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ORIGINAL PAPER

# A fluctuation removal based univariate integration over prescribed nodes: certain important aspects of one node fluctuation free integration

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**Abstract** This work aims at the evaluation of a univariate integral whose integrand except the weight function is assumed to be analytic inside a region containing the integration interval as an interior line in the complex plane of the independent variable. The method developed here is based on the idea of fluctuation removal which is the basic root of fluctuation free integration and Gauss quadratures. To this end, first, weight function generating subspaces are constructed. Then various possibilities to use a true weight function in the integration are discussed. All analyses here are for one node integration although higher order fluctuation removal possibilities are also restrictedly discussed. Certain illustrative applications are also distributed in side the sections to support the ideas of the work.

**Keywords** Univariate integration · Quadrature · Fluctuation free representation · Moments · Weight functions · Hilbert spaces

## 1 Introduction

Since the evaluations of the univariate or multivariate integrals are frequently encountered tasks in mathematical chemistry, the approximation methods for these purposes

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are important needs to this end. Although there are many standing numerical approximation techniques for both univariate and multivariate integrations, there is still some rooms to develop new methods to get higher efficiency and accuracy. Since many multivariate integration methods are based on the univariate integration it is quite natural to focus on univariate integration first in the development of a new method. Hence, we deal with the univariate integrals here and what we will obtain will be applicable to multivariate integrals by using the multidimensional grids instead of univariate ones.

The method we develop here is somehow based on the fluctuation free integration which is another way of expressing Gauss quadratures [1–3] via polynomials in terms of matrix representation approximations. Although we will not get into the details, it is important to note that for some probabilistic events such as in Nonequilibrium Statistical Mechanics [4] and Quantum Chemistry [5–8], fluctuations have an important place.

The fluctuation free integration [9–17] does not require to use polynomials only. It can use any appropriate basis function structure although the general tendency is to use polynomials since a lot of formulae be come quite simple in those cases.

To recall mainlines of the fluctuation free integration we consider a function $f(x)$ and the Hilbert space [18,19] of functions, $\mathcal{H}$, which are analytic [20] and therefore square integrable over a finite interval $[a, b]$ and under a given weight function $W(x)$. We define the inner product of two functions in this space, $\mathcal{H}$, as follows

$$(g_1, g_2) \equiv \int_a^b dx\, W(x) g_1(x) g_2(x), \qquad g_1(x),\ g_2(x) \in \mathcal{H} \tag{1}$$

where the arguments of the functions in the inner product are not explicitly shown at the left hand side since $x$ is dummy integration variable of the inner product. We assume that we have constructed the basis functions spanning $\mathcal{H}$ and orthonormalized them if they are not. The general tendency is to start from a linearly independent complete set to span the space $\mathcal{H}$ and to choose the power set $x^0, x^1, \ldots, x^n, \ldots$ first and then to orthonormalize [21–23] them al though this is not the only way to this end. This choice produces an orthonormal polynomial set. Some other nonpolynomial structures in the initialization enable us to use nonpolynomial structures [24]. Without specifying the individual structures we denote the orthonormalized basis functions as follows

$$\mathcal{U} \equiv \{u_i(x)\}_{i=1}^{\infty}, \qquad \left(u_i, u_j\right) = \delta_{i,j} \tag{2}$$

where $\delta_{i,j}$ stands for the Kronecker's delta symbol which becomes 1 if its subindices match and vanishes otherwise. This basis set is denumerably infinite hence needs to be approximated by its following finite truncations

$$\mathcal{U}_n \equiv \{u_i(x)\}_{i=1}^{n}, \qquad n = 1, 2, 3, \ldots \tag{3}$$

which urges us to define the following basis vector function

$$\mathbf{u}_n(x) \equiv [u_1(x)\ \ldots\ u_n(x)\ ,]^T \qquad n = 1, 2, 3, \ldots \tag{4}$$

and to write the inner product matrix equality

$$\left(\mathbf{u}_n, \mathbf{u}_n^T\right) = \mathbf{I}_n, \qquad n = 1, 2, 3, \ldots \tag{5}$$

Now we can consider the independent variable operator [9,11] which multiplies its operand by the independent variable as follows

$$\widehat{x}g(x) \equiv xg(x), \qquad x \in [a, b], \qquad g \in \mathcal{H}. \tag{6}$$

If $\mathbf{X}^{(n)}$ denotes the matrix representation of this operator on $\mathcal{H}_n$ which is spanned by $\mathcal{U}_n$ then we can write

$$\mathbf{X}^{(n)} \equiv \left(\mathbf{u}_n, \widehat{x}\,\mathbf{u}_n^T\right), \qquad n = 1, 2, 3, \ldots \tag{7}$$

which is another inner product matrix structure.

We can define another algebraic operator [9,11,18] which multiplies its operand by the value of the function $f(x)$ as follows

$$\widehat{f}g(x) \equiv f\left(\widehat{x}\right) g(x) = f(x)g(x), \qquad x \in [a, b], \qquad g \in \mathcal{H} \tag{8}$$

which permits us to write the following matrix representation, $\mathbf{M}_f^{(n)}$ of this operator on $\mathcal{H}_n$

$$\mathbf{M}_f^{(n)} \equiv \left(\mathbf{u}_n, \widehat{f}\,\mathbf{u}_n^T\right) = \left(\mathbf{u}_n, f\left(\widehat{x}\right)\mathbf{u}_n^T\right), \qquad n = 1, 2, 3, \ldots \tag{9}$$

The fluctuationlessness theorem [9,11] dictates us that this matrix representation can be approximated as follows if all transitions, single or consecutively multiple, between the subspace $\mathcal{H}_n$ and its complement, $\mathcal{H}_n^{\perp}$, are ignored

$$\mathbf{M}_f^{(n)} \approx f\left(\mathbf{X}^{(n)}\right), \qquad n = 1, 2, 3, \ldots \tag{10}$$

In plain English, this means that the image of the matrix representation of the independent variable operator on $\mathcal{H}_n$ under the function $f$ becomes equal to the matrix representation of $f$ when all contributions involving integrals whose integrands are related to the single or multiple transitions between the subspace $\mathcal{H}_n$ and its complement to $\mathcal{H}$, $\mathcal{H}_n^{\perp}$ are ignored. We call the matrix $\mathbf{X}^{(n)}$ Universal Matrix since it does not depend on the function $f$ and once it is evaluated it can be used indefinitely many times in function operator matrix representations.

