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FLUCTUATION EXPANSION FOR A UNIVARIATE FUNCTION'S MATRIX REPRESENTATION

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ABSTRACT. The matrix representation of a univariate function operator is considered. A rapidly converging scheme is constructed via a fluctuation operator projecting to the complement of the space spanned by a finite number of bases. We give only first two terms although the construction of whole approximation is possible.

Keywords: Hilbert spaces, matrix representation, fluctuation expansion, approximate quadrature.

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1. Introduction

Matrix representations enable us to use cartesian space tools for computations and convert the operator related problems to matrix algebraic ones. One of the most abundantly matrix representation employing fields is quantum mechanics. Schrödinger operator's matrix representation over an appropriately chosen set of basis set is used in both energy and expected value evaluations and evolution determination of the quantum systems. Since reader can find an enormous number of references on these topics without remarkable efforts we do not intend to refer any resource about them. Quantum mechanics uses linearity in equations by definition. However, recent researches about the optimal control of quantum systems by using an external agent like laser and/or magnetic fields revealed the possibility of dealing with PDEs and functional equations with nonlinearity [8]-[13], [18, 19, 25, 26, 28]. The nonlinearity which is generally cubic comes from the unknown external field components and does not prevent the utilization of the matrix representations of the linear operators existing in the forward and backward evolution equations. In fact all theories using probabilistic notions somehow involve matrix representations.

There are certain preliminary works of the author and his group about the matrix representations of the linear operators whose domains and ranges are same Hilbert spaces [2, 4, 5, 21, 31, 32, 34], [14]-[17]. Amongst these, two fluctuation free matrix representation related ones [16, 17] are quite fundamental reports and can be considered as the basis to this work since we extend the ideas there to the fluctuation contributing terms systematically here.

We consider the algebraic operators which multiply their operands by a function, here, in this work. The operators map from a Hilbert space to (or into) itself. The Hilbert space under consideration ($\mathcal{H}$) is assumed to be composed of functions which are analytic and therefore square integrable over a given interval under a given weight function $w(x)$ assumed to be continuous and to have unit integral over this interval. The interval can be chosen open, half open, or closed

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by keeping in mind the fact that the continuity can imply the square integrability only in the case of closed intervals. Here we prefer to use closed intervals in most general point of view, and, more specifically $[\,0,1\,]$ in implementations, to avoid certain complications which are not in fact important for actual applications.

The inner product of any two functions, $g_1(x)$ and $g_2(x)$, from this space is defined as

$$(g_1, g_2) \equiv \int_a^b dx w(x) g_1(x) g_2(x), \tag{1}$$

where the dependence of g_1 and g_2 on the independent variable is not shown explicitly in the notation of the inner product naturally, since the independent variable is somehow a continuous summation index and therefore an internal agent.

We can consider the algebraic operator $\widehat{x}$ which multiplies its argument by the independent variable x and write the following equality for any function $g(x)$ from $\mathcal{H}$

$$\widehat{x} g(x) \equiv x g(x), \qquad x \in [\,a, b\,]\,. \tag{2}$$

This operator is bounded as long as the integration interval is bounded as can be concluded from (2). Indeed, for finite intervals the norm of the image of $g(x)$ under $\widehat{x}$ is bounded due to Cauchy–Schwartz inequality. The division of this norm by the norm of $g(x)$ gives a finite bound without depending on $g(x)$, and therefore, the norm of the operator $\widehat{x}$ is bounded for finite intervals. If the interval is semi–infinite or infinite then appropriate choices of the weight function enables us to get bounded $\widehat{x}$ operator.

Now we can define the following operator $\widehat{f}$ over $\mathcal{H}$

$$\widehat{f} g(x) \equiv f(x) g(x), \qquad x \in [\,a, b\,], \qquad g(x) \in \mathcal{H}, \tag{3}$$

where the function $f(x)$ is assumed to be in $\mathcal{H}$. If we denote the i–th element of an orthonormal set of basis functions in $\mathcal{H}$ by $u_i(x)$ and write

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

then the matrix representation of $\widehat{f}$, $\mathbf{M}\left(\widehat{f}\right)$ can be explicitly defined as follows

$$\mathbf{M}\left(\widehat{f}\right) = \begin{bmatrix} \left(u_1, \widehat{f} u_1\right) & \cdots & \left(u_1, \widehat{f} u_n\right) & \cdots \\ \vdots & \ddots & \vdots & \cdots \\ \left(u_n, \widehat{f} u_1\right) & \cdots & \left(u_n, \widehat{f} u_n\right) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \tag{5}$$

where u_is satisfy the following equalities because of the orthonormality

$$(u_i, u_j) \equiv \int_a^b dx w(x) u_i(x) u_j(x) = \delta_{ij}, \qquad i, j = 1, 2, ..., \tag{6}$$

where $\delta_{i\,j}$ stands for the Kroenecker's delta symbol which produces 1 when $i = j$ otherwise 0. This representation is an infinite by infinite type matrix, and of course, requires sufficient payment of care to certain convergence issues not to get unexpected results in the practical utilization.

Since infinite dimensionality is not a desired structure unless certain particular cases are under consideration, we intend to truncate this representation to get finite dimensional matrices and then try to find certain rather simple ways dealing with those finite matrices. To this end we consider the subspace of $\mathcal{H}$, which is denoted by $\mathcal{H}_n$ and spanned by the basis functions

$u_1(x)$, ..., $u_n(x)$. We can also consider the matrix representation of $\widehat{f}$'s restriction from this subspace to same subspace. If we denote this representation by $\mathbf{M}^{(n)}\left(\widehat{f}\right)$ then we can write

$$\mathbf{M}^{(n)}\left(\widehat{f}\right) = \left[\begin{array}{ccc} \left(u_1, \widehat{f}u_1\right) & \cdots & \left(u_1, \widehat{f}u_n\right) \\ \cdots & \ddots & \cdots \\ \left(u_n, \widehat{f}u_1\right) & \cdots & \left(u_n, \widehat{f}u_n\right) \end{array} \right]. \tag{7}$$

The most important issue here is, perhaps, to get rid of the integrals in the matrix construction or to approximate them by certain universal (not depending on f) integrals.

The paper is organised as follows. The second section contains the Cauchy contour integral representation of the operator $\widehat{f}$ via resolvent of $\widehat{x}$ and the space folding from whole Hilbert space $\mathcal{H}$ to its subspace $\mathcal{H}_n$ for the resolvent and then the finding of the explicit structure of $\mathbf{M}^{(n)}\left(\widehat{f}\right)$. The third section is about the construction of the fluctuation expansion of $\mathbf{M}^{(n)}\left(\widehat{f}\right)$. The fourth section involves the evaluation of the zeroth and first order components of the expansion. The fifth and sixth sections cover illustrative implementations and concluding remarks respectively.

2. Finite dimensional approximation for the matrix representation

The operator $\widehat{f}$ can be expressed through Cauchy contour integral over the resolvent of the operator $\widehat{x}$ as follows

$$\widehat{f} = -\frac{1}{2\pi i}\oint_C d\zeta f(\zeta)\left[\widehat{x} - \zeta\widehat{I}\right]^{-1}, \tag{8}$$

where C stands for a counterclockwise contour which covers a ζ–complex plane region involving entire interval $[\,a, b\,]$ as a set of interior points .

Let us define

$$\widehat{L} \equiv \widehat{x} - \zeta\widehat{I}, \qquad \widehat{R} \equiv \left[\widehat{x} - \zeta\widehat{I}\right]^{-1}, \tag{9}$$

where ζ is permitted to take the values making $\widehat{L}$ invertable. The domains and the ranges of these operators are same, $\mathcal{H}$. Since $\mathcal{H}$ is direct sum of two orthogonal subspaces, $\mathcal{H}_n$ and its complement, it is quite natural to decompose these operators as follows

$$\begin{aligned} \widehat{L} &\equiv \widehat{L}_{ss} + \widehat{L}_{sc} + \widehat{L}_{cs} + \widehat{L}_{cc}, \\ \widehat{R} &\equiv \widehat{R}_{ss} + \widehat{R}_{sc} + \widehat{R}_{cs} + \widehat{R}_{cc}, \end{aligned} \tag{10}$$

where the subindices of the right hand side components, s and c, recall subspace $\mathcal{H}_n$ and its complement respectively. The explicit expressions of the operator $\widehat{L}$'s components are given below

$$\begin{aligned} \widehat{L}_{ss} &\equiv \widehat{P}^{(n)}\widehat{L}\widehat{P}^{(n)}, & \widehat{L}_{sc} &\equiv \widehat{P}^{(n)}\widehat{L}\left[\widehat{I} - \widehat{P}^{(n)}\right], \\ \widehat{L}_{cs} &\equiv \left[\widehat{I} - \widehat{P}^{(n)}\right]\widehat{L}\widehat{P}^{(n)}, & \widehat{L}_{cc} &\equiv \left[\widehat{I} - \widehat{P}^{(n)}\right]\widehat{L}\left[\widehat{I} - \widehat{P}^{(n)}\right], \end{aligned} \tag{11}$$

where

$$\widehat{P}^{(n)} \equiv \sum_{i=1}^{n}\widehat{P}_i \tag{12}$$

and

$$\widehat{P}_i g(x) \equiv u_i(x)\left(u_i, g\right), \qquad 1 \le i \le n, \qquad g(x) \in \mathcal{H}_n. \tag{13}$$

The components of $\widehat{R}$ can be obtained from (11) just by replacing all appearences of $\widehat{L}$ with $\widehat{R}$.

