Chapter

The Inverse of the Discrete Momentum Operator

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Abstract

In the search of a quantum momentum operator with discrete spectrum, we obtain some properties of the discrete momentum operator for nonequally spaced spectrum. We find the inverse operator. We use the matrix representation of these operators, and we find that there is one more eigenvalue and eigenfunction than the dimension of the matrix. We apply the results to obtain the discrete adjoint of the momentum operator. We conclude that we can have discrete operators which can be self-adjoint and that it is possible to define a self-adjoint extension of the corresponding Hilbert space. These results help us understand the quantum time operator.

Keywords: discrete quantum mechanics, discrete momentum operator, inverse of the momentum operator, nonstandard finite differences derivative, exact discrete integration

1. Introduction

Nonstandard finite difference derivatives help determine the discrete versions of some differential equations and their solutions [1–10]. This method uses nonstandard expressions of the finite differences derivative in such a way that they give the exact result when applied to a particular function.

Another benefit of nonstandard finite difference for the derivative of a function is that it can be used as a discrete quantum operator to deal with quantum mechanical operators with discrete spectrum [11, 12]. Since some quantum operators have a discrete spectrum, a discrete derivative can be very useful in quantum mechanics theory [11, 12].

In Section 2, we define and obtain some properties of the discrete derivative operator from a global point of view, i.e., considering all the values of a function on all the points of a mesh at once. This is done by defining a matrix that collects the derivatives for each mesh point when applied to a given vector. We find the eigenvalues and eigenvectors of the derivative matrix. We also discuss the commutation properties between the derivative and coordinate matrices. The canonical commutator is satisfied only along some directions.

The summation by parts theorem and the adjoint of the momentum operator are found in Section 3. We introduce the discrete symmetric operator definition similar to continuous variables functions in a Hilbert space.

An interesting result is that the considered matrices have more eigenvalues and corresponding *almost* eigenvectors (the last entry of the eigenvector is null) beside the usual number due to their dimension of them. For a semi-infinite matrix, the last entry is of little effect, and such additional eigenvalues will belong to the matrix spectrum when seen as an operator. Such additional eigenvalues and eigenvectors are common to all the considered matrices. With these results, we can say that there are also self-adjoint discrete operators and that we can also have discrete self-adjoint extensions in the corresponding Hilbert space. These results are beneficial when dealing with the question of the existence of a time operator in quantum mechanics [12].

We introduce the discrete inverse matrix of the discrete derivative operator in Section 4. The difference between the scheme we address in this work with other proposals for a discrete derivative is a modification in the derivative matrix for the final point of a grid of points, which causes the derivative matrix to have an inverse.

We can deal with any mesh without asking for equidistant points. At the end of this paper, there are some concluding remarks.

2. Discrete derivation

Let us consider a partition $\mathcal{P} = \{q_0, q_1, q_2, \dots, q_N\}$ of the interval $[q_0, q_N]$ and vectors $\mathbf{f} = (f_0, f_1, \dots, f_N)^T$, and $\mathbf{g} = (g_0, g_1, \dots, g_N)^T$ associated to this partition. The distances $\Delta_j = q_{j+1} - q_j$, for each j, are not supposed to be equal.

The finite differences derivative matrix $\mathbf{D}$ is defined as

$$\mathbf{D} = \begin{pmatrix} -\frac{1}{\xi_0} & \frac{1}{\xi_0} & 0 & \dots & 0 & 0 \\ 0 & -\frac{1}{\xi_1} & \frac{1}{\xi_1} & \dots & 0 & 0 \\ 0 & 0 & -\frac{1}{\xi_2} & \dots & 0 & 0 \\ \vdots & & & & & \\ 0 & 0 & 0 & \dots & -\frac{1}{\xi_{N-1}} & \frac{1}{\xi_{N-1}} \\ 0 & 0 & 0 & \dots & 0 & -\frac{1}{\xi_N} \end{pmatrix}, \tag{1}$$

where

$$\xi_j = \Delta_j e^{-ip\Delta_j/2} \operatorname{sinc}\left(\frac{\Delta_j}{2} p\right), \quad j = 0, \dots, N-1, \tag{2}$$

$$\xi_N = -\frac{i}{p}. \tag{3}$$

The function $\operatorname{sinc}(z)$ is the entire function equal to one at $z = 0$ and $z^{-1} \sin z$ otherwise. The continuous parameter p in this expression is related to the conjugate variable to the discrete variable q_j, see Eq. (11) below. The choice of ξ_j ensures that the finite differences derivative (d-derivative) delivers the exact result when acting on the complex exponential function e^{-ipq}.

