Numerical calculations can be realized by using any software which is capable of doing what we want. Here we have used MuPAD Computer System Algebra developed by Paderborn University in Germany[7] because its capability of performing calculations at any desired level of accuracy and also its symbolic programming features. We report the results for 5, 10, and 15 values of n here. They are given below

$n = 5$

$$\xi_{1,5} = -\xi_{5,5} = 2.02018287045608563293$$
$$\xi_{2,5} = -\xi_{4,5} = 0.95857246461381850711$$
$$\xi_{3,5} = 0.00000000000000000000$$
$$w_{1,5} = w_{5,5} = 0.01125741132772068893$$
$$w_{2,5} = w_{4,5} = 0.22207592200561264440$$
$$w_{3,5} = 0.53333333333333333333$$

$n = 10$

$$\xi_{1,10} = -\xi_{10,10} = 3.43615911883773760333$$
$$\xi_{2,10} = -\xi_{9,10} = 2.53273167423278979641$$
$$\xi_{3,10} = -\xi_{8,10} = 1.75668364929988177345$$
$$\xi_{4,10} = -\xi_{7,10} = 1.03661082978951365418$$
$$\xi_{5,10} = -\xi_{6,10} = 0.34290132722370460879$$
$$w_{1,10} = w_{10,10} = 0.00000431065263071828$$
$$w_{2,10} = w_{9,10} = 0.00075807093431221767$$
$$w_{3,10} = w_{8,10} = 0.01911158050077028561$$
$$w_{4,10} = w_{7,10} = 0.13548370298026773556$$
$$w_{5,10} = w_{6,10} = 0.34464233493201904288$$

$n = 15$

$$\xi_{1,15} = -\xi_{15,10} = 4.49999070730939155366$$
$$\xi_{2,15} = -\xi_{14,15} = 3.66995037340445253473$$
$$\xi_{3,15} = -\xi_{13,15} = 2.96716692790560324849$$
$$\xi_{4,15} = -\xi_{12,15} = 2.32573248617385774545$$
$$\xi_{5,15} = -\xi_{11,15} = 1.71999257518648893242$$
$$\xi_{6,15} = -\xi_{10,15} = 1.13611558521092066632$$
$$\xi_{7,15} = -\xi_{9,15} = 0.56506958325557574853$$
$$\xi_{8,15} = 0.00000000000000000000$$

$$w_{1,15} = w_{15,15} = 0.00000000085896498996$$
$$w_{2,15} = w_{14,15} = 0.00000059754195979206$$
$$w_{3,15} = w_{13,15} = 0.00005642146405189017$$
$$w_{4,15} = w_{12,15} = 0.00156735750354995621$$
$$w_{5,15} = w_{11,15} = 0.01736577449213760635$$
$$w_{6,15} = w_{10,15} = 0.08941779539984440217$$
$$w_{7,15} = w_{9,15} = 0.23246229360973223332$$
$$w_{8,15} = 0.31825951825951825952$$

These result are obtained within 100 decimal digit accuracy under MuPAD and only first 20 fractional digits are reported. the fractional digits beyond the twentieth one are rounded to 20th fractional digit. The symmetry in the results is easily noticable. The sum of weights are all equal to 1. This makes meaningful to use the word "weight" for the naming of these entities.

4 Numerical Efficiency

We have applied our presented method to various functions. All of them are encouraging and promising although higher values of n may be required depending on how continuous $f(x)$ is or how the Taylor series expansion of $f(x)$ converges. We do not intend to report anyone of them. Instead, we are going to give the comparison between the exact and approximate values of the Taylor series expansion of the integral's value with respect to t. To this end we can start with (15) and obtain the following equation by an appropriate coordinate transformation

$$\mathcal{I}(t,u) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx e^{-x^2} f(u+tx) \quad (48)$$

which can be rewritten as follows

$$\mathcal{I}(t,u) = \sum_{k=0}^{\infty} \frac{1+(-1)^k}{2} \frac{\Gamma\left(\frac{k+1}{2}\right)}{k!\sqrt{\pi}} f^{(k)}(u)t^k \quad (49)$$

by expanding $f(u+tx)$ into a power series of t.