The universal matrix is symmetric and its spectrum is com posed of single real values located in the interval $[a, b]$ (therefore there is no multiplicity) [9,11]. If we denote the eigenvalues and corresponding normalized eigenvectors by $\xi_i$ and $\mathbf{x}_i\,(i = 1, 2, \ldots, n)$ respectively then one can write

$$\mathbf{X}^{(n)} = \sum_{i=1}^{n} \xi_i \mathbf{x}_i \mathbf{x}_i^T, \qquad n = 1, 2, 3, \ldots \tag{11}$$

which implies

$$\mathbf{M}_f^{(n)} \approx \sum_{i=1}^{n} f\left(\xi_i\right) \mathbf{x}_i \mathbf{x}_i^T, \qquad n = 1, 2, 3, \ldots \tag{12}$$

Now we can consider the following univariate integral

$$\mathcal{I}_{W,a,b}\left(f\right) \equiv \int_a^b dx\, W(x) f(x) \tag{13}$$

and write

$$\begin{aligned}
&\mathcal{I}_{W,a,b}\left(f\right) \\
&= \int_a^b dx\, W(x) u_1(x) f(x) u_1(x) = \int_a^b dx\, W(x) u_1(x) f\left(\widehat{x}\right) u_1(x) \\
&= \int_a^b dx\, W(x) \mathbf{e}_1^T \mathbf{u}(x) f\left(\widehat{x}\right) \mathbf{u}(x)^T \mathbf{e}_1 = \mathbf{e}_1^T \left( \int_a^b dx\, W(x) \mathbf{u}(x) f\left(\widehat{x}\right) \mathbf{u}(x)^T \right) \mathbf{e}_1 \\
&= \mathbf{e}_1^T \left( \mathbf{u}, f\left(\widehat{x}\right) \mathbf{u}^T \right) \mathbf{e}_1 = \mathbf{e}_1^T \mathbf{M}_f^{(n)} \mathbf{e}_1 \approx e_1^T f\left(\mathbf{X}^{(n)}\right) \mathbf{e}_1 = \sum_{i=1}^{n} f\left(\xi_i\right) \left( \mathbf{e}_1^T \mathbf{x}_i \right)^2
\end{aligned} \tag{14}$$

where $\mathbf{e}_1$ stands for the cartesian unit vector whose only nonzero element resides at the first position, as long as $u_1(x)$ is identical to 1. This identicality is a matter of choice of the first basis function as a constant and requires the integral normalization of the weight (its integral is assumed to be 1). The result at the rightmost part of (14) is a quadrature like formula with $n$ values of the function $f(x)$ at the nodes $\xi_1, \ldots, \xi_n$ with the weight parameters which are the squares of the first element squares of the $\mathbf{x}_i$ eigenvectors.

Although we have stated that the so-called fluctuation terms are ignored we have not explicitly recalled these terms. Despite concerned reader can find documents about these terms it is better to give some brief details. If the function $f(x)$ is expandable to a Taylor series [22,23,25] which is around a point (say $c$) of the inter val $[a, b]$ and converges throughout that interval then we can write

$$f(x) = \sum_{i=0}^{\infty} \frac{f^{(i)}(c)}{i!} (x - c)^i \tag{15}$$

which means

$$\mathbf{M}_f^{(n)} = \left(\mathbf{u}_n,\, f\left(\widehat{x}\right)\,\mathbf{u}_n^T\right) = \sum_{i=0}^{\infty} \frac{f^{(i)}(c)}{i!}\left(\mathbf{u}_n,\, \left(\widehat{x} - c\widehat{I}\right)^i\,\mathbf{u}_n^T\right), \qquad n = 1, 2, 3, \ldots \tag{16}$$

where $\widehat{I}$ stands for the unit operator. We can define the following matrices whose first one is the universal matrix

$$\mathbf{X}_i^{(n)} \equiv \left(\mathbf{u}_n, \widehat{x}^i \mathbf{u}_n^T\right), \qquad i = 1, 2, 3, \ldots \quad n = 1, 2, 3, \ldots \tag{17}$$

and use them to write

$$\left(\mathbf{u}_n, \left(\widehat{x} - c\widehat{I}\right)^i\,\mathbf{u}_n^T\right) = \sum_{j=0}^{i} \binom{i}{j} c^{i-j} \mathbf{X}_j^{(n)}, \qquad i = 1, 2, 3, \ldots \qquad n = 1, 2, 3, \ldots \tag{18}$$

which can be rewritten ($f$ in the superscript being addressing to the word "fluctuation" and $\mathbf{I}_n$ denoting $n \times n$ type unit matrix) as follows

$$\begin{aligned}\left(\mathbf{u}_n, \left(\widehat{x} - c\widehat{I}\right)^i\,\mathbf{u}_n^T\right) &= \sum_{j=0}^{i} \binom{i}{j} c^{i-j} \left[\mathbf{X}^{(n)}\right]^j + \sum_{j=2}^{i} \binom{i}{j} c^{i-j} \mathbf{X}_j^{(f,n)}, \\ &= \left(\mathbf{X}^{(n)} - c\mathbf{I}_n\right)^i + \sum_{j=2}^{i} \binom{i}{j} c^{i-j} \mathbf{X}_j^{(f,n)}, \\ &\qquad i = 1, 2, 3, \ldots \qquad n = 1, 2, 3, \ldots \end{aligned} \tag{19}$$

where

$$\mathbf{X}_j^{(f,n)} \equiv \mathbf{X}_j^{(n)} - \left[\mathbf{X}^{(n)}\right]^j, \qquad j = 2, 3, 4, \ldots \qquad n = 1, 2, 3, \ldots \tag{20}$$

which can be called "Fluctuation Matrices" and we have used the fact that (20) produces zero matrices when $j$ takes values 0 or 1. It is not unique to define a fluctuation matrix and these ones are a little bit different than the fluctuation mat rices we defined earlier [9,11]. To emphasize on this fact we can consider the case where $j = 2$ in the last identity and write

$$\mathbf{X}_2^{(f,n)} \equiv \mathbf{X}_2^{(n)} - \left[\mathbf{X}^{(n)}\right]^2 = \left(\mathbf{u}_n, \widehat{x}\left[\widehat{I} - \widehat{P}^{(n)}\right]\widehat{x}\,\mathbf{u}_n^T\right), \qquad n = 1, 2, 3, \ldots \tag{21}$$

where $\widehat{P}^{(n)}$ stands for the projection operator [9,11] whose explicit form is given below

$$\widehat{P}^{(n)} g(x) \equiv \sum_{i=1}^{n} u_i(x)\,(u_i, g), \qquad g \in \mathcal{H}, \qquad n = 1, 2, 3, \ldots \tag{22}$$

For $i = 1$, the right hand side of (21) matches first of our relevant previous fluctuation matrices whose explicit definitions are given below

$$\boldsymbol{\Phi}_i^{(n)} \equiv \left(\mathbf{u}_n, \widehat{x}\left\{\left[\widehat{I} - \widehat{P}^{(n)}\right]\widehat{x}\right\}^i \mathbf{u}_n^T\right), \qquad i = 1, 2, 3, \ldots \qquad n = 1, 2, 3, \ldots \tag{23}$$

