Matrix Weighted Multivariate Hausdorff Moment Problem
Arising From Quantum Mechanical Applications of
Probabilistic Evolution Approach

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Abstract: This study is the extension of accompanying work entitled "Multivariate Hausdorff Moment Problem Arising From Quantum Mechanical Applications of Probabilistic Evolution Approach." In this study, multivariate finite interval Hausdorff moment problem under matrix weight arising from quantum mechanical applications of Probabilistic Evolution Approach is defined. Existence of the solution of this problem is proved. It also has been proven that the problem may have infinitely many solution. Moreover, solution procedure is presented in huge detail.

Key–Words: Hausdorff Moment Problem, Quantum Mechanics, Probabilistic Evolution Approach, Kronecker Product, Kronecker Power Series

1 Introduction

Doing quantum mechanics without explicitly solving Schrödinger wave equation is a dream or not? That is the question which scientists try to answer in last decades. Considering quantum many body system the number of the freedom of the system under consideration growth exponentially in the coordinates and this situation makes it impossible to solve Schrödinger equation even in the modern computer architectures. Density Functional Theory one of the seminal work related to answer that question and answering partly yes lead to the Nobel Prize. In last years, some variants of that theory such as Orbital Free Density Functional theory developed. All these approaches requires solution of not the Schrödinger but the reduced number of other partial differential equations. Beside these leading research, Quantum Monte Carlo methods search for the answer and they all have the ability of calculation of ground state of the system under consideration.

In addition to the quantum many body systems, optimal control of the quantum phenomena requires computationally sophisticated algorithms due to the huge number of iterations and the necessity of the solving Schrödinger equation up to a high degree of numerical accuracy. Since most of the numerical algorithms require discretization, the solution may fail to converge due to the errors arising out of discretization.

Our research focuses on the same topic yet by following different path. In most of the cases, expectation values of the certain entities such as position and momentum operators contains all the information about the system under consideration. The time evolution of the expectation value dynamics can be determined not by partial differential equations but by ordinary differential equations which we know about more then partial differential equations. The main difficulty arise here is closeness of the commutator algebra group can be satisfied in infinite dimension for most of the quantum mechanical systems. That means countably may set of nonlinear ODEs.

Our recently proposed method Probabilistic Evolution Approach can deal with the above mentioned difficulties to some extend. [3,4,9–16]This is achieved by the linearization of the given nonlinear set of ODEs in terms of the unknown system entities such as expectation values of position and momentum operators in quantum mechanical case. The linearization procedure produces linear set of ODEs in infinite dimension. This restriction is transcended by space extension methodologies and the solution of the recurrence relations as a finite sum. To make the description more concrete, lets consider the following Heisenberg equation of motion.

\[
\frac{d\langle s \rangle(t)}{dt} = \left\langle \frac{i}{\hbar} \left[\hat{H} - s \hat{H} \right] \right\rangle
\]

(1)

Where \( \hat{H} \) denotes the Hamiltonian of the quantum mechanical system under consideration and \( s \) denotes so called system vector whose explicit structure is given as follows.
After all these steps, countably many sets of linear ODEs can be obtained in the following form.

$$\frac{d\mathbf{s}}{dt} = \mathbf{E}\xi(t)$$  \hspace{1cm} (7)

where:

$$\xi(t) = \begin{bmatrix} \langle \mathbf{s}^{(0)} \rangle (t) \\ \langle \mathbf{s}^{(1)} \rangle (t) \\ \vdots \\ \langle \mathbf{s}^{(n)} \rangle (t) \end{bmatrix}^T$$  \hspace{1cm} (8)

and the formal solution is as follows.

$$\xi(t) = e^{t\mathbf{E}}\xi(0)$$  \hspace{1cm} (9)

The equation (7) are the Probabilistic Evolution Approach equations and the equation (9) is its formal solution. But due to the infinite dimensional structure of the evolution matrix, equation (9) is impractical. To overcome this issue we will generate recurrence relations. These recurrent relations may be cumbersome, if evolution matrix has many number of blocks in diagonals. Some space extension possibilities such as nonlinear space extension and the constancy added space extension are proposed both to reduce the number of diagonals and to change their structure [4–6, 17–20]. For the two banded structure in evolution matrix, this is also the case in fourth order quantum anharmonic oscillator, the formal solution as a finite sum can be given as follows.