On the other hand, (43) can be treated in the same manner as well. This gives

$$\mathcal{I}(t,u) \approx \sum_{k=0}^{\infty} \frac{f^{(k)}(u)}{k!} \left(\sum_{j=1}^{n} w_{j,n}\xi_{j,n}^k\right)t^k \quad (50)$$

which urges us to compare the coefficients of t^k in the last two equalities. In both (49) and (50) all odd powers of t vanish. This, in fact, spontaneously removes the positivity requirement on t. For $n = 5$, the coefficient of $f^{(2k)}(u)t^{2k}$ in the approximate expression

(50) deviates from its counterpart in the exact expression (49) when k is greater than or equal to 5. The other coefficients match within 19 fractional decimal digit accuracy. Indeed the coefficients of $f^{(10)}(u)t^{10}$ for the exact and approximate expressions are roughly 8.138×10^{-6} and 7.105×10^{-6} respectively. In the case where $n = 10$ situation is almost same however first 19 coefficients match instead of 9 and matching is not at the level of 19 but 15 fractional decimal digit accuracy. Remarkable deviations start from the 20. coefficient. Similar behavior is observed for the case where $n = 15$. All these mean that the number of the correct digits should be increased in the weight and node values to get always same precision and the accuracy is about $o(t^{2n})$. We suffice with this discussion here although this is rather qualitative and not precise error estimation since it is out of the scope of this work.

5 Concluding Remarks

We have presented a new extended form of the recently developed fluctuation expansion method in the evaluation of univariate integrals having Gaussian type weight function.

The new extension of the fluctuation method here is the utilization of a subspace spanned by not just a single but more than one functions in the Hilbert space of the square integrable functions over the domain of the integral. We do not take the first and higher order contributions in the fluctuation expansion. We keep only the terms having no fluctuation functions in the expansion. At the final form, we could have been able to get a Gauss quadrature like expression by using matrix algebraic tools.

The parameter t appearing in the denominator of the Gaussian weight function plays the most important role in the analysis. Its vanishing value makes the weight function a Dirac's delta distribution located at the point where $x = u$ in the interval. Hence the series expansion of the integral in powers of t somehow corresponds to the expansion of the weight function to a linear combination of Dirac's delta function and its derivatives.

Two items are important in the numerical efficiency of the formula constructed here. First one is the approximate match between the approximation formula derived here and the series expansion of the integral in powers of t. Exact match occurs for a finite number of the coefficients of these two entities in ascending powers of t and this finite number depends on the value of the method's subspace's dimension n. Denumerably infinite number of remaining terms related to higher powers of t in approximate formula deviate from their counterparts in the exact formula.

The second important thing is the need for increasing high precision in the calculations as n grows. For the first item, we do not always need power series expansions in fact. Only the values of $f(x)$ at nodes are required unless we are enforced to use power series for some mathematical reasons. On the other hand, high accuracy in the calculations when it is necessary requires the employment of the multiprecision algorithms. This can be done mostly by using symbolic and/or high performance computational softwares like MuPAD, Mathematica, REDUCE, Maple, Macsyma and so on.

References:
[1] M. Demiralp, A Fluctuation Expansion Method for the Evaluation of a Function's Expectation Value, *ICNAAM, International Conference on Numerical Analysis and Applied Mathematics - 2005 Extended Abstracts, Eds: T.E.Simos, G. Psihoyios, Ch. Tsitouras*, 2005, pp. 711-714.

[2] M. Demiralp, Determination of Quantum Expectation Values Via Fluctuation Expansion, *Lecture Series on Computer and Computational Sciences, (Proceedings of ICCMSE - 2005, International Conference of Computational Methods in Science and Engineering)*, 2005, pp. 146-149.

[3] N. A. Baykara and M. Demiralp, Fluctuation Expansion in the Quantum Optimal Control of One Dimensional Perturbed Harmonic Oscillator, *Lecture Series on Computer and Computational Sciences, (Proceedings of ICCMSE - 2005, International Conference of Computational Methods in Science and Engineering)*, 2005, pp. 56-59.

[4] E. Meral and M. Demiralp, Phase Space Consideration in Quantum Dynamical Fluctuation Expansion, *Lecture Series on Computer and Computational Sciences, (Proceedings of ICCMSE - 2005, International Conference of Computational Methods in Science and Engineering)*, 2005, pp. 406-409.

[5] A. H. Zemanian, *Distribution Theory and Transform Analysis: An Introduction to Generalized Functions, With Applications*, Dover Publications Co., 1987.

[6] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products,* Academic Press. Inc., 1979.

[7] Paderborn University, *MuPAD, A Computer Algebra System: http://www.mupad.com/*