The operator $\widehat{P}^{(n)}$ projects from $\mathcal{H}$ to $\mathcal{H}_n$ and is the unit operator of $\mathcal{H}_n$. Its additive complement to unit operator $\widehat{I}$, $\left[\widehat{I} - \widehat{P}^{(n)}\right]$, projects from $\mathcal{H}$ to $\mathcal{H} - \mathcal{H}_n$ and it is the unit operator of that subspace. The binary products of these two operators, without regarding the order, vanish because of the projection operators' idempotency.

Our purpose here is to get the explicit expression of $\widehat{R}_{ss}$ since it is somehow corresponding to $\mathbf{M}^{(n)}\left(\widehat{f}\right)$. This can be done by using the fact that $\widehat{R}$, the resolvent of $\widehat{x}$, is the inverse of $\widehat{L}$. Therefore the product of $\widehat{L}$'s right hand side with the right hand side of $\widehat{R}$ in (10) must be equal to $\widehat{I}$ whose decomposition components are $\widehat{P}^{(n)}$ and $\left[\widehat{I}-\widehat{P}^{(n)}\right]$. If this equality is written and the binary products of the operator's components, whose first factor's second subindex does not match the first subindex of the second factor, are eliminated since they vanish due to mismatching projections, then we obtain

$$\begin{aligned}\widehat{L}_{ss}\widehat{R}_{ss} \;&+\; \widehat{L}_{ss}\widehat{R}_{sc}+\widehat{L}_{sc}\widehat{R}_{cs}+\widehat{L}_{sc}\widehat{R}_{cc}+\widehat{L}_{cs}\widehat{R}_{ss}+\widehat{L}_{cs}\widehat{R}_{sc}+\\ &+\; \widehat{L}_{cc}\widehat{R}_{cs}+\widehat{L}_{cc}\widehat{R}_{cc}=\widehat{I}.\end{aligned} \tag{14}$$

The pre and post multiplication of this equality by $\widehat{P}^{(n)}$ results in

$$\widehat{L}_{ss}\widehat{R}_{ss}+\widehat{L}_{sc}\widehat{R}_{cs}=\widehat{P}^{(n)} \tag{15}$$

after using the idempotency and annihilating–each–other's–image property of the projection operators. This contains two unknowns, $\widehat{R}_{ss}$ and $\widehat{R}_{cs}$ and enforces us to get another equation involving only these unknowns. It can be obtained by multiplying both sides of (14) with $\left[\widehat{I}-\widehat{P}^{(n)}\right]$ from left and with $\widehat{P}^{(n)}$ from right.

$$\widehat{L}_{cs}\widehat{R}_{ss}+\widehat{L}_{cc}\widehat{R}_{cs}=\widehat{0}. \tag{16}$$

Now we can write

$$\widehat{L}_{cc}=\widehat{x}_{cc}-\zeta\left[\widehat{I}-\widehat{P}^{(n)}\right]=\left[\widehat{x}_{cc}-\zeta\widehat{I}\right]\left[\widehat{I}-\widehat{P}^{(n)}\right]=\left[\widehat{I}-\widehat{P}^{(n)}\right]\left[\widehat{x}_{cc}-\zeta\widehat{I}\right], \tag{17}$$

where

$$\widehat{x}_{cc}=\left[\widehat{I}-\widehat{P}^{(n)}\right]\widehat{x}\left[\widehat{I}-\widehat{P}^{(n)}\right]. \tag{18}$$

The operator $\widehat{L}_{cc}$ behaves as zero operator on $\mathcal{H}_n$ and maps from $\mathcal{H}-\mathcal{H}_n$ to $\mathcal{H}-\mathcal{H}_n$. Its inverse on $\mathcal{H}-\mathcal{H}_n$ is defined and produces $\left[\widehat{I}-\widehat{P}^{(n)}\right]$ when it multiplies $\widehat{L}_{cc}$ from left or right. If we denote this inverse by using standard notation, that is, $\widehat{L}_{cc}^{-1}$ then we can write its explicit structure as follows

$$\widehat{L}_{cc}^{-1}=\left[\widehat{x}_{cc}-\zeta\widehat{I}\right]^{-1}\left[\widehat{I}-\widehat{P}^{(n)}\right]=\left[\widehat{I}-\widehat{P}^{(n)}\right]\left[\widehat{x}_{cc}-\zeta\widehat{I}\right]^{-1}. \tag{19}$$

This enables us to express $\widehat{R}_{cs}$ as follows in terms of the other entities of (16)

$$\widehat{R}_{cs}=-\left[\widehat{I}-\widehat{P}^{(n)}\right]\left[\widehat{x}_{cc}-\zeta\widehat{I}\right]^{-1}\widehat{L}_{cs}\widehat{R}_{ss}. \tag{20}$$

which puts (15) into the following form

$$\left[\widehat{x}_{ss}-\zeta\widehat{I}-\widehat{x}_{sc}\left(\widehat{x}_{cc}-\zeta\widehat{I}\right)^{-1}\widehat{x}_{cs}\right]\widehat{R}_{ss}=\widehat{P}^{(n)}, \tag{21}$$

where

$$\widehat{x}_{ss}\equiv\widehat{P}^{(n)}\widehat{x}\widehat{P}^{(n)},\qquad \widehat{x}_{sc}\equiv\widehat{P}^{(n)}\widehat{x}\left[\widehat{I}-\widehat{P}^{(n)}\right],\qquad \widehat{x}_{cs}\equiv\left[\widehat{I}-\widehat{P}^{(n)}\right]\widehat{x}\widehat{P}^{(n)}. \tag{22}$$

The coefficient operator at the left hand side of (21) gives zero images for all elements of $\mathcal{H}-\mathcal{H}_n$, that is, it is zero operator on this subspace. On the other hand the image of any function in $\mathcal{H}_n$ under this operator remains in the same subspace and never becomes zero function for appropriate ζ values. Therefore it has a region of ζ–complex plane, on which it is invertable. For such values of ζ we can write

$$\begin{aligned}\widehat{R}_{ss} &= \left[\widehat{x}_{ss} - \zeta\widehat{I} - \widehat{x}_{sc}\left(\widehat{x}_{cc} - \zeta\widehat{I}\right)^{-1}\widehat{x}_{cs}\right]^{-1}\widehat{P}^{(n)} = \\ &= \widehat{P}^{(n)}\left[\widehat{x}_{ss} - \widehat{I} - \widehat{x}_{sc}\left(\widehat{x}_{cc} - \zeta\widehat{I}\right)^{-1}\widehat{x}_{cs}\right]^{-1}\widehat{P}^{(n)}.\end{aligned} \tag{23}$$

Let us go back to $\mathbf{M}^{(n)}\left(\widehat{f}\right)$. We can consider $\mathbf{M}^{(n)}(.)$ as a mapping from the linear operators on $\mathcal{H}$ to the $n\times n$ matrices whose (i,j)–th element is the inner product of the image of $u_j(x)$ under the considered operator with $u_i(x)$. First of all this mapping is linear. It is not so hard to write the following properties for this operator

$$\mathbf{M}^{(n)}\left(\widehat{O}\widehat{P}^{(n)}\right) = \mathbf{M}^{(n)}\left(\widehat{P}^{(n)}\widehat{O}\right) = \mathbf{M}^{(n)}\left(\widehat{P}^{(n)}\widehat{O}\widehat{P}^{(n)}\right) = \mathbf{M}^{(n)}\left(\widehat{O}\right), \tag{24}$$

$$\mathbf{M}^{(n)}\left(\widehat{O}\left[\widehat{I} - \widehat{P}^{(n)}\right]\right) = \mathbf{M}^{(n)}\left(\left[\widehat{I} - \widehat{P}^{(n)}\right]\widehat{O}\right) = \mathbf{0}, \tag{25}$$

$$\mathbf{M}^{(n)}\left(\widehat{O}_1\widehat{P}^{(n)}\widehat{O}_2\right) = \mathbf{M}^{(n)}\left(\widehat{O}_1\right)\mathbf{M}^{(n)}\left(\widehat{O}_2\right), \qquad \mathbf{M}^{(n)}\left(\widehat{P}^{(n)}\right) = \mathbf{I}_n. \tag{26}$$

In these formulae, $\widehat{O}$, $\widehat{O}_1$ and $\widehat{O}_2$ are arbitrary bounded linear operators from $\mathcal{H}$ to $\mathcal{H}$ and $\mathbf{I}_n$ stands for the n–dimensional unit matrix.