This does not mean that all $\mathbf{X}_i^{(f,n)}$ matrices match these matrices. However, they are related to each other. For example, one can write the following equality for the new third fluctuation matrix

$$\mathbf{X}_3^{(f,n)} \equiv \mathbf{X}_3^{(n)} - \left[\mathbf{X}^{(n)}\right]^3 = \boldsymbol{\Phi}_2^{(n)} + \mathbf{X}^{(n)}\boldsymbol{\Phi}_1^{(n)} + \boldsymbol{\Phi}_1^{(n)}\mathbf{X}^{(n)}, \qquad n = 1, 2, 3, \ldots \tag{24}$$

The other $\mathbf{X}_i^{(f,n)}$ matrices can also be ex pressed in similar type formulae. The important difference between $\mathbf{X}_i^{(f,n)}$s and $\boldsymbol{\Phi}_i^{(n)}$s is the number of appearance of the operator $\left[\widehat{I} - \widehat{P}^{(n)}\right]$. It appears exactly $i$ times in $\boldsymbol{\Phi}_i^{(n)}$ while $\mathbf{X}_i^{(f,n)}$ is composed of terms each of which may have a different number of appearance for $\left[\widehat{I} - \widehat{P}^{(n)}\right]$ but even in this case $\left[\widehat{I} - \widehat{P}^{(n)}\right]$ can appear at most $i$ times in a single additive term.

The operator $\widehat{P}^{(n)}$ has the property of being idempotent [9,11] as can be easily shown. It projects any vector belonging to $\mathcal{H}$ to its finite dimensional subspace $\mathcal{H}_n$. If its operand lies in $\mathcal{H}_n$ then it produces the same vector. In other words, it is unit operator of $\mathcal{H}_n$. Similarly, the operator $\left[\widehat{I} - \widehat{P}^{(n)}\right]$ projects from $\mathcal{H}$ to $\mathcal{H}_n^{\perp}$, the orthogonal complement of $\mathcal{H}_n$ to $\mathcal{H}$. It is also a unit operator but now for $\mathcal{H}_n^{\perp}$. The image of a vector in $\mathcal{H}_n$ under the operator $\widehat{x}$ may or may not have components in $\mathcal{H}_n^{\perp}$ depending on its operand. This image is pruned by the operator $\left[\widehat{I} - \widehat{P}^{(n)}\right]$ hence the operator $\left[\widehat{I} - \widehat{P}^{(n)}\right]\widehat{x}$ can produce images either zero or lying in $\mathcal{H}_n^{\perp}$. On the other hand the operator $\widehat{x}\left[\widehat{I} - \widehat{P}^{(n)}\right]\widehat{x}$ can produce images having components in both $\mathcal{H}_n$ and in its orthogonal complement $\mathcal{H}_n^{\perp}$ depending on its operand. However the fluctuation matrices $\boldsymbol{\Phi}_i^{(n)}$ are the matrix representation of this operator restricted to $\mathcal{H}_n$. Therefore they reflect the transitions between the subspace $\mathcal{H}_n$ and its orthogonal complement. These transitions are corresponding to the contributions co ming from the basis functions $u_{n+1}(x), u_{n+2}(x), \ldots$ which become more oscillatory as their subindices increase. These oscillations give the appearance of quite random changes, or in more correct word, fluctuations. This is the reason why we call the related matrices "Fluctuation Matrices".

It is not hard to show that the fluctuation matrices de noted by $\mathbf{X}_j^{(f,n)}$s tend to vanish as the subspace dimension $n$ grows unboundedly although the rate of diminishing decelerates as $j$ increases. This can be shown via a norm analysis for more precise statements and seems to be quite natural since the matrix representation of any power of $\widehat{x}$ approaches to the same power of the matrix representation of $\widehat{x}$ as the subspace $\mathcal{H}_n$ tends to approach to entire Hilbert space $\mathcal{H}$. This phenomenon can be more clearly observed when an orthogonal polynomial basis set [9,11] is used. In that case, the three consecutive term involving recursions are obtained amongst the basis functions which are orthonormal polynomials. This results in universal matrices whose only nonzero elements are located at the main diagonal and its two nearest neighbor diagonals. Then one can easily show that the first fluctuation matrix $\mathbf{X}_2^{(f,n)}$ has just a single nonzero element located at the rightmost bottom position [9,11]. As the sub index of $\mathbf{X}_j^{(f,n)}$, $j$, increases other lo cations become to be filled by nonzero values to up and left directions. The norms of these matrices quite small in comparison with corresponding power of the universal matrix. We do not intend to give more details about these points here. These can perhaps be used to develop a nonlinear analysis in future works of us or someones else.

As we have investigated above, the nodes for the fluctuation free integration come from the spectrum of the universal matrix $\mathbf{X}^{(n)}$. This spectrum changes as $n$ varies and the nodes for $n$ are nested in the nodes for $(n+1)$. Unless the function to be integrated is not known on these nodes we can not use the fluctuation free integration scheme as it stands. The locations of the nodes depend not only on $n$ but basis functions, interval, and weight function. Hence, we may seek some ways to change the weight of the integral without changing its certain important features like analyticity. This work somehow tries to do this task.

The paper is organised as follows. Section 2 is devoted to the construction of a subspace that we call "Weight Function Generating Subspace". The one node integration via orthonormalized power set works for certain restricted values of the single node under consideration. Section 3 attempts to change this restricted subinterval. Section 4 focuses on nonpolynomial basis functions in the weight function generating subspace construction. Section 5 finalizes the paper via concluding remarks. The case where more than one condition are imposed for the above mentioned subspace construction is given in some details by the companion of this paper [26]. Certain illustrative implementations are distributed throughout the sections.

## 2 Single node integration: weight function generators

The main purpose in this paper to construct an approximation scheme having the efficiency of Fluctuation Free Integration which is equivalent to Gauss Quadrature for polynomial basis set. What we are intending to do for this aim is the construction of a new weight function and then to use it in the integration to get a quadrature like formula. To explain our basic idea we start with the simple case having just a single node where the value of the function to be integrated will be used in the formulae for simplicity. We will consider the integral as follows

$$\mathcal{I} = \int_0^1 dx f(x) \tag{25}$$

where the moments are defined through the following formulae

$$\mu_i \equiv \int_0^1 dx x^i = \frac{1}{i+1}, \qquad i = 0, 1, \ldots \tag{26}$$