$$\langle \mathbf{s}^{(j+1)} \rangle (0) = e^{\beta t} \sum_{j=0}^{\infty} \frac{1}{j!} \left( \frac{e^{\beta t} - 1}{\beta} \right)^j \mathbf{T}_j \langle \mathbf{s}^{(j)} \rangle (0)$$  \hspace{1cm} (10)

where $\mathbf{T}_j$ is a rectangular matrix of $n \times n^j$ type. Since the right hand side of the above equation (1) contains new unknowns, it is necessary to define their time evolution.

$$\frac{d\langle \mathbf{s}^{(j)} \rangle (t)}{dt} = \sum_{k=0}^{\infty} \mathbf{E}_{j,k} \langle \mathbf{s}^{(k)} \rangle (t), \quad j = 1, 2, \ldots$$  \hspace{1cm} (4)

Where $\mathbf{E}_{j,k}$ explicitly defined as follows.

$$\mathbf{E}_{j,k} \equiv \sum_{k=0}^{j-1} \left( \mathbf{I}_n^{\otimes k} \otimes \mathbf{H}^{(c)}_{m-j+1}(t) \otimes \mathbf{I}_n^{\otimes (j-k-1)} \right)$$  \hspace{1cm} (5)

Evolution matrix contains $\mathbf{E}_{j,k}$ matrices as its blocks and can be placed as follows.

$$\mathbf{E} = \begin{bmatrix} \mathbf{E}_{0,0} & \cdots & \mathbf{E}_{0,j} & \cdots & \mathbf{E}_{0,j} & \cdots \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots \\ \mathbf{E}_{j,0} & \cdots & \mathbf{E}_{j,j} & \cdots & \mathbf{E}_{j,j} & \cdots \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots \end{bmatrix}$$  \hspace{1cm} (6)

After all these steps, countably many sets of linear ODEs can be obtained in the following form.

$$\frac{d\xi(t)}{dt} = \mathbf{E}\xi(t)$$  \hspace{1cm} (7)

where;

$$\xi(t) = \begin{bmatrix} \langle \mathbf{s}^{(0)} \rangle (t) \\ \langle \mathbf{s}^{(1)} \rangle (t) \\ \vdots \\ \langle \mathbf{s}^{(n)} \rangle (t) \end{bmatrix}^T$$  \hspace{1cm} (8)

and the formal solution is as follows.

$$\xi(t) = e^{t\mathbf{E}}\xi(0)$$  \hspace{1cm} (9)

The definition and the solution of matrix weighted multivariate Hausdorff Moment Problem Arising From Quantum Mechanical Applications of Probabilistic Evolution Approach. In this study, we will extend this issue by using matrix weights for better modeling correlations between expectation values of the operators appearing in the Kronecker powers of the system vector. The definition of the matrix weighted multivariate finite interval Hausdorff moment problem as follows.

$$\mu_j \equiv \int_V dV \mathbf{W}_j(x) x^{\otimes j}, \quad j = 0, 1, 2, \ldots$$  \hspace{1cm} (11)

where $\mu_j$ corresponds to the $\langle \mathbf{s}^{(j)} \rangle (0)$ and $\mathbf{W}_j(x)$ are unknown weight functions and $\mathbf{x}$ is an $n$ dimensional vector containing independent variables of the weight functions. As in the previous case, $V$ denotes finite hypercube and its boundary conditions will be defined accordingly to satisfy the positivity of the weight function in that hypercube.

The definition and the solution of matrix weighted multivariate finite interval Hausdorff moment problem of that type is the main contribution of this study both in the research area of moment problem and of Probabilistic Evolution Approach.

If the moment problem is solved the solution of Probabilistic Evolution Approach given in equation
(10) can be written in the following form.
\[ \langle S \rangle (t) = \int_V dV W_j(x) e^{\beta t} \sum_{j=0}^{\infty} \frac{1}{j!} \left( e^{\beta t} - 1 \right)^j T_j x^{\otimes j} \]

This is the more eligible form to reduce the computational task because of the direct usage of the Kronecker powers of vector and also some algorithms currently developed for this purpose.