Now from (8) and above properties we can write

$$\mathbf{M}^{(n)}\left(\widehat{f}\right) = -\frac{1}{2\pi i}\oint_C d\zeta f(\zeta)\,\mathbf{M}^{(n)}\left(\widehat{R}\right) = -\frac{1}{2\pi i}\oint_C d\zeta f(\zeta)\,\mathbf{M}^{(n)}\left(\widehat{R}_{ss}\right), \tag{27}$$

which urges us to evaluate $\mathbf{M}^{(n)}\left(\widehat{R}_{ss}\right)$. To this end we can rewrite (21) as follows by considering the fact that $\widehat{I}\widehat{R}_{ss} = \widehat{P}^{(n)}\widehat{R}_{ss}$

$$\left[\widehat{x}_{ss} - \zeta\widehat{P}^{(n)} - \widehat{x}_{sc}\left(\widehat{x}_{cc} - \zeta\widehat{I}\right)^{-1}\widehat{x}_{cs}\right]\widehat{R}_{ss} = \widehat{P}^{(n)}. \tag{28}$$

If we take the matrix representation on $\mathcal{H}_n$ of both sides and use the above matrix representation properties we can obtain

$$\left[\mathbf{X}^{(n)} - \zeta\mathbf{I}_n + \mathbf{\Phi}(\zeta)\right]\mathbf{M}^{(n)}\left(\widehat{R}_{ss}\right) = \mathbf{I}_n, \tag{29}$$

where

$$\mathbf{X}^{(n)} \equiv \mathbf{M}^{(n)}\left(\widehat{x}\right), \qquad \mathbf{\Phi}(\zeta) \equiv \mathbf{M}^{(n)}\left(\widehat{x}_{sc}\left[\zeta\widehat{I} - \widehat{x}_{cc}\right]^{-1}\widehat{x}_{cs}\right). \tag{30}$$

These enable us to conclude

$$\mathbf{M}^{(n)}\left(\widehat{f}\right) = \frac{1}{2\pi i}\oint_C d\zeta f(\zeta)\left[\zeta\mathbf{I}_n - \mathbf{X}^{(n)} - \mathbf{\Phi}(\zeta)\right]^{-1}. \tag{31}$$

This is the compact matrix kernel integral representation of the finite space matrix representation for the operator $\widehat{f}$. Its matrix kernel is in a matrix resolvent type structure and the deviation from the pure resolvent structure is characterized by $\mathbf{\Phi}(\zeta)$.

3. Fluctuation expansion

Let us focus on the matrix $\mathbf{\Phi}(\zeta)$ which can be expanded to the following series

$$\mathbf{\Phi}(\zeta) = \mathbf{M}^{(n)}\left(\widehat{x}_{sc}\left[\zeta\widehat{I} - \widehat{x}_{cc}\right]^{-1}\widehat{x}_{cs}\right) = \sum_{i=0}^{\infty}\zeta^{-i-1}\mathbf{\Phi}_{i+1}(\zeta), \tag{32}$$

where

$$\mathbf{\Phi}_{i+1} \equiv \mathbf{M}^{(n)}\left(\widehat{x}_{sc}\widehat{x}_{cc}^{i}\widehat{x}_{cs}\right) = \mathbf{M}^{(n)}\left(\widehat{x}\left\{\left[\widehat{I} - \widehat{P}^{(n)}\right]\widehat{x}\right\}^{i+1}\right), \qquad i = 0, 1, 2, ... \tag{33}$$

The utilization of (32) in the matrix inverse of (31) enables us to write

$$\left[\zeta\mathbf{I}_n - \mathbf{X}^{(n)} - \mathbf{\Phi}(\zeta)\right]^{-1} = \left[\zeta\mathbf{I}_n - \mathbf{X}^{(n)} - \sum_{i=0}^{\infty}\zeta^{-i-1}\mathbf{\Phi}_{i+1}\right]^{-1}. \tag{34}$$

As can be noticed easily $\mathbf{\Phi}_{i+1}$ is i–th degree homogeneous matrix functional of the operator $\left[\widehat{I} - \widehat{P}^{(n)}\right]$. This property can be used as an ordering agent. To be more clear we can define

$$\mathbf{Z}(\zeta, \epsilon) \equiv \left[\zeta\mathbf{I}_n - \mathbf{X}^{(n)} - \sum_{i=0}^{\infty}\frac{\epsilon^{i+1}}{\zeta^{i+1}}\mathbf{\Phi}_{i+1}\right]^{-1}, \tag{35}$$

which implies

$$\mathbf{Z}(\zeta, 1) = \left[\zeta\mathbf{I}_n - \mathbf{X}^{(n)} - \sum_{i=0}^{\infty}\zeta^{-i-1}\mathbf{\Phi}_{i+1}\right]^{-1}. \tag{36}$$

If we expand $\mathbf{Z}(\zeta, \epsilon)$ in ascending natural number powers of ϵ we can write

$$\mathbf{Z}(\zeta, \epsilon) = \sum_{i=0}^{\infty}\epsilon^{i}\mathbf{Z}_i(\zeta), \tag{37}$$

where

$$\mathbf{Z}_i(\zeta) \equiv \frac{1}{i!}\left\{\frac{\partial^i}{\partial\epsilon^i}\left[\zeta\mathbf{I}_n - \mathbf{X}^{(n)} - \sum_{j=0}^{\infty}\frac{\epsilon^{j+1}}{\zeta^{j+1}}\mathbf{\Phi}_{j+1}\right]^{-1}\right\}_{\epsilon=0}, \qquad i = 0, 1, 2, ... \tag{38}$$

By assuming the convergence of the series at the right hand side of (37) at $\epsilon = 1$ we can write

$$\left[\zeta\mathbf{I}_n - \mathbf{X}^{(n)} - \sum_{i=0}^{\infty}\zeta^{-i-1}\mathbf{\Phi}_{i+1}\right]^{-1} = \sum_{i=0}^{\infty}\mathbf{Z}_i(\zeta) \tag{39}$$

which implies

$$\mathbf{M}^{(n)}\left(\widehat{f}\right) = \sum_{i=0}^{\infty}\mathbf{F}_i, \tag{40}$$

where

$$\mathbf{F}_i = \frac{1}{2\pi i}\oint_C d\zeta f(\zeta)\mathbf{Z}_i(\zeta), \qquad i = 0, 1, 2, ... \tag{41}$$

We can define the following approximants

$$\mathbf{F}^{(k)} = \sum_{i=0}^{k}\mathbf{F}_i \tag{42}$$

and write

$$\mathbf{M}^{(n)}\left(\widehat{f}\right) \approx \mathbf{F}^{(k)}, \qquad k = 0, 1, 2, ... \tag{43}$$

A careful look at the definition of $\mathbf{Z}_i(\zeta)$ shows that it contains the matrices $\mathbf{\Phi}_1$, ..., $\mathbf{\Phi}_i$ in finite number of factor containing products in such a way that the operator $\left[\widehat{I}-\widehat{P}^{(n)}\right]$ appears exactly i times in each product. In other words the number of appearence of this operator is equal to i, the index of $\mathbf{Z}_i(\zeta)$. We call this index and therefore the number of the appearence of $\left[\widehat{I}-\widehat{P}^{(n)}\right]$ as the "order" of the relevant matrix. To give a good interpretation to this order we need to investigate the structure of $\mathbf{\Phi}_{i+1}$. We can go back to (33) for this purpose. We see that the most important agent is the operator $\left[\widehat{I}-\widehat{P}^{(n)}\right]\widehat{x}$. The operator $\widehat{x}$ always creates two orthogonal components, one in $\mathcal{H}_n$ and the other in $(\mathcal{H}-\mathcal{H}_n)$ unless its operand has a specific nature. This splitting feature diminishes the norms of the resulting components. The image of $\widehat{x}$ is chopped by the operator $\left[\widehat{I}-\widehat{P}^{(n)}\right]$ to annihilate the component in $\mathcal{H}_n$. Therefore the norm of the operand's image under $\left[\widehat{I}-\widehat{P}^{(n)}\right]\widehat{x}$ becomes smaller. This event, that is, the splitting of the operand and then chopping one component can be called as "Fluctuation" because of the transfers between two orthogonal subspaces. Since this binary product operator appears i times in $\mathbf{\Phi}_{i+1}$ we call $\mathbf{\Phi}_{i+1}$ "i–th Order Fluctuation Matrix". This is reflected to $\mathbf{F}_i$ as "i–th Order Fluctuation Component". Therefore, we call (40) "Fluctuation Expansion". We call the finite sum defined in (42) "k–th Order Fluctuation Approximant".