In the one node integration we need to consider just a single node and accompanying weight constant which are denoted by $x_1$ and $w_1$ respectively. The fluctuation free integration (or Gauss quadrature) dictates us that the following conditions should hold,

$$w_1 = \widetilde{\mu}_0, \qquad w_1 x_1 = \widetilde{\mu}_1 \tag{27}$$

where the symbols $\widetilde{\mu}_0$ and $\widetilde{\mu}_1$ stand for the first two moments of the unknown weight function $\widetilde{w}(x)$ which is somehow considered as the distorted form of the original constant unit weight function $w_c(x) = 1$ by a scaling factor $s(x)$, that is, $\widetilde{w(x)} = w_c(x)s(x)$. We will focus on $s(x)$ here. We want to construct of weight functions in the Hilbert space of functions which are analytic in a region containing the interval [0, 1] in the complex plane of the independent variable $x$. We prefer to deal with a subspace which contain s (not necessarily composed of them only) weight functions we need. The subspace we need can be constructed by imposing certain conditions. However, the positivity everywhere except a finite number of points, which is the fundamental property of the weight functions, and the inhomegeneous conditions in (27) are not convenient to this end. On the other hand, we can de rive a homogeneous condition from the conditions of (27) as follows

$$\begin{aligned} \widetilde{\mu}_0 = \int_0^1 dx s(x), \qquad \widetilde{\mu}_1 = \int_0^1 dx s(x) x, \\ \longrightarrow \quad \widetilde{\mu}_1 \int_0^1 dx s(x) - \widetilde{\mu}_0 \int_0^1 dx s(x) x = 0 \\ \longrightarrow \quad x_1 \int_0^1 dx s(x) - \int_0^1 dx s(x) x = 0 \end{aligned} \tag{28}$$

We call the last equation “Single Node Weighing Con dition”. We can assume that the function $s(x)$ is analytic in the analyticity region of the function to be integrated. This enables us to use Taylor expansions. For symmetry reasons we prefer to use the expansion at the midpoint of the integration interval. Thus

$$s(x) = \sum_{j=0}^{\infty} s_j \left(x - \frac{1}{2}\right)^j \tag{29}$$

which gives the following relation amongst the coefficients

$$\begin{aligned} s(x) &= \sum_{j=0}^{\infty} s_j \left( x_1 \int_0^1 dx \left(x - \frac{1}{2}\right)^j - \int_0^1 dx \left(x - \frac{1}{2}\right)^j x \right) \\ &= \sum_{j=0}^{\infty} s_j \left[ \frac{1}{2^j (j+1)} \frac{1 + (-1)^j}{2} \left(x_1 - \frac{1}{2}\right) - \frac{1}{2^{j+1}(j+2)} \frac{1 - (-1)^j}{2} \right] = 0 \end{aligned} \tag{30}$$

The solution of $s_0$ in terms of the remaining coefficients gives

$$s_0 = -\sum_{j=1}^{\infty} s_j \left[ \frac{1}{2^j (j+1)} \frac{1 + (-1)^j}{2} - \frac{1}{2^{j+1}(j+2)} \frac{1 - (-1)^j}{2} \left(x_1 - \frac{1}{2}\right)^{-1} \right] \tag{31}$$

which can be used in (29) to eliminate $s_0$ to produce

$$s(x) = \sum_{j=1}^{\infty} s_j p_j(x) \tag{32}$$

where

$$\begin{aligned} p_j(x) = \left(x - \frac{1}{2}\right)^j - \frac{1 + (-1)^j}{2^{j+1}(j+1)} + \frac{1 - (-1)^j}{2^{j+2}(j+2)} \left(x_1 - \frac{1}{2}\right)^{-1}, \\ j = 1, 2, 3, \ldots \end{aligned} \tag{33}$$

The root loci of these polynomials should be investigated since the product of their reciprocals with the function to be integrated will be used as the function of the quadrature we want to construct. We will use the follow ing equalities for approximating the integral

$$\int_0^1 dx f(x) \equiv \int_0^1 dx s(x) \widetilde{f}(x), \qquad \widetilde{f}(x) \equiv \frac{f(x)}{s(x)} \tag{34}$$

where $s(x)$ and $\widetilde{f}(x)$ now will be conside red as the weight and the function to be integrated. A careful analysis shows that the even degree polynomials in (33) have node free zeros. They are distributed on a circle centered at the point $(1/2, 0)$ of the $x$ complex plane with same angles between two consecutive complex roots. The radii

of these circles are less than $1/2$ and tend to be $1/2$ as the degree of the polynomial under consideration increases unboundedly. This means that the even degree $p_j$ polynomials' reciprocals can not be analytic over the entire do main of the integration, $[0, 1]$.

The odd degree $p$ polynomials above have roots which are again distributed on a circle centered at the point $(1/2, 0)$ of the $x$ complex plane with same angles between two consecutive roots. However, this time, the radii of the circles are proportional to the reciprocal of an odd integer root of the term $(x_1 - 1/2)$. This brings analyticity on the entire integration domain whose extent becomes larger as $x_1$ approaches $1/2$. As a matter of fact, the polynomial $p_1(x)$ has the largest analyticity domain for its reciprocal since its only zero denoted by $x_z$ can be expressed as follows

$$x_z = \frac{1}{2} - \frac{1}{12}\left(x_1 - \frac{1}{2}\right)^{-1} \tag{35}$$

If the node $x_1$ approaches $1/2$ from right then $x_z$ goes to plus infinity. As $x_1$ gets apart to the right from this midpoint $x_z$ gets smaller and when $x_1$ be comes $2/3$ the root vanishes by destroying the reciprocal analyticity. On the other hand, as $x_1$ gets apart to the left from the midpoint $1/2$, $x_z$ starts to grow from minus infinity until it destroys the reciprocal analyticity at $x_1$'s value of $1/3$ where $x_z$ vanishes. All these mean that $p_1(x)$ can be used as a weight function for $x_1 \in \left(\frac{1}{3}, \frac{2}{3}\right)$. Al though this interval gives the weight function character to $p_1(x)$ it is safer to use a narrower $x_1$ subinter val centered at the midpoint $1/2$ for better quality in fluctuation free integration. The larger analyticity do main the better efficiency in the use of the fluctuation free integration. Figure 1 depicts the normalized form of first polynomial ba sis function in the $[0, 1]$ interval for the weight function constructed above for several nodal values. As can be noticed immediately the line segments remain positive for all $x$ values as long as $x_1$ remains between $1/3$ and $2/3$. The color ing used to distinguish the plots are also given through legend property of the plotting. This figure implies that normalized form of $p_1(x)$ can be used as a weight for nodal values between $1/3$ and $2/3$ exclusive. The next figure, Fig. 2, depicts the even degree polynomials for the degrees 2, 4, 6, 8, 10 with different colors given through the legend of the figure.