The remaining part of the paper is organized as follows. Following section covers the provement of existence of the solution of the problem beside its explicit solution and some detailed discussions. The paper will be finalized with concluding remarks and future directions of research as always.

2 Solution of Multivariate Hausdorff Moment Problem

2.1 Existence of the Solution

As stated in the accompanying study and the early works of Felix Hausdorff univariate finite interval moment problem has a unique solution in the case of positive definiteness of Hankel matrix \[1,2\]. In that study, we have shown that this property may not hold for the multivariate case under matrix weight. In the definition of the problem, we have countably many matrix weight functions. Firstly, we will begin to investigate the positive definiteness of these matrix weight function. For this purpose, Hankel matrix can be defined in the block structure for multivariate case in the following form.

\[ H_m \equiv \begin{bmatrix} M_{0,0} & M_{0,1} & \ldots & \ldots \\ M_{1,0} & M_{1,1} & \ldots & \ldots \\ \ldots & \ldots & \ddots & \ldots \\ \ldots & \ldots & \ldots & M_{m,m} \end{bmatrix} \] (12)

where:

\[ M_{j,k} \equiv \int_V dV W_j(x) x^{\otimes j} x^{\otimes kT} \] (13)

Here, we will follow the identical steps given in the accompanying paper. To prove the positivity of Hankel matrix, the following equation must be satisfied for all vectors \( y \) by definition.

\[ y^\dagger H_m y > 0 \] (14)

Using (13) in (14) implies:

\[ q = \sum_{j,k} m_j y^\dagger M_{j,k} y_k \]
\[ = \int_V dV W_j(x) \left[ \sum_{j=0}^{m} y_j^\dagger x^{\otimes j} \right] \left[ \sum_{k=0}^{m} x^{\otimes kT} y_k \right] \]
\[ q = \int_V dV W_j(x) ||\phi(x, y)||^2 \] (15)

Where:

\[ \phi(x, y) = \sum_{k=0}^{m} x^{\otimes kT} y_k \] (16)

The equation (15) is sufficient to complete the proof if all countably many matrices \( W_j(x) \) is positive definite in the studied hypercube. However, the boundaries of the hypercube is not initially imposed and can be selected to satisfy that condition, this is a strong condition to be satisfied. It is again important to point out that in our applications, the solution of the problem has not to be present moment. It is sufficient for our applications to produce an integral transformation whose kernel has no singularities in the studied hypercube.

2.2 Explicit Solution

The decomposition of the matrices \( F_j(x) \) as \( F_j(x) = W_j(x) \Omega_j(x)^{-1} \) transforms matrix weighted multivariate moment problem to the following form.

\[ \mu_j \equiv \int_V dV F_j(x) \Omega_j(x) x^{\otimes j}, \quad j = 0, 1, 2, \ldots \] (17)

Kronecker power series expansion of the functions \( F_j(x) \) may be written in the following form. Since the analyticity in weight functions assumed this series always exist, no other assumption is required.

\[ F_j(x) = \sum_{k=0}^{\infty} A^{(j)}_k (x^{\otimes k}) \] (18)

The explicit structure of \( A^{(j)}_k \) is as follows.

\[ A^{(j)}_k (x^{\otimes k}) \equiv \begin{bmatrix} f_k^{(1,1)} x^{\otimes k} & f_k^{(1,2)} x^{\otimes k} & \ldots & \ldots \\ f_k^{(2,1)} x^{\otimes k} & f_k^{(2,2)} x^{\otimes k} & \ldots & \ldots \\ \ldots & \ldots & \ddots & \ldots \\ \ldots & \ldots & \ldots & f_k^{(n_1,n_1)} x^{\otimes k} \end{bmatrix} \]
Variables $x$ dependence of this matrix can be separated by the help of following expansion.

$$ A_k^{(j)}(x^\otimes k) = \sum_{r=1}^{n^j} u_r^T \otimes B_r^{k,j} x^\otimes k $$  \hspace{1cm} (19)