4. Zeroth and first order terms of fluctuation expansion

We give the explicit expressions of $\mathbf{F}_0$ and $\mathbf{F}_1$ below since we concern with only these terms in this work.

$$\mathbf{F}_0=\frac{1}{2\pi i}\oint_C d\zeta f(\zeta)\,\mathbf{Z}_0(\zeta)=\frac{1}{2\pi i}\oint_C d\zeta f(\zeta)\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}=f\left(\mathbf{X}^{(n)}\right), \tag{44}$$

$$\mathbf{F}_1=\frac{1}{2\pi i}\oint_C d\zeta f(\zeta)\,\frac{1}{\zeta}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{\Phi}_1\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}, \tag{45}$$

where the contour integral of the second formula can not be immediately evaluated as we have done in the formula of $\mathbf{F}_0$. However it has an analytic result which can be obtained after a sufficiently detailed analysis. To this end we need to separate the ζ dependent matrix kernel into simple inverses (just the inverse or inverse power of a first degree matrix polynomial). For this purpose, first, we can write the following identity

$$\frac{1}{\zeta}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}=\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{X}^{(n)^{-1}}-\frac{1}{\zeta}\mathbf{X}^{(n)^{-1}}, \tag{46}$$

which permits us to write

$$\begin{aligned}\frac{1}{\zeta}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{\Phi}_1\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}=\mathbf{X}^{(n)^{-1}}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{\Phi}_1\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}-\\ -\frac{1}{\zeta}\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1},\end{aligned} \tag{47}$$

where we have used commutativity of $\mathbf{X}^{(n)}$ with a matrix function of $\mathbf{X}^{(n)}$. The rightmost term of the last equation can be expressed as follows by using (46)

$$\begin{aligned}\frac{1}{\zeta}\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1} &= \mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{X}^{(n)^{-1}}-\\ &\quad -\frac{1}{\zeta}\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1\mathbf{X}^{(n)^{-1}}\end{aligned} \tag{48}$$

which produces the following result when it is combined with (47)

$$\frac{1}{\zeta}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{\Phi}_1\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}=\mathbf{X}^{(n)^{-1}}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{\Phi}_1\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}-$$

$$-\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1\mathbf{X}^{(n)^{-1}}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}+\frac{1}{\zeta}\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1\mathbf{X}^{(n)^{-1}}, \tag{49}$$

where we have considered the commutativity of $\mathbf{X}^{(n)}$ with a matrix function of $\mathbf{X}^{(n)}$ again. The previously given Cauchy contour integral over each of the right hand side terms except the first one in (49) can be analytically evaluated. This urges us to decompose the first right hand side term of (49) to simple terms each of which permits us to evaluate the Cauchy contour integral analytically. To this end we can define

$$\mathbf{\Phi}_1^{(1)}=\sum_{i=1}^{n}\left(\mathbf{x}_i^T\mathbf{\Phi}_1\mathbf{x}_i\right)\mathbf{x}_i\mathbf{x}_i^T \tag{50}$$

and

$$\mathbf{\Phi}_1^{(2)}=\sum_{\substack{i,j=1\\ i\neq j}}^{n}\frac{\left(\mathbf{x}_i^T\mathbf{\Phi}_1\mathbf{x}_j\right)}{\xi_i-\xi_j}\mathbf{x}_i\mathbf{x}_j^T, \tag{51}$$

where $\mathbf{x}_i$ stands for the i–th eigenvector of $\mathbf{X}^{(n)}$ with unit Frobenius norm (the corresponding eigenvalue is denoted by ξ_i).

A careful investigation shows that $\mathbf{\Phi}_1^{(1)}$ commutes with $\mathbf{X}^{(n)}$. This allows us to write

$$\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{\Phi}_1^{(1)}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}=\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-2}\mathbf{\Phi}_1^{(1)}. \tag{52}$$

On the other hand we can write

$$\mathbf{\Phi}_1-\mathbf{\Phi}_1^{(1)}=\sum_{\substack{i,j=1\\ i\neq j}}^{n}\left(\mathbf{x}_i^T\mathbf{\Phi}_1\mathbf{x}_j\right)\mathbf{x}_i\mathbf{x}_j^T \tag{53}$$

which takes us to the following equality

$$\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\left[\mathbf{\Phi}_1-\mathbf{\Phi}_1^{(1)}\right]\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}=\sum_{\substack{i,j=1\\ i\neq j}}^{n}\frac{\left(\mathbf{x}_i^T\mathbf{\Phi}_1\mathbf{x}_j\right)}{(\zeta-\xi_i)(\zeta-\xi_j)}\mathbf{x}_i\mathbf{x}_j^T=$$

$$=\sum_{\substack{i,j=1\\ i\neq j}}^{n}\frac{\left(\mathbf{x}_i^T\mathbf{\Phi}_1\mathbf{x}_j\right)}{(\zeta-\xi_i)(\xi_i-\xi_j)}\mathbf{x}_i\mathbf{x}_j^T-\sum_{\substack{i,j=1\\ i\neq j}}^{n}\frac{\left(\mathbf{x}_i^T\mathbf{\Phi}_1\mathbf{x}_j\right)}{(\xi_i-\xi_j)(\zeta-\xi_j)}\mathbf{x}_i\mathbf{x}_j^T=$$

$$=\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{\Phi}_1^{(2)}-\mathbf{\Phi}_1^{(2)}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1} \tag{54}$$

(52) and (54) enables us to write the following identity

$$\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{\Phi}_1\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}=$$

$$=\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-2}\mathbf{\Phi}_1^{(1)}+\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{\Phi}_1^{(2)}-\mathbf{\Phi}_1^{(2)}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}. \tag{55}$$

This takes us to the ultimate expression of the ζ–dependent matrix part of the matrix representation for $\widehat{f}$.

$$\frac{1}{\zeta}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{\Phi}_1\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}=\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-2}\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1^{(1)}+$$

$$+\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1^{(2)}-\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1^{(2)}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}-$$
$$-\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1\mathbf{X}^{(n)^{-1}}\left[\zeta\mathbf{I}_n-\mathbf{X}^{(n)}\right]^{-1}+\frac{1}{\zeta}\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1\mathbf{X}^{(n)^{-1}}. \tag{56}$$

The employment of this result in (45) gives the following expression after performing the Cauchy contour integrations

$$\mathbf{F}_1=f'\left(\mathbf{X}^{(n)}\right)\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1^{(1)}+f\left(\mathbf{X}^{(n)}\right)\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1^{(2)}-\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1^{(2)}f\left(\mathbf{X}^{(n)}\right)-$$
$$-\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1\mathbf{X}^{(n)^{-1}}f\left(\mathbf{X}^{(n)}\right)+f(0)\mathbf{X}^{(n)^{-1}}\mathbf{\Phi}_1\mathbf{X}^{(n)^{-1}}. \tag{57}$$

(44) states a very important fact: if all fluctuations are omitted then the matrix representation of $\widehat{f}$ on $\mathcal{H}_n$ is equal to the image of the matrix representation of $\widehat{x}$ on $\mathcal{H}_n$ under the function f. This was given as a theorem and proved quite recently [16]. We call that theorem "Fluctuationlessness Theorem". Its first comprehensive utilization to get matrix representations in any desired precision for various functions in practice has also been reported [17]. There had been certain efforts from author's group to use fluctuation expansion in its preliminary form for expected value evaluation in quantum mechanics and quantum optimal control [5, 14, 15]. However, in those works, the fluctuationlessness theorem was not proved and the fluctuation expansion was not systematically constructed yet although there were many signals about the existence of them. The five successful works which were reported as conference proceedings [2, 4, 21, 31, 32, 34] were based on the fluctuationlessness theorem which was proven but not published yet at those days.

Fluctuationlessness theorem defines a very good approximation for $\mathbf{M}^{(n)}\left(\widehat{f}\right)$. The quality of the approximation decreases if the curvature of $f(x)$ increases. However this decrease can always be compensated by increasing the dimension of $\mathcal{H}_n$. The analyticity of $f(x)$ on the interval is an essential requirement. As long as it is fulfilled, the quality of the fluctuationlessness approximation (approximation by retaining only $\mathbf{F}_0$) is controllable via n. This approximation requires the evaluation of $\mathbf{X}^{(n)}$ which is in fact a universal entity (does not depend on $f(x)$). It is done just once and then can be used indefinitely many times for the matrix representation calculation of any given function. To this end certain libraries or data files including the eigenpairs of $\mathbf{X}^{(n)}$ for various n values can be constructed to be used by certain programming or scripting languages in computer applications.