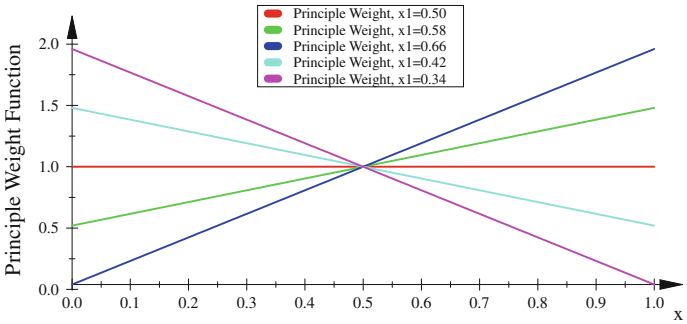


**Fig. 1** The variations of the principal weight polynomial for several nodal values

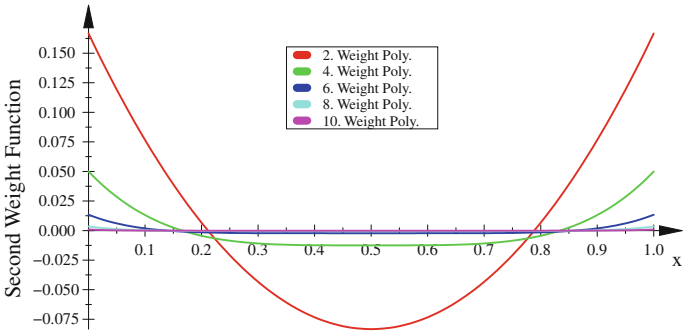


**Fig. 2** The variations of the second, fourth, sixth, eighth and tenth polynomial from the weight generating subspace

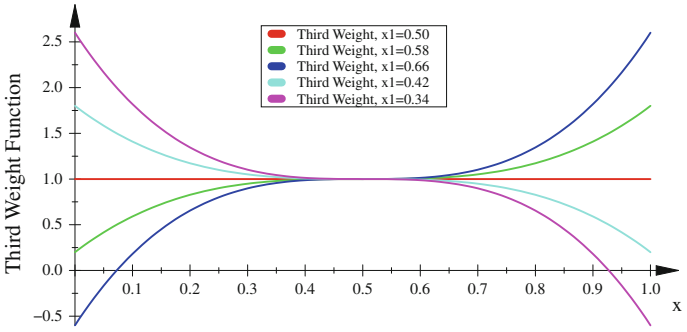


**Fig. 3** The variations of the third polynomial from the weight generating subspace for several nodal values

Since the integral of these polynomials are equal to 0 in the interval [0, 1], they can not be normalized in this interval, so that they can not be used as weight functions. The third figure (Fig. 3) depicts the normalized form of third polynomial in [0, 1] interval for the same nodal values as in Fig. 1 with the same coloring. The lack of positivity everywhere is apparent for all function plots corresponding to some different nodal values. However, there seems to be some subinterval for $x_1$, where the polynomial is positive everywhere throughout the inter val.

We call the subspace spanned by $p$ polynomials "First Order Single Node Weight Generators". As we have noticed above these polynomials except the first one are not positive for all $x_1$ values between $1/3$ and $2/3$ exclusive. However, the positivity of the first polynomial for this open interval of the node, is sufficient to create new polynomials which remain positive between $1/3$ and $2/3$ exclusive. Towards this goal certain linear combinations containing $p_1(x)$ amongst $p$ polynomials can be constructed although we do not in tend to give details here. Thus we can state that a denumerable infinite number of basis function can be constructed for this subspace. Then, certain linear combinations which can be constructed in accordance with the needs can be used for approximate integration. This is a quite comprehensive issue and we suffice to use only the first polynomial $p_1(x)$ we call "Principal Weight Gene rator"for the first order single node quadrature. Another important issue is the integral

normalization. We will approximate the integral under consideration as follows (as we mentioned above)

$$\mathcal{I} = \int_0^1 dx p_1(x) \left[ \frac{f(x)}{p_1(x)} \right] \tag{36}$$

where we have had to consider the reciprocal of $p_1(x)$ as a part of the function to be integrated to be able to use $p_1(x)$ as a weight function. This may work as long as the reciprocal of $p_1(x)$ remains analytic everywhere in the interval [0, 1] since the requirement for being analytic in a region containing this integration interval as an interior subregion in the comp lex plane of $x$ is fulfilled. According to our analyses above this property happens to exist and therefore we can approximate (36) as follows by using the single node fluctuation free integration under the weight $p_1(x)$

$$\mathcal{I} \approx \frac{1}{p_1(x_1)} f(x_1) \tag{37}$$

which means that the reciprocal of $p_1(x_1)$, which is guaranteed to be positive takes the duty of one node integration weight constant. Since the equality in (36) is invariant under the scaling of the function $p_1(x)$, we prefer to normalize $p_1(x)$ to make unit its integral between 0 and 1. We can denote the resulting function by $w_1(x)$ for our further analyses. Due to particular structure of $p_1(x)$ it is exactly same as $w_1(x)$. Thus, we can write

$$\mathcal{I} \approx \frac{1}{w_1(x_1)} f(x_1) \tag{38}$$

Figure 4 contains the exact and approximate integrals of the function $exp(\alpha x)$. The approximate integrals obtained using (37) are for $x_1 = 0.42, 0.50, 0.58, 0.60$. They are depicted against the $\alpha$ values between 0 and 2. Same plotting for $\alpha$ values between 2 and 7 are depicted in Fig. 5.