In case it is needed, for small Δ_j we have the power series expansion

$$\xi_j \approx \Delta_j - i\frac{p}{2}\Delta_j^2 - \frac{p^2}{6}\Delta_j^3, \quad 0 \le j < N. \tag{4}$$

We see that ξ_j is similar to the difference Δ_j of the usual finite differences derivative. However, we will only consider the case where Δ_j has a finite value.

Let us discuss some properties of the d-derivative matrix. The action of the d-derivative matrix $\mathbf{D}$ when acting to the left, on the vector $\mathbf{f}^T = (f_0, f_1, \dots, f_N)$, results in

$$\mathbf{f}^T\mathbf{D} = \left(-\frac{f_0}{\xi_0}, -(\mathcal{D}\mathbf{f})_1, -(\mathcal{D}\mathbf{f})_2, \dots, -(\mathcal{D}\mathbf{f})_N\right), \tag{5}$$

where

$$(\mathcal{D}\mathbf{f})_j = \frac{f_j}{\xi_j} - \frac{f_{j-1}}{\xi_{j-1}}, \tag{6}$$

is a finite differences approximation to the derivative of a function extended to the complex plane. These improved increments ξ_j are defined over the complex plane. For a small difference Δ_j, we have that

$$(\mathcal{D}\mathbf{f})_j \approx \left(\frac{f_{j+1}}{\Delta_{j+1}} - \frac{f_j}{\Delta_j}\right) + i\frac{p}{2}\left(f_{j+1} - f_j\right) + \frac{p^2}{12}\left(f_{j+1} - f_{j+1}\right)\Delta_{j+1}. \tag{7}$$

We see that we have another discrete approximation to the derivative of a function.

Now, the action to the right of the derivative matrix on a vector is:

$$\mathbf{Dg} = \left((\mathrm{D}g)_0, (\mathrm{D}g)_1, \dots, (\mathrm{D}g)_{N-1}, -\frac{f_N}{\xi_N}\right)^T, \tag{8}$$

where

$$(\mathrm{D}g)_j = \frac{g_{j+1} - g_j}{\xi_j}, \tag{9}$$

is a modified finite differences derivative of $g(q)$ at q_j. In case Δ_j is small, we have that

$$(\mathrm{D}\mathbf{g})_j \approx \frac{g_{j+1} - g_j}{\Delta_j} + i\frac{p}{2}\left(g_{j+1} - g_j\right) - \frac{p^2}{12}\Delta_j\left(g_{j+1} - g_j\right). \tag{10}$$

The first term in this approximation is the usual finite differences derivative of a function.

Note that for in the limiting case, $\Delta_j \to 0$, both nonstandard finite differences (Eq. 5) and (Eq. 8) reduce to the usual forward finite difference approximation to the derivative.

The eigenvalues of the derivative matrix $\mathbf{D}$ are $\lambda_j = -1/\xi_N, -1/\xi_{N-1}, \dots, -1/\xi_0$, and the corresponding eigenvectors are

$$\left\{ \begin{pmatrix} \dfrac{\xi_N^N}{\prod_{n=0}^{N-1}(\xi_N - \xi_n)} \\ \dfrac{\xi_N^{N-1}}{\prod_{n=1}^{N-1}(\xi_N - \xi_n)} \\ \dfrac{\xi_N^{N-2}}{\prod_{n=2}^{N-1}(\xi_N - \xi_n)} \\ \vdots \\ 1 \end{pmatrix}, \begin{pmatrix} \dfrac{\xi_{N-1}^{N-1}}{\prod_{n=0}^{N-2}(\xi_{N-1} - \xi_n)} \\ \dfrac{\xi_{N-1}^{N-2}}{\prod_{n=1}^{N-2}(\xi_{N-1} - \xi_n)} \\ \dfrac{\xi_{N-1}^{N-3}}{\prod_{n=2}^{N-3}(\xi_{N-1} - \xi_n)} \\ \vdots \\ 0 \end{pmatrix}, \dots, \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \right\}. \tag{11}$$