Fluctuation free matrix representation stated by the fluctuationlessness theorem expresses the matrix representation of a function as a finite linear combination of the function values evaluated at the eigenvalues of the independent variable matrix representation with the matrix coefficients such that the matrix coefficient of the function value at a specific eigenvalue projects to the eigenspace corresponding that eigenvalue. In this sense, the expression is a quadrature like formula. This urges us to seek similarities to the numerical quadratures which are generally based on interpolation [24, 29]. Trapezoidal [6], Newton-Cotes [1, 20, 27, 30], Simpson [3] rules are all based on interpolations. However, most important quadrature which has a strong analogy to fluctuation free matrix representation is the Gauss quadrature [23]. Its extended version[7, 22, 33] increased the power of the quadrature. As quite recently proven the Jacobi matrix of Gauss quadrature is the matrix representation of the independent variable over the quadrature's intervals and under its weight. However, Gauss quadrature is based on Lagrange interpolation and therefore uses polynomials as basis functions. In this perspective, the fluctuation free matrix representation and integration are based on any type of basis function set. That is, it takes the

Gauss quadrature as a subclass for numerical integration. This makes it somehow a very powerful and flexible extension to Gauss quadrature for integration.

Similar things can also be said for $\mathbf{F}_1$. However its structure is a little bit complicated than the one for $\mathbf{F}_0$ since it requires derivative values of the function beside its value at zero. This complication increasingly continues as we consider higher and higher fluctuation components although we do not deal with them explicitly here. $\mathbf{F}_1$ is an alternative to increasing n in fluctuationlessness approximation (the use of $\mathbf{F}_0$ only) to get higher quality. One may anticipate to get better results even for $n = 1$ at the expense of using more information about the function under consideration. In other words, the use of $\mathbf{F}_1$ can be considered as an indirect way of increasing n with different function informations.

5. Illustrative implementations

We consider the case where the interval and the weight function are $[\,0, 1\,]$ and 1 respectively. We concern with the worst quality case, that is, we take $n = 1$. Then we can write the following equalities for various entities

$$u_1(x) \equiv 1, \qquad \mathbf{M}^{(1)}\left(\widehat{f}\right) = \left(u_1, f\left(\widehat{x}\right) u_1\right) = \int_0^1 dx f(x), \tag{58}$$

$$\mathbf{X}^{(1)} \equiv (u_1, xu_1) = \int_0^1 dx x = \frac{1}{2}, \qquad \mathbf{F}_0 = f\left(\frac{1}{2}\right), \tag{59}$$

$$\mathbf{\Phi}_1 \equiv \left(u_1, \widehat{x}\left[\widehat{I} - \widehat{P}^{(n)}\right]\widehat{x}u_1\right) = \left(u_1, x^2 u_1\right) - \left(u_1, xu_1\right)^2 = \frac{1}{12}, \tag{60}$$

$$\mathbf{\Phi}_1^{(1)} = \mathbf{\Phi}_1, \qquad \mathbf{\Phi}_1^{(2)} = 0, \tag{61}$$

$$\mathbf{F}_1 = \frac{1}{6}\left(\frac{\mathrm{d}f}{\mathrm{dx}}\right)_{x=\frac{1}{2}} - \frac{1}{3} f\left(\frac{1}{2}\right) + \frac{1}{3} f(0). \tag{62}$$

We have chosen first $f(x) = \mathrm{e}^{\alpha x}$ where α can be considered as the curvature parameter because its higher values correspond to higher derivative values and therefore higher curvatures. Figure 1 contains three curves each of which takes α as independent variable: (1) the exact analytical result of the integral of the function, (2) the fluctuationlessness aproximant, (3) The first order fluctuation approximant.

Figure 1 takes the domain of α as $[\,0, 7\,]$. The results in Figure 1 show that the exact integral, zeroth and first order fluctuation approximants are indistinguishable unless the numerical results are compared (even there the discrepancy is at quite high decimal digits) in $[\,0, 3\,]$. Starting from $\alpha = 3$ the curves become distinguishable and the differences amongst them increases. This implies that the increasing α values cause decreasing approximation quality in fluctuationlessness approximation and first order fluctuation approximation. However, first order fluctation approximant is better than the fluctuationlessness approximation (zeroth order fluctuation approximant). The function $\mathrm{e}^{\alpha x}$ is analytic everywhere except infinity. Its analyticity domain in x complex plane contains the interval $[\,0, 1\,]$ as an interior region. There is no singularity of the function in the close vicinity of the interval $[\,0, 1\,]$. This causes high approximation quality in fluctuation approximant as we observe from the results in Figure 1. However, the approximation is better for low curvatures. This is not only peculiar to this function. It is general because the high curvature means low convergence rate in power series and therefore lower quality in analyticity.

Our next example focuses on $f(x) \equiv \sin\left(\alpha x\right)$. The results are depicted in Figure 2 in exactly same way as the previous one.

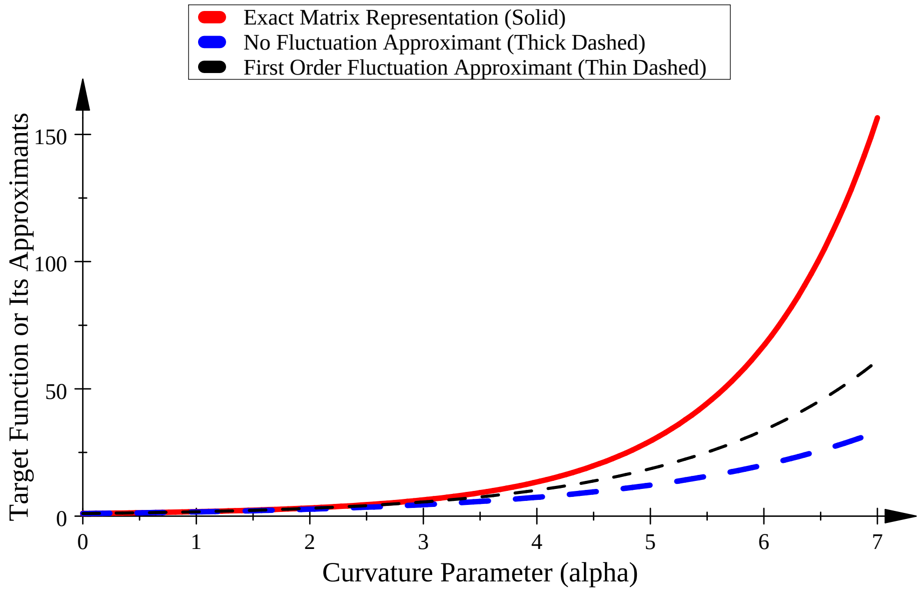

Figure 1. Results for $e^{\alpha x}$

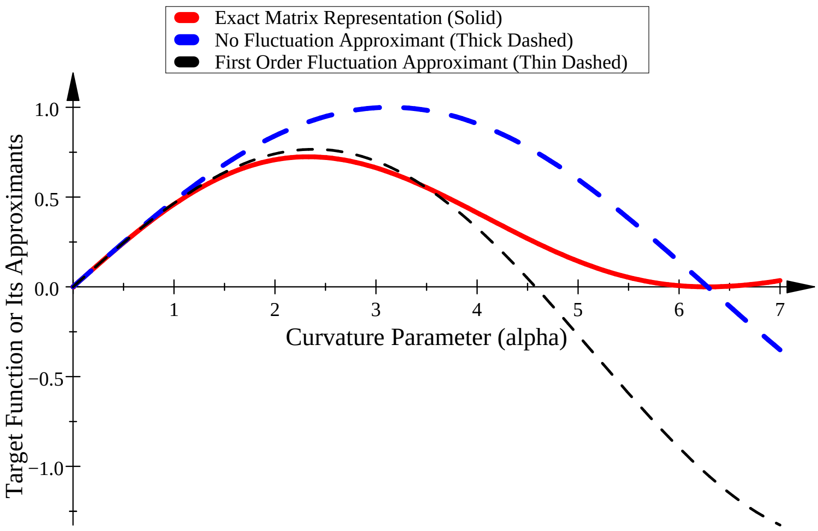

Figure 2. Results for $\sin(\alpha x)$

Similar behavior of the previous case is observed here. The approximating power of the first order fluctuation approximant is apparent. However, again, the quality decreases as the curvature parameter α increases. The function of this case has no singularity in any finite region of x complex plane. Its all singular nature is at infinity. In other words this function is analytic everywhere in finite regions. Hence this is reflected to the quality positively.

Our third example deals with a polar singularity. The function is explicitly given below.

$$f(x) \equiv \frac{1}{1+\frac{\alpha}{\beta}x}, \tag{63}$$

where the parameters α and β are given positive values (We use two parameters, although a single parameter seems to be sufficient, to distinguish the effects of curvature and singularity location). This function has a simple pole located at $x = -\beta/\alpha$. The greater β value the greater approximation quality in this structure since the location of the pole moves in the direction to minus infinity as β increases and therefore weaken the effect of the singularity to the analiticity domain and hence convergence domain of powers series of the function.

The results for this function when $\beta = 1$ are depicted in Figure 3. A careful investigation on

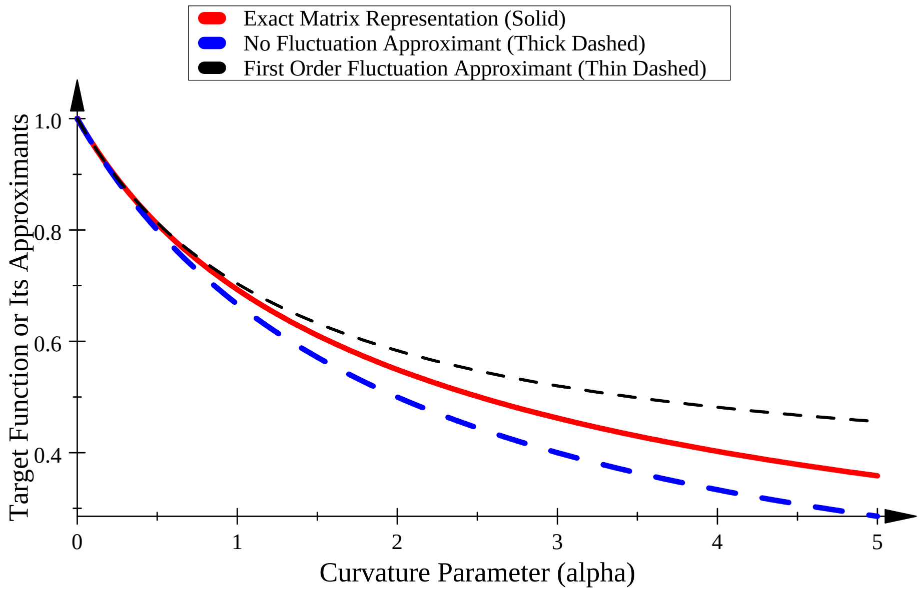

Figure 3. Results for $\frac{1}{1+\frac{\alpha}{\beta}x}$

the zeroth and first order fluctuation approximants shows that curves match in a small domain of α as we move from left to right . Then they become apart. However, in a domain bounded from right by a critical value (can be considered turning point), the deviation of the first order approximant is less than the one of the fluctuationlessness aproximation in absolute value. At the critical point these deviations become identical in absolute value. From this point to right the deviation of the first order fluctuation approximant grows more rapidly than the one for fluctuationless approximation. Our more detailed experimentations verify this observation. The theoretical explanation of this observation is the asymptotic behaviors of the approximants under consideration as α increases towards infinity. What we can extract from this case is that the negative effect of the polar singularity on the quality of the approximation is obvious, and, the negativity increases as the pole gets closer to the concerned interval of the approximation. Many different investigations on the cases with polar singularities having single or multiple poles can be made. We made such investigations, all of which confirm what we conclude in this example.

Our fourth example considers the following function

$$f(x) \equiv \sqrt{1 + \frac{\alpha}{\beta}x}, \tag{64}$$

where α and β scalars taking positive real number values. The plots for this case are given in Figure 4 for $\beta = 1$. This case can be discussed exactly in the same lines of explanations as the third example case. However, here the singularity is branch point type. Indeed, the function under consideration has two branch points: one at infinity, one at $x = -\beta/\alpha$. The square root structure of the function causes the existence of two Riemann sheets. This is one of the simplest branch cut cases and we can ask about the role of the number of Riemann sheets. The location

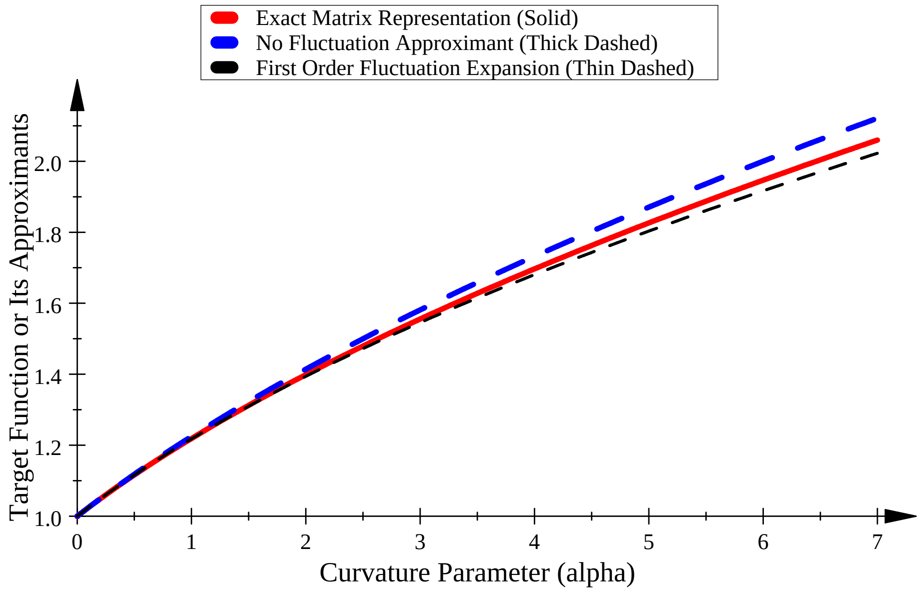

Figure 4. Results for $\sqrt{1+\frac{\alpha}{\beta}x}$

of the finite point branch point affects the quality as our observations say. This is quite expected because the branch point closer to the concerned interval affects the convergence properties and therefore matrix representations. However, this example alone, can not reveal the role of the number of the Riemann sheets. To understand this we need another example. Although there are a lot of function structures which have more than two Riemann sheets in finite numbers, we just jump to the case of simplest infinite Riemann sheets.

Therefore, we consider the following function

$$f(x) \equiv \ln\left(1+\frac{\alpha}{\beta}x\right), \tag{65}$$

where, as before, the parameters α and β are considered as positive real values.

The results for this case are shown in Figure 5. As can be seen from this figure, the increasing number of Riemann sheets has a negative effect on the quality of the first order fluctuation expansion. However, this is not so dramatic although some other functions may give higher deviations.

Until now we have dealt with the one dimensional subspace of the Hilbert space $\mathcal{H}$. This assumption has discarded the off–diagonal terms of the first order fluctuation matrix since they are nonexistent in fact. Now, to take those terms into consideration we increase the dimension to 2 which is the next simplest case. The basis functions we need for this case are as follows

$$u_1(x) \equiv 1, \qquad u_2(x) \equiv \sqrt{3}\,(2x-1)\,. \tag{66}$$

We will concern with the case where

$$f(x) \equiv e^{\alpha x} \tag{67}$$

as the only example since just one single example will be good enough to see the contribution of the first order fluctuation approximant. All we have stated before can be exactly applied to this case by the interested reader.

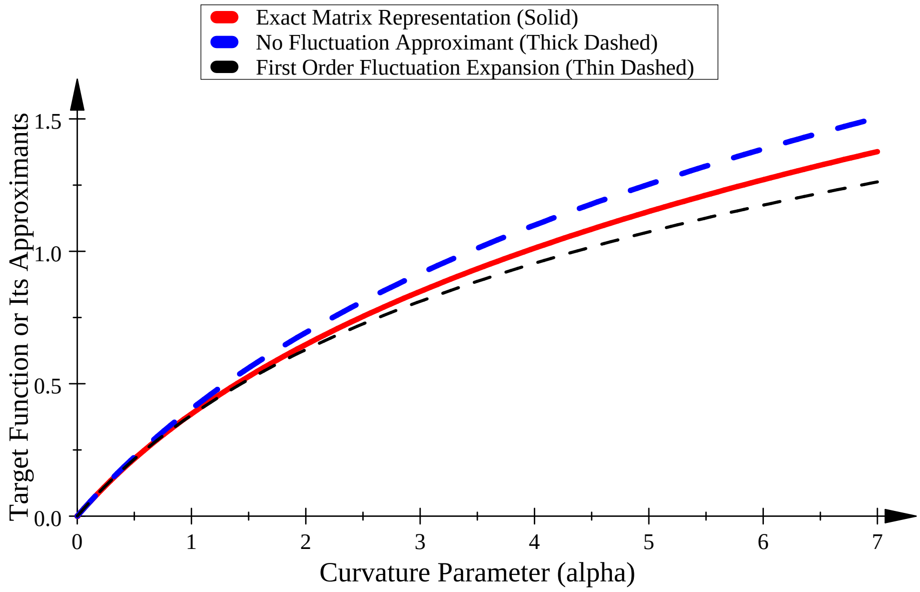

Figure 5. Results for $\ln 1 + \frac{\alpha}{\beta} x$

The (2×2) matrix representation of this function is given below

$$\left[\mathbf{M}^{(2)}\left(f\right)\right]_{1,1} \equiv \frac{e^{\alpha}-1}{\alpha}, \tag{68}$$

$$\left[\mathbf{M}^{(2)}\left(f\right)\right]_{1,2} \equiv \left[\mathbf{M}^{(2)}\left(f\right)\right]_{2,1} \equiv 2\sqrt{3}\,\frac{e^{\alpha}(\alpha-1)+1}{\alpha^2} - \sqrt{3}\,\frac{e^{\alpha}-1}{\alpha}, \tag{69}$$

$$\left[\mathbf{M}^{(2)}\left(f\right)\right]_{2,2} \equiv \frac{e^{\alpha}\left(3\alpha^2-12\alpha+24\right)-\left(3\alpha^2+12\alpha+24\right)}{\alpha^3}. \tag{70}$$

(2×2) matrix representation of the operator $\widehat{x}$ and its eigenpairs are given below

$$\mathbf{X}^{(2)} \equiv \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{6} \\ \frac{\sqrt{3}}{6} & \frac{1}{2} \end{bmatrix}, \tag{71}$$

$$\xi_1 \equiv \frac{1}{2} + \frac{\sqrt{3}}{6}, \qquad \xi_2 \equiv \frac{1}{2} - \frac{\sqrt{3}}{6}, \tag{72}$$

$$\mathbf{x}_1 \equiv \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}, \qquad \mathbf{x}_2 \equiv \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}. \tag{73}$$

The fluctuationlessness approximation is given below

$$\mathbf{F}_0 = e^{\frac{\alpha}{2}} \begin{bmatrix} \cosh\frac{\sqrt{3}}{6} & \sinh\frac{\sqrt{3}}{6} \\ \sinh\frac{\sqrt{3}}{6} & \cosh\frac{\sqrt{3}}{6} \end{bmatrix}. \tag{74}$$

The first order fluctuation matrix and related terms are given below

$$\mathbf{\Phi} = \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{15} \end{bmatrix}, \qquad \mathbf{\Phi}^{(1)} = \begin{bmatrix} \frac{1}{30} & 0 \\ 0 & \frac{1}{30} \end{bmatrix}, \qquad \mathbf{\Phi}^{(2)} = \begin{bmatrix} 0 & \frac{\sqrt{3}}{30} \\ -\frac{\sqrt{3}}{30} & 0 \end{bmatrix}. \tag{75}$$

We are not going to give the explicit structure of the first order fluctuation approximant because it is quite complicated in typographical point of view.

The results for this case are depicted in Figure 6. They are quite similar to the case of $n = 1$. The effect of n on the modification coming from the first order fluctuation term is not so clear although one can expect that the increasing n values may increase the contribution of first order fluctuation term. This investigation should be done not on the graphics but on the analytical structure. This dependence may be affected by the function under consideration. We do not intend to realize any such kind of investigation here since our purpose is to show how first order fluctuation approximants strengthen the fluctuationlessness approximant.

At this point we need to ask one important question. "Which is better, to increase n in fluctuationlessness approximant or without changing n to use the first order fluctuation approximant?". In fact, the increasing n value does not change the matrix structure of the fluctuationlessness approximation very much except the need to evaluate more eigenpairs due to dimension increase. So this may seem to be more attractive. On the other hand, when we need to find the matrix representation of some other type operators especially in the case of the operators as products of certain number of operators, at least one interior factor of which is the operator $\left[\widehat{I}-\widehat{P}^{(n)}\right]$, the fluctuationlessness term (in other words, zeroth order fluctuation term) vanishes. If the number of the interior factors equal to $\left[\widehat{I}-\widehat{P}^{(n)}\right]$ is more than 1 then the number of the vanishing leading fluctuation terms increases. This situation enforces us to evaluate not just the first order but some number of higher order terms.

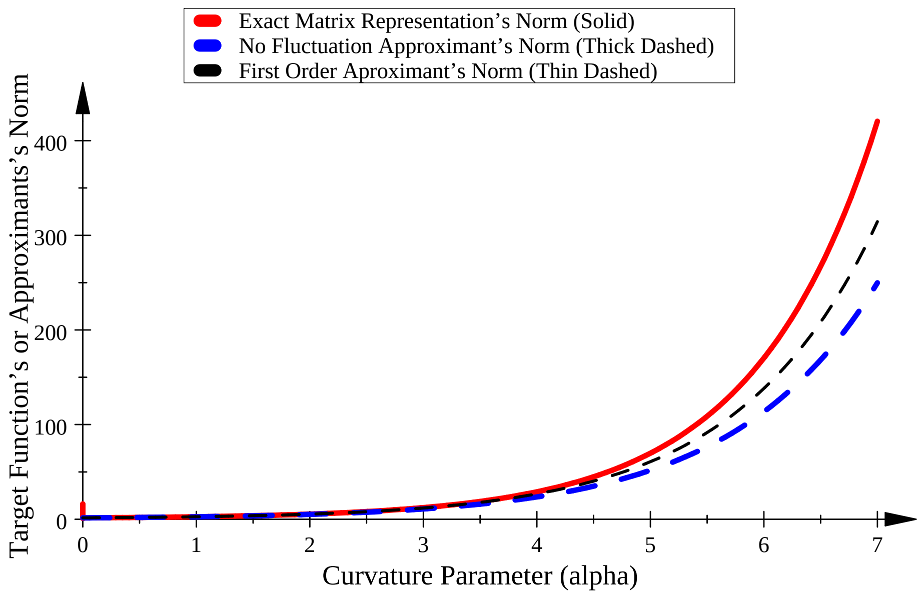

Figure 6. Results for $e^{\alpha x}$ and $n = 2$

6. Concluding remarks

In this work we have developed an expansion for a function's matrix representation on the considered Hilbert space's ($\mathcal{H}$) subspace ($\mathcal{H}_n$) spanned by a finite number of functions from the basis set of $\mathcal{H}$, in ascending number of appearences of the operator projecting from the Hilbert space to its considered subspace's complement. The first term of this expansion can also be called zeroth order term and has a very specific but easy–to–use structure. It is the image of the matrix representation of the independent variable on $\mathcal{H}_n$ under f, the function whose matrix representation is concerned. Hence, once the matrix representation of the independent variable is evaluated for a given dimension of the subspace then it can be used arbitrarily many times in applications for different functions but same dimensionality. That is, the evaluation is based on highly universal structure. This was investigated in previous works of the author. The expansion here is based on the resolvent operator's matrix representation on the finite subspace and Cauchy contour integration. The infinite dimensional resolvent is somehow folded to a finite dimensional matrix resolvent structure with certain perturbation terms coming from the fluctuations which are created by the powers of the operator $\left[\widehat{I}-\widehat{P}^{(n)}\right]\widehat{x}$. These terms are disintegrated to individual terms which are ordered in ascending number of appearence of the operator $\left[\widehat{I}-\widehat{P}^{(n)}\right]$. The analytical structures of these terms seem to be becoming complicated as the number of the appearence increases. Hence we confined ourselves on the cases of zeroth and first order terms only since our main purpose is to show that a fluctuation expansion construction is possible and even the first order contribution affects the approximation quality positively.

There seem to be existing two alternatives to increase the quality of the approximation although some other ways may be found in future: (1) increasing the dimension of the subspace $\mathcal{H}_n$; (2) considering the contribution of the fluctuation expansion terms. The former one seems to be more practical because of the simplicity of the formula to be used and the high level universality in the evaluation. However, we need to emphasize on the fact that the independent variable matrix representation's use in the evaluation is generally based on its eigenpairs and its eigenvalues tend to spread over the interval $[\,0,1\,]$ as the dimension grows. In other words, the number of the eigenvalues close to zero increases by making the spectral determination process ill–posed. That is, ill–posedness increases as n grows. This may require high precision calculations. Hence it is better to use scripting languages or libraries permitting to use arbitrary precision in computer applications. On the other hand this determination is needed just once for each n and its results can be stored for future uses repeatedly.

The other alternative focuses on the first order fluctuation expansion truncation first. The formula is a little bit more complicated than the no–fluctuation case. It contains more individual terms including the first derivative or itself of the function with the argument $\mathbf{X}^{(n)}$, the matrix representation of the independent variable on $\mathcal{H}_n$. The number of the terms and the derivatives of the function increases as the order of the fluctuation expansion grows. This may make the evaluations more ill–posed because of the possible differences of the almost equal entities. Hence, this enforces to use higher and higher precisions as the order of the fluctuation expansion goes up to infinity. The universality is also existing in this case and same considerations are valid as before. Therefore, one prefers the former case, that is, the increasing the dimensions of the subspace in the zeroth order term as long as the zeroth order term does not vanish. Otherwise first or higher order of fluctuation term evaluation becomes the only alternative to approximate the matrix representation of f on $\mathcal{H}_n$. These cases which require the employment of the first or higher order of fluctuation terms is another interesting issue. However, we have not intended to focus on them here.

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References

[1] Abramowitz, M., Stegun, I.A., eds, (1972), Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, Dover, New York.

[2] Altay, N., Demiralp, M., (2008), Numerical Solution of Ordinary Differential Equations in Fluctuationlessness Theorem Perspective, Proceedings of the 1st WSEAS International Conference on Multivariate Analysis and its Application in Science and Engineering (MAASE'08), May 27-30, Istanbul, Turkey, pp.162–167.

[3] Atkinson, K.A., (1989), An Introduction to Numerical Analysis (2nd edition), John Wiley and Sons, ISBN 0-471-50023-2.

[4] Baykara, N.A., Gürvit, E., Demiralp, M., (2008), A Hybridized Finite Taylor Formula by Fluctuation Free Remainder Term for Univariate Function Approximation, Proceedings of the International Conference on Numerical Analysis and Applied Mathematics (ICNAAM 2008), September 15-19, Kos, Greece, pp.87-91.

[5] Baykara, N.A., 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 Comput. Methods in Sci. and Eng. (ICCMSE 2005), Redderbrick BV, Loutraki, Greece, Sept. 16–20, pp.4A:56-59.

[6] Burden, R.L., Faires, J.D., (2000), Numerical Analysis (7th edition), Brooks/Cole, ISBN 0-534-38216-9.

[7] Clenshaw C.W., Curtis, A.R., (1960), A method for numerical integration on an automatic computer, Numerische Mathematik, 2, 197p.

[8] Demiralp M., Tunga, B., (2005), Instantaneous Stability and Robustness Investigations in Quantum Optimal Control: Harmonic Oscillator Under Linear Dipole and Quadratic Control Agents, ANACM, 2, pp.60–69.

[9] Demiralp, M., Rabitz, H., (1998), Assessing Optimality and Robustness of Control Over Quantum Dynamics, Phys. Rev. A, 57, pp.2420-2425.

[10] Demiralp, M., Rabitz, H., (2000), Assessing Optimality and Robustness for the Control of Dynamical Systems, Phys. Rev. A, 61, pp.2569-2578.

[11] Demiralp, M., Rabitz H., (1994), Optimal Control in Classical Molecular Dynamics: A Perturbation Formulation and the Existence of Multiple Solutions, J. Math. Chem., 16, pp.185-209.

[12] Demiralp, M., Rabitz, H., (1995), Upper and Lower Bounds on the Control Field and the Quality of Achieved Optimally Controlled Quantum Molecular Motion, J. Math. Chem., 19, pp.337-357.

[13] Demiralp, M., Rabitz H., (1993), Optimally Controlled Quantum Molecular Dynamics: A Perturbation Formulation and the Existence of Multiple Solutions, Phys. Rev. A, 47, pp.809-816.

[14] Demiralp, M., (2005), A Fluctuation Expansion Method for the Evaluation of a Function's Expectation Value, Proceddings of the Int. Conf. on Numer. Anal. and Appl. Math., (ICNAAM2005), Wiley, Rhodes, Greece, Sept. 16–20, pp.711-714.

[15] Demiralp, M., (2005), Determination of Quantum Expectation Values Via Fluctuation Expansion, Lecture Series on Computer and Computational Sciences, Selected Papers from Int. Conf. of Comput. Methods in Sci. and Eng. (ICCMSE 2005), Redderbrick BV, Loutraki, Greece, Sept. 16–20, pp.4A:146-149.

[16] Demiralp, M., (2009), Fluctuationlessness Theorem to Approximate Univariate Functions's Matrix Representations, WSEAS Transac. on Math., 8(6), pp.258-267.

[17] Demiralp, M., (2009), No fluctuation approximation in any desired precision for univariate function matrix representations, J. Math. Chem., 47(4), pp.99-110.

[18] Demiralp, M., Rabitz, H., (1997), Dispersion-free Wave Packets and Feedback Solitonic Motion in Controlled Quantum Dynamics, Phys. Rev. A, 55, pp.673-677.

[19] Demiralp, M., Rabitz, H., (1993), Optimally Controlled Quantum Molecular Dynamics: The Effect of Nonlinearities on the Magnitude and Multiplicity of Control–Field Solutions, Phys. Rev. A, 47, pp.831-837.

[20] Forsythe, G.E., Malcolm, M.A., Moler, C.B., (1977), Computer Methods for Mathematical Computations, Prentice–Hall, Englewood Cliffs, NJ.

[21] Gürvit, E., Baykara, N.A., Demiralp, M., (2008), Evaluation of Univariate Integrals via Fluctuationlessness Theorem, Proceedings of the International Conference on Numerical Analysis and Applied Mathematics (ICNAAM 2008), September 15-19, Kos, Greeece, AIP 1048, pp.231-234.

[22] Gentleman, W.M., (1972), Implementing Clenshaw–Curtis quadrature I: Methodology and experience, Comm. of the ACM, 15(5), pp. 337-342.

[23] Gil, A., Segura, J., Temme, N.M., (2007), Numerical Methods for Special Functions, SIAM, ISBN 978-0-898716-34-4.

[24] Kincald, D., Cheney, W., (2002), Numerical Analysis (3rd edition) Brooks/Cole, ISBN 0-534-38905-8, Chapter 6.

[25] Kurşunlu, A., İYaman, I., Demiralp, M., (2003), Optimal Control of One Dimensional Quantum Harmonic Oscillator Under an External Field With Quadratic Dipole Function and Penalty on Momentum: Construction of the Linearised Field Amplitude Integral Equation, ANACM, WILEY-VCH, 1, pp.270-279.

[26] Li, G., Artamonov, M., Rabitz, H., Wang, S.-W., Georgopoulos, P.G., Demiralp, M., (2003), High Dimensional Model Representations Generated from Low Order Terms, –lp–RS–HDMR, J. Comput. Chem., 24, pp.647-656.

[27] Press, W.H., Flannery, B.P., Teukolsky, S.A., Vetterling, W.T., (1988), Numerical Recipes in C, Cambridge University Press, Cambridge, UK.

[28] Rabitz, H., Ho, T.-S., Hsieh, M., Kosut, R., Demiralp, M., (2006), Topology of optimally controlled quantum mechanical transition probability landscapes, Phys. Rev. A, 74, pp.012721-(1-9).

[29] Schatzman, M., (2002), Numerical Analysis: A Mathematical Introduction, Clarendon Press, Oxford, ISBN 0-19-850279-6, Chapter 4 and 6.

[30] Stoer, J., Bulirsch, R., (1980), Introduction to Numerical Analysis, Springer–Verlag, New York.

[31] Tunga, B., Demiralp, M., (2008), Fluctuationlessness Approximation Towards Orthogonal Hyperprismatic Grid Construction, Proceedings of 1st WSEAS International Conference on Multivariate Analysis and its Application in Science and Engineering (MAASE'08), May 27-30, Istanbul, Turkey, pp.193–197.

[32] Üsküplü, S., Demiralp, M., (2008), Univariate Integration via Space Extension Based No Fluctuation Approximation, Proceedings of the International Conference on Numerical Analysis and Applied Mathematics, ICNAAM, September 15–19, Kos, Greece, AIP 1048, pp.566-569.

[33] Waldvogel, J., (2004), Fast construction of the Fejér and Clenshaw–Curtis quadrature rules, BIT Numerical Mathematics, 43(1), pp.001-018.

[34] Yaman, I., Demiralp, M., (2008), An Integration Free Universal Approximation Method Based on Orthogonal Polynomials, Proceedings of the International Conference on Numerical Analysis and Applied Mathematics, ICNAAM, September 15–19, Kos, Greece, AIP 1048, pp.601-604.

Metin Demiralp, for a photograph and biography, see TWMS J. Pure Appl. Math., V.1, N.1, 2010, p.53