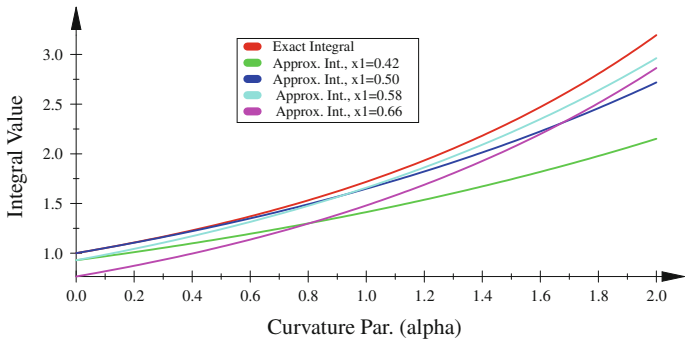


**Fig. 4** The exact and approximate values of the integrals of $exp(\alpha x)$ versus $\alpha$ values from 0 to 2

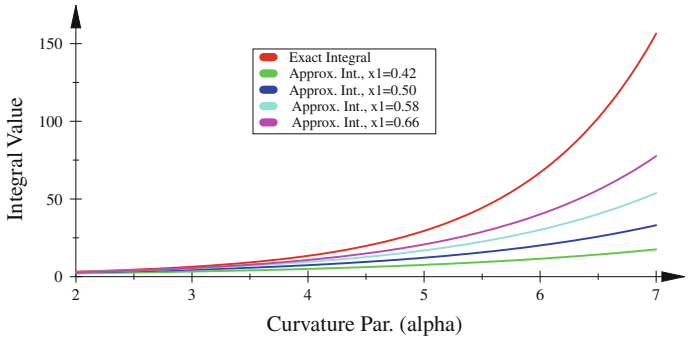


**Fig. 5** The exact and approximate values of the integrals of $exp(\alpha x)$ versus $\alpha$ values from 2 to 7

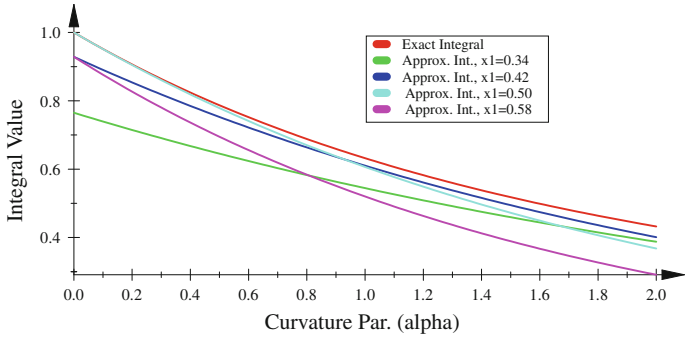


**Fig. 6** The exact and approximate values of the integrals of $exp(-\alpha x)$ versus $\alpha$ values from 0 to 2

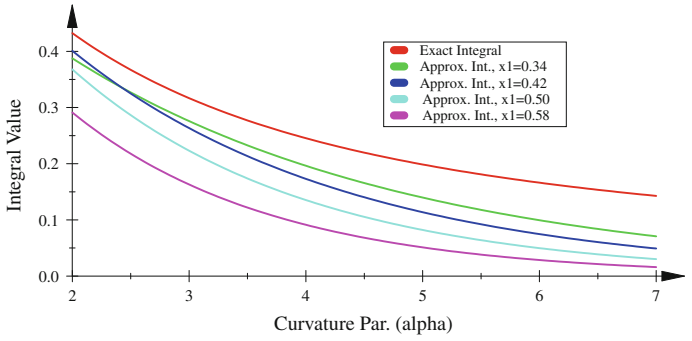


**Fig. 7** The exact and approximate values of the integrals of $exp(-\alpha x)$ versus $\alpha$ values from 2 to 7

These plots are constructed for monotously increasing functions to understand what happens when the curvature of the function to be integrated increases. We could equivalently investigate the case of monotously decreasing functions in the same way. The Figs. 6 and 7 are designed to this end by using the function $exp(-\alpha x)$ for various $\alpha$ values.

What we have extracted from these plots can be itemized as follows

1. If $\alpha$ is approaches 0 then the exponential function under consideration tends to be constant unit function. In that case the nodal value $x_1 = 0.50$ produces the best approximation which matches the exact integral. This can be generalized as the conclusion "flat (almost constant)"functions can be characterized by the nodes in the close vicinity of $x_1 = 0.50$. That is, the nodes around the midpoint produce the best approximation to the flat function integrations.
2. As $\alpha$ increases from 0 the curvature of the exponential function grows. The required node for the best integral value moves from the midpoint to the right. This means that we can expect high qualities from the one node integration for the functions with high curvature and monotonous increasing feature, by using nodal points close to 1.
3. As $\alpha$ decreases from 0 the curvature of the exponential function increases with a monotonous decrease. The required node for the best integral value moves from the midpoint to the left. This means that we can expect high qualities from the one node integration for the functions with high curvature and monotonous decreasing feature, by using nodal points close to 0.
4. If the function under consideration is known nowhere except the node $x_1$ then there is nothing to do with the se formulation beyond using the formula given by (37). However we can say something qualitative about the approximation performance if we have some extra qualitative information about the function.
5. If the function under consideration is analytically known everywhere then it becomes flexible to choose best $x_1$ nodal value to get best approximation. The location of $x_1$ for best integration is not universal, it changes from function to function. To find the best location is a function dependent comprehensive issue we find out of the scope of this paper.

## 3 Changing the one node fundamental interval

The analysis in the previous section shows that $x_1$ can take values from only one third of the entire interval. This is of course an undesired situation and should be removed to get more practical applicability. As we found the method we have developed until now uses the open interval $(1/3, 2/3)$ as the largest interval possibility. However, for the sake of larger reciprocal analyticity we prefer to use some interior subinterval, say $\left[x_1^{(min)}, x_1^{(max)}\right]$. Fortunately this is possible. We have used unit constant weight function in the previous section although we do not have to do so in fact. We can transform the integration variable and rewrite integral under consideration as follows

$$\mathcal{I} = \int_0^1 dx(k+1)x^k f\left(1 - x^{k+1}\right) \tag{39}$$

where we have used the transformation $x \to 1 - x^{k+1}$ for a nonnegative integer value of $k$. The function $W(x)$ defined below can be considered as a weight since it has all features of a weight function in the interval [0, 1]

$$W(x) \equiv (k+1)x^k, \qquad k = 0, 1, 2, \ldots \tag{40}$$

which includes the unit constant weight as a particular case. If the only value of function $f$ to be used in integration is at the node where $x = x_1$ then the one node fluctuation free integration's node is located at $x = \widetilde{x}_1$ which is related to $x_1$ through the equality

$$\widetilde{x}_1 \equiv (1 - x_1)^{\frac{1}{k+1}}, \qquad k = 0, 1, 2, \ldots \tag{41}$$

We are going to try to find the region for $x_1$ to produce a desired reciprocal analyticity domain.

We can write the new form of (28) for this weight as follows

$$\begin{aligned} \widetilde{\mu}_0 = \int_0^1 dx\, W(x)s(x), \qquad \widetilde{\mu}_1 = \int_0^1 dx\, W(x)s(x)x, \\ \longrightarrow \widetilde{\mu}_1 \int_0^1 dx\, W(x)s(x) - \widetilde{\mu}_0 \int_0^1 dx\, W(x)s(x)x = 0 \\ \longrightarrow \widetilde{x}_1 \int_0^1 dx\, W(x)s(x) - \int_0^1 W(x)dxs(x)x = 0 \end{aligned} \tag{42}$$

where (29) maintains its validity while (30) should take the following form

$$s(x) = \sum_{j=0}^{\infty} s_j \left( \widetilde{x}_1 \int_0^1 dx\, W(x) \left(x - \frac{1}{2}\right)^j - \int_0^1 dx\, W(x) \left(x - \frac{1}{2}\right)^j x \right) \tag{43}$$

If we define

$$\begin{aligned} \sigma_j = \left( \widetilde{x}_1 \int_0^1 dx\, W(x) \left(x - \frac{1}{2}\right)^j - \int_0^1 dx\, W(x) \left(x - \frac{1}{2}\right)^j x \right), \\ j = 0, 1, 2, \ldots \end{aligned} \tag{44}$$

then we can solve $s_0$ in terms of other $s_i$ coefficients as follows

$$s_0 = -\sum_{j=1}^{\infty} s_j \frac{\sigma_j}{\sigma_0} \tag{45}$$

which can be used in (43) for the elimination of $s_0$ to get

$$s(x) = \sum_{j=1}^{\infty} s_j p_j(x) \tag{46}$$

where

$$p_j(x) = \left(x - \frac{1}{2}\right)^j - \frac{\sigma_j}{\sigma_0}, \qquad j = 1, 2, 3, \ldots \tag{47}$$

$\sigma$ coefficients in the above analysis can be analytically determined although we do not give their explicit structures since we do not intend to deal with $p$ polynomials except the first one as we did before. Since the evaluation of $p_1(x)$ necessitates $\sigma_0$ and $\sigma_1$ we give them explicitly below

$$\sigma_0 = \widetilde{x}_1 - \frac{k+1}{k+2}, \qquad \sigma_1 = \frac{k}{2(k+2)}\sigma_0 - \frac{k+1}{(k+2)^2(k+3)}. \tag{48}$$

These formulae enable us to write

$$p_1(x, \widetilde{x}_1, k) = x - \frac{1}{2} - \frac{k}{2(k+2)} + \frac{k+1}{(k+2)(k+3)\left[(k+2)\widetilde{x}_1 - (k+1)\right]} \tag{49}$$

whose zero $x_z\,(x_1, k)$ is explicitly given be low

$$x_z\,(\widetilde{x}_1, k) = \frac{1}{2} + \frac{k}{2(k+2)} - \frac{k+1}{(k+2)(k+3)\left[\,(k+2)\widetilde{x}_1 - (k+1)\,\right]} \tag{50}$$

which should satisfy the following inequalities

$$x_z\,(\widetilde{x}_1, k) > \frac{1}{2} + \rho, \qquad x_z\,(\widetilde{x}_1, k) < \frac{1}{2} - \rho \tag{51}$$

where $\rho$ stands for the radius of the circle centered at $x = 1/2$, which defines the reciprocal analyticity domain. The simultaneous solutions of these inequalities al low us to find analytic solutions whose explicit structures in terms of $k$ and $\rho$ are given below by skipping the intermediate algebra

$$\widetilde{x}_1^{(min)}(k, \rho) < \widetilde{x}_1 < \widetilde{x}_1^{(max)}(k, \rho) \tag{52}$$

where

$$\widetilde{x}_1^{(max)}(k, \rho) \equiv \frac{(k+1)\left[(2\rho+1)\,k + (6\rho+1)\right]}{(k+3)\left[(2\rho+1)\,k + 4\rho\right]} \tag{53}$$

$$\widetilde{x}_1^{(min)}(k, \rho) \equiv \frac{(k+1)\left[(2\rho-1)\,k + (6\rho-1)\right]}{(k+3)\left[(2\rho-1)\,k + 4\rho\right]} \tag{54}$$

which enable us to write

$$1-\widetilde{x}_1^{(max)}(k,\rho)^{k+1} < x_1 < 1-\widetilde{x}_1^{(min)}(k,\rho)^{k+1}. \tag{55}$$

These bounds for $x_1$ get closer and approach a common limit which is $1-e^{-2}$ (greater than 0.86466 in decimal digits after the fifth one), where $e$ is the base of the natural logarithm, as $k$ goes to infinity. All this analysis shows that it is possible to change the reciprocal analyticity interval by using appropriate co ordinate transformations. We have used the integer powers of the independent variable here as weights. This enforced the reciprocal analyticity interval to shift right. If we would use

$$\mathcal{I}=\int_0^1 dx(k+1)x^k f\left(x^{k+1}\right) \tag{56}$$

then we would shift the reciprocal analyticity interval to the left for each $k$ and $\rho$ values and what we would immediately notice that these intervals would get closer and approach the common limit $e^{-2}$ (less than 0.135336 in decimal digits after the fifth one). This interval extension and/or shift completely depends on the structure of the weight function $W(x)$ coming from the transformation we used in the integral. The important property of the weight functions here is the fact that they increase from either left or right endpoint of the integration interval here. The rate of the increase determines the amount of the shifting to the left or right. Hence, one can seek appropriate weight functions to shift the reciprocal analyticity interval to the desired position with the accompaniment of the interval contraction. We have not performed a sufficiently detailed analysis to find whether it is possible to get access to endpoints. In other words here it seems to be possible to find map pings enabling us to use almost entire region of the integration interval for $x_1$ nodal value. Nevertheless, we have shown that we can deal with the nodes satisfying $e^{-2} < x_1 < 1-e^{-2}$ inequalities. We find all the remaining issues like to find weight functions constructing larger domains out of the scope of this paper although they may be considered as interesting for mathematical point of view.

Now, in the light of above discussions, the one node integration formulae given in (37) and (38) remain valid for these cases as long as the restrictions given for $x_1$ in this section are not destroyed and this sections' structures for $p_1$ and $w_1$ are used.

## 4 Nonpolynomial weight function generators

In the previous sections we have focused on the construction of polynomial weight function generators. Our at tempts revealed the fact that it is impossible to construct polynomials remaining positive at every point of the interval $[0, 1]$ for the nodal value $x_1$. All the polynomials of the first order weight function generators satisfy the single fluctuation removal condition but it is impossible to find a polynomial which behaves as a weight function for all $x_1$ values between 0 and 1 inclusive. This quite restricted situation is however peculiar to the polynomial structures. We will show that

it is possible to construct a nonpolynomial structure which is a power series in fact, and, can be used as a weight function for all $x_1$ values between 0 and 1 inclusive. We may choose the function $s(x)$ as follows

$$s(x, \nu) \equiv \mathrm{e}^{\nu\left(x-\frac{1}{2}\right)} \tag{57}$$

where $\nu$ is assumed to be a real value. First order fluctuation removal condition dictates us that

$$\begin{aligned}
&\left(x_1 - \frac{1}{2}\right) \int_0^1 dx s(x, \nu) - \int_0^1 dx s(x, \nu) \left(x - \frac{1}{2}\right) \\
&= \left(x_1 - \frac{1}{2}\right) \int_0^1 dx \mathrm{e}^{\nu\left(x-\frac{1}{2}\right)} - \int_0^1 dx \mathrm{e}^{\nu\left(x-\frac{1}{2}\right)} \left(x - \frac{1}{2}\right) \\
&= \left(x_1 - \frac{1}{2} + \frac{1}{\nu}\right) \frac{2}{\nu} \sinh\left(\frac{\nu}{2}\right) - \frac{1}{\nu} \cosh\left(\frac{\nu}{2}\right) = 0
\end{aligned} \tag{58}$$

whose analytic solution for $\nu$ in terms of $x_1$ is almost impossible. However we can give numerical solution as the inverse of the function presented in Fig. 8. As can be easily noticed $x_1$ nodal values vary between 0 and 1 inclusive as $\nu$ moves from left to right on the real axis. The endpoints where $x_1$ becomes either 0 or 1 correspond the minus and plus infinite limits of the $\nu$ parameter. This is somehow an expected result since we have lived the trouble for getting the interval endpoint values of $x_1$ into the reciprocal analyticity domain. In fact, it corresponds to the singularities of the end points in quadratures which are generally constructed for open intervals. The interesting thing here is the one to one correspondence between $x_1$ and $\nu$ and the coverage of the entire domain of the nodal values. This is just a single example which reveals the fact that one can construct infinite series by using infinite linear combinations (exponential function has a such structure) in the weight generator subspace. We do not intend to at tempt a rigorous analysis for these types construction here since our purpose was just to show the possibility of constructing weight functions covering for all possible nodal values. However, we will use this weight in the companion of this paper to get more sophistication.

Figure 9 contains the exact and approximate integrals of the function $exp(\alpha x)$. The approximate integrals obtained using (37) are for $\nu = 0.5, 1.0, 1.5, 2.0$. They are depicted against the $\alpha$ values between 0 and 2. Same plotting for $\alpha$ values between 2 and 7 are depicted in Fig. 10.The approximate integrals obtained using (37) are for $\nu = 5.0, 8.0, 9.0, 10.0$. As it is seen from the figures, as curvature of the function increases, we have to use a larger $\nu$ value in the weight function.

The Figs. 11 and 12 are designed to this end by using the function $exp(-\alpha x)$ for various $\alpha$ values.The approximate integrals obtained using (37) are for $\nu = -0.5$, $-1.0, -1.5, -2.0$ and $\nu = -2.5, -4.0, -6.0, -10.0$ respectively. This shows us, for

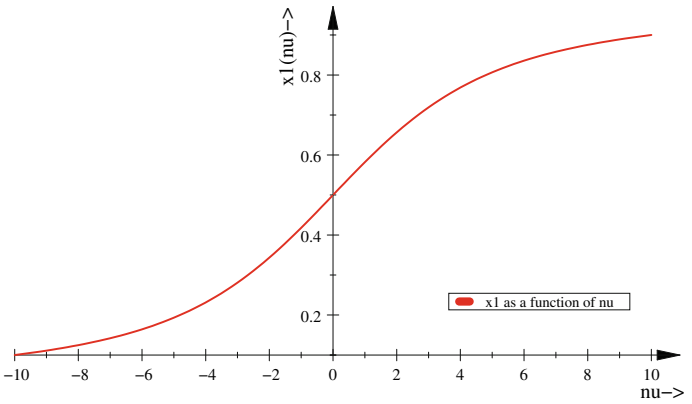


**Fig. 8** The variation of $x1$ nodal parameter values with $\nu$ exponential parameter values

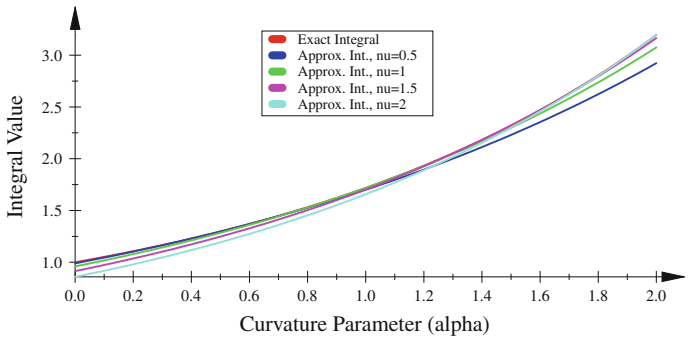


**Fig. 9** The exact and approximate values of the integrals of $exp(\alpha x)$ versus $\alpha$ values from 0 to 2

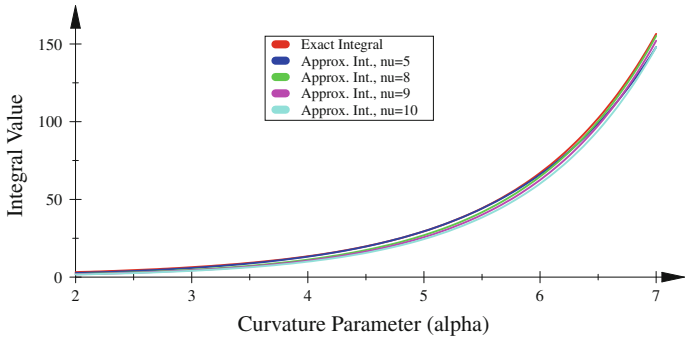


**Fig. 10** The exact and approximate values of the integrals of $exp(\alpha x)$ versus $\alpha$ values from 2 to 7

functions with negative arguments, $\nu$ parameter must have negative values and as curvature of the function increases with a monotonous decrease, the absolute value of $\nu$ parameter given in the weight function has to be larger.

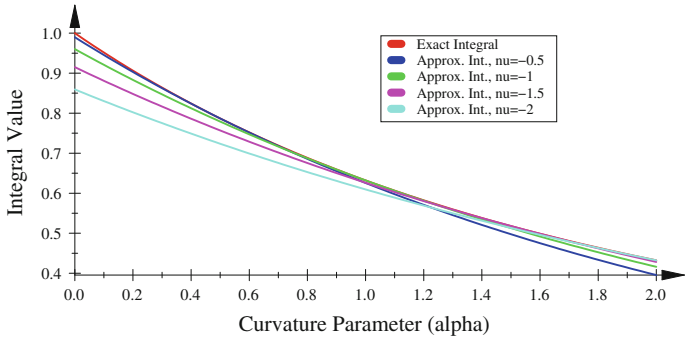


**Fig. 11** The exact and approximate values of the integrals of $exp(-\alpha x)$ versus $\alpha$ values from 0 to 2

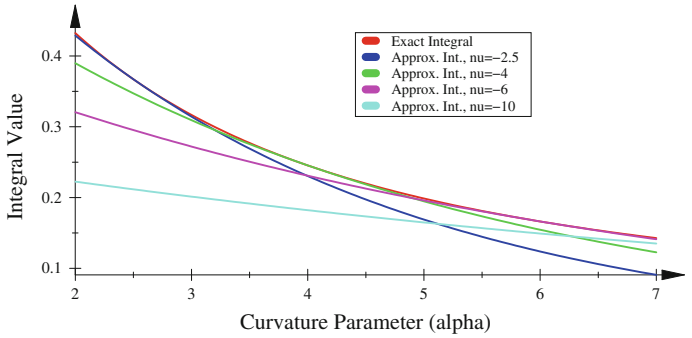


**Fig. 12** The exact and approximate values of the integrals of $exp(-\alpha x)$ versus $\alpha$ values from 2 to 7

## 5 Concluding remarks

In this work, we have tried to construct a specific subspace in the Hilbert space, to which the functions to be integrated belong, such that the elements of this subspace can be used if they are true weights. In this way we could be able to change the weight of the integration at the expense of appearing a new reciprocal factor in the function to be integrated. Our efforts have been not to destroy the analyticity properties of the function to be integrated. This enables us to change the location of the single node under consideration. However we observed that polynomial structures bring restrictions on the location of the single node under consideration. We have found the way to get rid of this unpleasant situation by using nonpolynomial structures. The exponential weight seem to be a very productive candidate to this end. The companion of this paper uses this weight comprehensively to increase the efficiency of one node fluctuation free integration. There, we give the formulation of one node fluctuation free integration under more than one (many) linear homogeneous conditions.

Practically speaking, the location of the single node seems to be very important due to the results of our various implementations, and, those locations are not universal, depending on the nature of the function to be integrated. From function to function, a

given node may require many conditions to be imposed for weight function generating subspace construction as we present in the companion paper.

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