Note that, due to the operator character of the matrix, there is an additional eigenvector, the exponential function $\mathbf{e} = \left(e^{-ipq_0}, e^{-ipq_1}, e^{-ipq_2}, \dots, e^{-ipq_N}\right)$, with eigenvalue $-ip$,

$$\mathbf{De} = -ip\,\mathbf{e}. \tag{12}$$

3. The adjoint of the discrete derivative

A sesquilinear form between vectors $\mathbf{f}$ and $\mathbf{g}$ is defined with the help of the summation matrix:

$$\mathbf{S} = \begin{pmatrix} \xi_0 & 0 & 0 & \dots & 0 & 0 \\ 0 & \xi_1 & 0 & \dots & 0 & 0 \\ 0 & 0 & \xi_2 & \dots & 0 & 0 \\ \vdots & & & & & \\ 0 & 0 & 0 & \dots & \xi_{N-1} & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \end{pmatrix}, \tag{13}$$

obtaining

$$\begin{aligned} & \mathbf{f}^T\,\mathbf{SDg} \\ & = -f_0 g_0 + f_0 g_1 - f_1 g_1 + f_1 g_2 - f_2 g_2 + f_2 g_3 - f_3 g_3 + \dots + f_N g_N \\ & = \mathbf{g}^T\left(\mathbf{B} - \mathbf{S}\tilde{\mathbf{D}}\right)\mathbf{f}, \end{aligned} \tag{14}$$

where

$$\tilde{\mathbf{D}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ -\dfrac{1}{\xi_1} & \dfrac{1}{\xi_1} & 0 & \dots & 0 & 0 \\ 0 & -\dfrac{1}{\xi_2} & \dfrac{1}{\xi_2} & \dots & 0 & 0 \\ \vdots & & & & & \\ 0 & 0 & 0 & \dots & \dfrac{1}{\xi_{N-1}} & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \end{pmatrix}. \tag{15}$$

and

$$\mathbf{B} = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & & & & & \\ 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 1 & 0 \end{pmatrix}. \tag{16}$$

Eq. (13) is the summation by parts equality in matrix form. We call the matrix $\tilde{\mathbf{D}}$ the d-adjoint of the discrete derivative matrix $\mathbf{D}$.

A row of the summation by parts matrix equality is:

$$\sum_{n=0}^{N-1} \xi_n f_n (\mathrm{D}\mathbf{g})_n + \sum_{n=1}^{N-1} \xi_n (\tilde{\mathrm{D}}\mathbf{f})_n g_n = f_{N-1} g_N - f_0 g_0, \tag{17}$$

which is the discrete version of the integration by parts theorem of the calculus of continuous variables.

The previous results are useful in quantum mechanics theory when considering the momentum or the Hamiltonian operators with a discrete spectrum.

We define the discrete momentum operator at q_j as

$$\hat{P}_j = -i(\mathrm{D})_j, \quad 0 \le j < N, \tag{18}$$

and its adjoint

$$\hat{P}_j^\dagger = -i(\tilde{\mathrm{D}})_j, \quad 0 < j < N. \tag{19}$$

The summation by parts provides the adjoint of the momentum operator and its symmetry property. Explicitly, Eq. (16) is rewritten as

$$\sum_{n=0}^{N-1} \xi_n f_n^* (-i\mathbf{D}\mathbf{g})_n - \sum_{n=1}^{N} \xi_n \left[\left(-i\tilde{\mathbf{D}}^* \mathbf{f} \right)_n \right]^* g_n = -if_{N-1}^* g_N + if_0^* g_0, \tag{20}$$

This equality yields

$$\langle f | \hat{P} g \rangle = \langle \tilde{P} f | g \rangle = -if_{N-1}^* g_N + if_0^* g_0. \tag{21}$$

Thus, we say that the discrete momentum operator $\hat{P}$ is d-symmetric, if $f_{N-1} = e^{i\theta} f_0$ and $g_N = e^{i\theta} g_0$, as is the case for continuous variables operators.

It is also possible to consider self-adjoint extensions for the discrete momentum operator, as it is done for the case of the continuous variable momentum operator [13].

3.1 Commutator between the d-derivative and the coordinate

In general, a discrete canonical commutation relationship $[A, B] = I$ is not possible for finite-dimensional matrices A and B because the trace of this relationship results in a contradiction ((0 = 1) [14]. However, there are some directions in which the commutator evaluates to a constant different from zero: the directions pointed at by its eigenvectors, for example. In addition, the matrix can be considered as an operation with additional eigenfunctions [15].

If we call $\mathbf{Q} = \text{diag}\left(q_j\right)$ to the coordinate matrix, the usual commutator between the d-derivative and coordinate matrices is:

$$[\mathbf{D}, \mathbf{Q}] = \begin{pmatrix} 0 & \frac{\Delta_0}{\xi_0} & 0 & \dots & 0 & \dots & 0 \\ 0 & 0 & \frac{\Delta_1}{\xi_1} & \dots & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 0 & \dots & \frac{\Delta_{N-1}}{\xi_{N-1}} \\ 0 & 0 & 0 & \dots & 0 & \dots & 0 \end{pmatrix}. \tag{22}$$

This matrix shifts and rescales the vector entries on which it acts. This matrix approaches an identity matrix when $\Delta_j \to 0$.

For a finite Δ_j, we look for the eigenvectors of the commutator matrix to obtain a diagonal matrix. The eigenvalues of the commutator (21), considered as a matrix, are all zero with multiplicity $N + 1$. The eigenvectors are $(1, 0, \dots, 0)^T$ and $(0, \dots, 0)^T$ with multiplicity N. In addition to considering the eigenvectors of this commutator matrix to obtain a diagonal matrix, we can take advantage of rescaling to cancel shifting and return to the original vector [15]. Then, the commutator matrix (21) has the additional eigenvector

$$\mathbf{h}^T = \left(\frac{1}{\lambda^{N-1}} \prod_{j=0}^{N-2} \frac{\Delta_j}{\xi_j}, \frac{1}{\lambda^{N-2}} \prod_{j=1}^{N-2} \frac{\Delta_j}{\xi_j}, \dots, \frac{\lambda \xi_{N-1}}{\Delta_{N-1}}\right)^T, \tag{23}$$

with an eigenvalue λ. The action of the commutator matrix on these vectors results in the same vector with the last entry equal to zero, which is almost an eigenvector.

Still another eigenvector, with eigenvalue one, is

$$\tilde{\mathbf{h}}^T = \left(1, \frac{\xi_0}{\Delta_0}, \dots, \prod_{n=0}^{N-1} \frac{\xi_n}{\Delta_n}\right)^T, \tag{24}$$

The commutator is equal to one along this direction. Then, the canonical commutation relationship is also valid in this direction.

Thus, along the mentioned directions, the d-derivative has similar properties as its continuous variable counterpart.

4. The inverse of the d-derivative

The d-derivative matrix that we use can be inverted. The determinant of the d-derivative matrix is

$$|\mathbf{D}| = \frac{1}{\xi_0\xi_1\xi_2\xi_3 \dots \xi_N}. \tag{25}$$

The inverse of the d-derivative matrix $\mathbf{D}$ is the negative of the progressive discrete integration matrix

$$\mathbf{I} = \begin{pmatrix} \xi_0 & \xi_1 & \xi_2 & \xi_3 & \dots & \xi_N \\ 0 & \xi_1 & \xi_2 & \xi_3 & \dots & \xi_N \\ 0 & 0 & \xi_2 & \xi_3 & \dots & \xi_N \\ 0 & 0 & 0 & \xi_3 & \dots & \xi_N \\ \vdots & & & & & \\ 0 & 0 & 0 & 0 & \dots & 0 \end{pmatrix}. \tag{26}$$

We discuss some properties of the d-integration matrix $\mathbf{I}$. When the d-integration matrix $\mathbf{I}$ is applied to the left to a vector $\mathbf{f}^T$ results in

$$\mathbf{f}^T\mathbf{I} = (\mathcal{I}_0\mathbf{f}, \mathcal{I}_1\mathbf{f}, \mathcal{I}_2\mathbf{f}, \dots, \mathcal{I}_N\mathbf{f}), \tag{27}$$

where

$$\mathcal{I}_j\mathbf{f} = \xi_j\left(f_0 + f_1 + \dots + f_j\right), \quad j \leq N. \tag{28}$$

The entries of the resulting vector are the progressive discrete integrations of $\mathbf{f}$ when the subintervals are of equal length ξ_j. When the d-integration matrix is applied to the right, we get

$$\mathbf{I}\mathbf{g} = \left(\mathrm{I}_0\mathbf{g}, \mathrm{I}_1\mathbf{g}, \mathrm{I}_2\mathbf{g}, \dots, \mathrm{I}_N\mathbf{g}\right), \tag{29}$$

where

$$\mathrm{I}_j\mathbf{g} = g_j\xi_j + g_{j+1}\xi_{j+1} + \dots + g_N\xi_N, \quad 0 \leq j \leq N. \tag{30}$$

This result is the progressive discrete integration of $\mathbf{g}$ when the subintervals are of different lengths.

The eigenvalues of $\mathbf{I}$ are $\xi_0, \dots, \xi_N$, and its eigenvectors are the same as for $\mathbf{D}$, Eq. (10). But, there is the additional eigenvector $\mathbf{e} = \left(e^{-ipq_0}, \dots, e^{-ipq_N}\right)^T$,

$$\mathbf{I}\mathbf{e} = \frac{i}{p}\mathbf{e}. \tag{31}$$

The d-derivative and its inverse are constant along the same directions. The domain of the d-derivative and d-integration is the same.

Now, the commutator between $\mathbf{S}$ and $\mathbf{Q}$ is

$$[\mathbf{Q}, \mathbf{I}] = \begin{pmatrix} 0 & \xi_1(q_1 - q_0) & \xi_2(q_2 - q_0) & \xi_3(q_3 - q_0) & \dots & -\xi_N(q_N - q_0) \\ 0 & 0 & \xi_2(q_2 - q_1) & \xi_3(q_3 - q_1) & \dots & -\xi_N(q_N - q_1) \\ 0 & 0 & 0 & \xi_3(q_3 - q_2) & \dots & -\xi_N(q_N - q_2) \\ \vdots & & & & & \\ 0 & 0 & 0 & 0 & \dots & -\xi_N(q_N - q_{N-1}) \\ 0 & 0 & 0 & 0 & \dots & 0 \end{pmatrix}, \tag{32}$$

which is the progressive discrete integral of $g(q)\left(q - q_j\right)$ when acting on the vector $\mathbf{g}$.

5. Conclusions

We have found another property of the d-derivative matrix: its inverse. The inverse of the d-derivative has the right properties; the properties of the continuous variable integration.

We discussed some of the properties of the discrete momentum operator when considering all of a subset of the spectrum points at once and its associated discrete integration matrices. The matrices are related by a common eigenvector for continuous variable functions. These results give us confidence that our choice is a good candidate for the discrete quantum momentum operator.

We also found that the matrices associated with the discrete derivative and the discrete integration have an additional eigenvalue and eigenvector, in contrast with the usual behavior of standard matrices. We have increased the number of eigenvalues and eigenvectors of a matrix by using it as an operator.

These operators are of help in defining a time operator and its eigenvalues and eigenvectors for use in nonrelativistic quantum mechanics [12]. They can also be used when the angular momentum on a circle is considered [16–18].

These results imply that we can deal with discrete quantum operators in almost the same way as for continuous variable operators case, including deficiency indices and self-adjoint extensions [13].

We have considered the exact discrete derivative for the complex exponential function, but these results are also valid for the real exponential function e^{-pq} with the replacements

$$\xi_N = \frac{1}{p}, \tag{33}$$

$$\xi_j = \frac{1 - e^{-p\Delta_j}}{p}, \quad j < N. \tag{34}$$

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