In that equality, $u_r$ stands for a $n^j \times 1$ dimensional unit vector whose $r$th element is equal to one and others are equal to zero. $B_r^{k,j}$ matrices are constant blocks of the matrix $A_k(x^\otimes k)$ and can be written explicitly as follows.

$$ B_r^{k,j} = \begin{bmatrix}
 f_{(1,r)}^T \\
 f_{(2,r)}^T \\
 \vdots \\
 f_{(n^j,r)}^T
\end{bmatrix} $$  \hspace{1cm} (20)

All these definitions help us to obtain following equality.

$$ \mu_j = \sum_{k=0}^{\infty} \sum_{r=1}^{n^j} \int_V dV \Omega_j(x) \left( u_r^T \otimes B_r^{k,j} x^\otimes k \right) x^\otimes j $$

$$ = \sum_{k=0}^{\infty} \sum_{r=1}^{n^j} \int_V dV \Omega_j(x) \left( u_r^T \otimes B_r^{k,j} \right) I_{n^j+k} x^\otimes j+k $$

$$ = \sum_{k=0}^{\infty} \sum_{r=1}^{n^j} \left( u_r^T \otimes B_r^{k,j} \right) \int_V dV \Omega_j(x) x^\otimes j+k $$

$$ \mu_j = \sum_{k=0}^{\infty} \tilde{A}_k^{(j)} \mathcal{M}_{j+k}^\Omega $$ \hspace{1cm} (21)

This final equation has known entities $\mu_j, \mathcal{M}_{j+k}^\Omega$ and has unknown entities $\tilde{A}_k^{(j)}$. If the unknown matrices can be find, the weight function can be produced from these values since it contains the coefficients of the Kronecker series expansion of the weight function. For this purpose, we will be interested for the case $j = m$, since it is straightforward for the other case. For the case $j = m$ following equation holds.

$$ \mu_m = \sum_{k=0}^{\infty} \tilde{A}_k^{(m)} \mathcal{M}_{m+k}^\Omega $$

$$ = \tilde{A}_1^{(m)} \mathcal{M}_{m+1}^\Omega + \tilde{A}_2^{(m)} \mathcal{M}_{m+2}^\Omega + \ldots $$ \hspace{1cm} (22)

To be able to satisfy this equality, we may write $\tilde{A}_j^{(m)}$ matrices as the outer product of the vectors $\mu_m$ and $\mathcal{M}_{m+j}^\Omega$ as follows.

$$ \tilde{A}_j^{(m)} = \sigma_j \mu_m \mathcal{M}_{m+j}^\Omega^T, \quad j = 0, 1, 2, \ldots $$ \hspace{1cm} (23)

The determination of the values $\sigma_j$ is of importance here and can be achieved by the following equality as can be easily seen from the equation (22).

$$ \sum_{j=0}^{\infty} \sigma_j \parallel \mathcal{M}_{m+j}^\Omega \parallel = 1 $$ \hspace{1cm} (24)

### 2.3 Discussions

The above equation can be satisfied by countably many $\sigma_j$ values. This mean that the matrix weighted multivariate finite interval Hausdorff moment problem my have infinitely many solutions. On the other hand, the following question must be replied. How many of these solutions satisfy the positivity property of the weight functions? The answer of that question vary depend on the given initial series and the boundaries of the hypercube. The advantage of the flexibility to determine boundaries can improve the chance of gathering solutions. As a final result, the matrix weighted moment problem may have none solution, unique solution or many solutions.

Here, it must be reemphasized that even if the gathered solutions does not satisfy the positivity property of the weight function, this does not obstruct the usage of solution in Probabilistic Evolution Approach as far as it does not have singularities in the studied hypercube.

### 3 Concluding Remarks

In this study, a matrix weighted multivariate finite interval Hausdorff moment problem is defined. Necessary and sufficient conditions for the existence of the solution to this problem is discussed. The main result and thus the main contribution of this study is that the defined problem may have infinitely many solution or no solution. Number of the solutions vary depending on the initial series under consideration and the selected boundaries of the hypercube studied hypercube.

The results and the solutions obtained in that work can facilitate analysis and the algorithm developments of the Probabilistic Evolution Approach for the quantum mechanical applications beside the systems whose initial conditions is not given with an accompanying Dirac delta initial probability density function.
References:


