Chapter 2

Matrices Which are Discrete Versions of Linear Operations

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Additional information is available at the end of the chapter

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Abstract

We introduce and study a matrix which has the exponential function as one of its eigenvectors. We realize that this matrix represents a set of finite differences derivation of vectors on a partition. This matrix leads to new expressions for finite differences derivatives which are exact for the exponential function. We find some properties of this matrix, the induced derivatives and of its inverse. We provide an expression for the derivative of a product, of a ratio, of the inverse of vectors, and we also find the equivalent of the summation by parts theorem of continuous functions. This matrix could be of interest to discrete quantum mechanics theory.

Keywords: exact finite differences derivative, exact derivatives on partitions, exponential function on a partition, discrete quantum mechanics

1. Introduction

We are interested on matrices which are a local, as well as a global, exact discrete representation of operations on functions of continuous variable, so that there is congruency between the continuous and the discrete operations and properties of functions. Usual finite difference methods [1–4] become exact only in the limit of zero separation between the points of the mesh. Here, we are interested in having exact representations of operations and functions for *finite* separation between mesh points.

The difference between our method and the usual finite differences method is the quantity that appears in the denominator of the definition of derivative. The appropriate choice of that denominator makes possible that the finite differences expressions for the derivative gives the exact results for the exponential function. We concentrate on the derivative operation, and we define a matrix which represents the exact finite difference derivation on a local and a global scale. The inverse of this matrix is just the integration operation. These are interesting subjects by itself, but they are also of interest in the quantum physics realm [5–7].

In this chapter, we will consider only the case of the derivative and the integration of the exponential function.

2. A matrix with the exponential function as an eigenvector

Here, we consider the $N \times N$ antisymmetric, tridiagonal matrix

$$\mathbf{D}_N := \begin{pmatrix} \frac{-e^{-v\Delta}}{2\chi(v,\Delta)} & \frac{1}{2\chi(v,\Delta)} & 0 & \dots & 0 & 0 & 0 \\ \frac{-1}{2\chi(v,\Delta)} & 0 & \frac{1}{2\chi(v,\Delta)} & \dots & 0 & 0 & 0 \\ 0 & \frac{-1}{2\chi(v,\Delta)} & 0 & \dots & 0 & 0 & 0 \\ \vdots & & & & & & \\ 0 & 0 & 0 & \dots & 0 & \frac{1}{2\chi(v,\Delta)} & 0 \\ 0 & 0 & 0 & \dots & \frac{-1}{2\chi(v,\Delta)} & 0 & \frac{1}{2\chi(v,\Delta)} \\ 0 & 0 & 0 & \dots & 0 & \frac{-1}{2\chi(v,\Delta)} & \frac{e^{v\Delta}}{2\chi(v,\Delta)} \end{pmatrix}, \tag{1}$$

where $v \in \mathbb{C}$—it can be pure real or pure imaginary—, $\Delta \in \mathbb{R}^+$, and $\chi(v,\Delta) := \sinh(v\Delta)/v \approx \Delta + v^2\Delta^3/6 + O(\Delta^5)$. This function $\chi(v,\Delta)$ is well defined for $v = 0$, with value $\chi(0,\Delta) = \Delta$. This matrix is interesting because, as we will see below, it represents a derivation on a partition. A rescaled matrix $\overline{\mathbf{D}}_N$ is defined as

$$\overline{\mathbf{D}}_N := \begin{pmatrix} -1/z & 1 & 0 & \dots & 0 & 0 & 0 \\ -1 & 0 & 1 & \dots & 0 & 0 & 0 \\ 0 & -1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & & & & & & \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & 0 & \dots & -1 & 0 & 1 \\ 0 & 0 & 0 & \dots & 0 & -1 & z \end{pmatrix}, \tag{2}$$

where $z = e^{v\Delta}$, and

$$\mathbf{D}_N := \frac{\overline{\mathbf{D}}_N}{2\chi(v,\Delta)}. \tag{3}$$

We are mainly interested in finding the eigenvalues and the corresponding eigenvectors of these matrices.

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We start our study with a result about the determinant of $\overline{\mathbf{D}}_N - \lambda \mathbf{I}_N$,

$$
\begin{aligned}
|\overline{\mathbf{D}}_N - \lambda \mathbf{I}_N| &= |\overline{\mathbf{D}}_N + \alpha \mathbf{I}_N| \\
&= \begin{vmatrix}
\alpha - 1/z & 1 & 0 & 0 & \dots & 0 & 0 & 0 \\
-1 & \alpha & 1 & 0 & \dots & 0 & 0 & 0 \\
0 & -1 & \alpha & 1 & \dots & 0 & 0 & 0 \\
0 & 0 & -1 & \alpha & \dots & 0 & 0 & 0 \\
\vdots & & & & & & & \\
0 & 0 & 0 & \dots & \alpha & 1 & 0 & 0 \\
0 & 0 & 0 & \dots & -1 & \alpha & 1 & 0 \\
0 & 0 & 0 & \dots & 0 & -1 & \alpha & 1 \\
0 & 0 & 0 & \dots & 0 & 0 & -1 & \alpha + z
\end{vmatrix} \\
&= \left(\alpha - \frac{1}{z}\right) \mathrm{A}_{N-1}(\alpha) + \mathrm{A}_{N-2}(\alpha),
\end{aligned}
\tag{4}
$$

where $\lambda = -\alpha$,

$$
\begin{aligned}
\mathrm{A}_j(\alpha) &:= \begin{vmatrix}
\alpha & 1 & 0 & \dots & 0 & 0 & 0 \\
-1 & \alpha & 1 & \dots & 0 & 0 & 0 \\
0 & -1 & \alpha & \dots & 0 & 0 & 0 \\
\vdots & & & & & & \\
0 & 0 & \dots & \alpha & 1 & 0 & 0 \\
0 & 0 & \dots & -1 & \alpha & 1 & 0 \\
0 & 0 & \dots & 0 & -1 & \alpha & 1 \\
0 & 0 & \dots & 0 & 0 & -1 & \alpha + z
\end{vmatrix} \\
&= (\alpha + z)\mathrm{B}_{j-1}(\alpha) + \mathrm{B}_{j-2}(\alpha),
\end{aligned}
\tag{5}
$$

and

$$
\mathrm{B}_j(\alpha) = \begin{vmatrix}
\alpha & 1 & 0 & \dots & 0 & 0 \\
-1 & \alpha & 1 & \dots & 0 & 0 \\
0 & -1 & \alpha & \dots & 0 & 0 \\
\vdots & & & & & \\
0 & 0 & \dots & \alpha & 1 & 0 \\
0 & 0 & \dots & -1 & \alpha & 1 \\
0 & 0 & \dots & 0 & -1 & \alpha
\end{vmatrix}.
\tag{6}
$$

Strikingly, we recognize the determinant $\mathrm{B}_j(\alpha)$ as the Fibonacci polynomial of index $j + 1$ [10, 11], i.e., $\mathrm{B}_j(\alpha)=\mathrm{F}_{j+1}(\alpha)$. Fibonacci polynomials are defined as

$$F_0(x) = 0, \quad F_1(x) = 1, \quad F_j(x) = xF_{j-1}(x) + F_{j-2}(x), \quad j \geq 2. \tag{7}$$

Since we have that $B_j(\alpha) = F_{j+1}(\alpha)$, and the recursion relationship for Fibonacci polynomials, we also have that

$$A_j(\alpha) = (\alpha + z)F_j(\alpha) + F_{j-1}(\alpha) = zF_j(\alpha) + F_{j+1}(\alpha), \tag{8}$$

and then

$$\begin{aligned} &|\overline{\mathbf{D}}_N + \alpha \mathbf{I}_N| \\ &= \left(\alpha - \frac{1}{z}\right)[zF_{N-1}(\alpha) + F_N(\alpha)] + zF_{N-2}(\alpha) + F_{N-1}(\alpha) \\ &= z[\alpha F_{N-1}(\alpha) + F_{N-2}(\alpha)] + \left(\alpha - \frac{1}{z}\right)F_N(\alpha) \\ &= \left(\alpha + z - \frac{1}{z}\right)F_N(\alpha). \end{aligned} \tag{9}$$

Then, the eigenvalues of the derivative matrix $\overline{\mathbf{D}}_N$ are $\lambda_1 = z - 1/z = e^{v\Delta} - e^{-v\Delta} = 2\sinh(v\Delta)$ and $\lambda_m = -\alpha_m$, where α_m is the m-th root of the N-th Fibonacci polynomial, which is a polynomial of degree $N - 1$ [10, 11].

The system of simultaneous equations for the eigenvector $\mathbf{e}_m^T = (e_{m,1} e_{m,2}, \ldots, e_N)$ corresponding to λ_m, can be put in a form similar to the recursion relationship for the Fibonacci polynomials, i.e.,

$$e_{m,2} = \lambda_m e_{m,1} + \frac{e_{m,1}}{z}, \tag{10}$$

$$e_{m,j+1} = \lambda_m e_{m,j} + e_{m,j-1}, \quad 1 < j < N, \tag{11}$$

$$ze_{m,N} = \lambda_m e_{m,N} + e_{m,N-1}. \tag{12}$$

This set of recursion relationships can be written as the matrix equation

$$\begin{pmatrix} e_{m,j} \\ e_{m,j+1} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & \lambda_m \end{pmatrix} \begin{pmatrix} e_{m,j-1} \\ e_{m,j} \end{pmatrix}, \quad j = 1, \ldots, N, \tag{13}$$

where $e_{m,0} = e_{m,1}/z$ and $e_{m,N+1} = ze_{m,N}$. Thus

$$\begin{pmatrix} e_{m,j} \\ e_{m,j+1} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & \lambda_m \end{pmatrix}^j \begin{pmatrix} e_{m,0} \\ e_{m,1} \end{pmatrix}, \quad j = 1, \ldots, N, \tag{14}$$

but

$$\begin{pmatrix} 0 & 1 \\ 1 & \lambda_m \end{pmatrix}^j = \begin{pmatrix} F_{j-1}(\lambda_m) & F_j(\lambda_m) \\ F_j(\lambda_m) & F_{j+1}(\lambda_m) \end{pmatrix}, \tag{15}$$

and then,

$$\begin{pmatrix} e_{m,j} \\ e_{m,j+1} \end{pmatrix} = \begin{pmatrix} F_{j-1}(\lambda_m) & F_j(\lambda_m) \\ F_j(\lambda_m) & F_{j+1}(\lambda_m) \end{pmatrix} \begin{pmatrix} e_{m,0} \\ e_{m,1} \end{pmatrix}, \quad j = 1, \ldots, N. \tag{16}$$

i.e., the j-th component of the m-th eigenvector is

$$e_{m,j} = \left[F_j(\lambda_m) + \frac{F_{j-1}(\lambda_m)}{z} \right] e_{m,1} \text{ for } j = 1, 2, \ldots, N. \tag{17}$$

For the case of the eigenvalue $\lambda_1 = z - 1/z$, we can rewrite Eq. (17) by noticing that if we let $x = w - w^{-1}$ $(w \in \mathbb{C})$, then $F_n(x) + F_{n-1}(x)/w = w^{n-1}$ for $n = 1, 2, \ldots$. This can be proved by induction method as follows. For $n = 1$, it is immediately verified. First, suppose that the equality holds for $n \le k$. Next, we compute the right-hand side of the equality for $k + 1$. Substituting $F_{k-1} = w\left(w^{k-1} - F_k\right)$ in the expression for $k + 1$, and using the properties of the Fibonacci polynomials, we obtain

$$\begin{aligned} F_{k+1}(x) + \frac{F_k(x)}{w} &= x F_k(x) + F_{k-1}(x) + \frac{F_k(x)}{w} \\ &= x F_k(x) + w^k - w F_k(x) + \frac{F_k(x)}{w} \\ &= w^k. \end{aligned} \tag{18}$$

Therefore, according to Eqs. (17) and (18), the eigenvector for the eigenvalue $\lambda_1 = 2\sinh(v\Delta)$ takes the form $\mathbf{e}_1 = c\left(1, z, \ldots, z^{N-1}\right)^T$, where c is a normalization constant. We can take advantage of the normalization constant and write

$$\mathbf{e}_1 = c\left(e^{vq_1}, , e^{vq_2}, \ldots, , e^{vq_N}\right)^T, \tag{19}$$

with eigenvalue $\lambda_1 = v$ (in original scaling, i.e., the eigenvalue of the matrix $\mathbf{D}_N$), q_1 is an arbitrary constant, and $q_j = q_1 + (j - 1)\Delta$. This means that the exponential function is an eigenvector of the derivative matrix which is a global representation of the derivative on the partition $\{q_1, q_2, \ldots, q_N\}$. Recall that the exponential function is an eigenfunction of the derivative of functions of continuous variable.

The remain of the eigenvectors have eigenvalues equal to the negative of the roots of the N-th Fibonacci polynomial $\lambda_m = -x_m$, $m = 1, 2, \ldots, N - 1$, and have the form

$$\mathbf{e}_m = c \begin{pmatrix} 1 \\ F_2(\lambda_m) + e^{-v\Delta} \\ F_3(\lambda_m) + e^{-v\Delta} F_2(\lambda_m) \\ \vdots \\ F_{N-1}(\lambda_m) + e^{-v\Delta} F_{N-2}(\lambda_m) \\ e^{-v\Delta} F_{N-1}(\lambda_m) \end{pmatrix} \tag{20}$$

The vector that we will be interested on is the one which is the exponential function (19) with eigenvalue v.

3. The matrix $\mathbf{D}_N$ represents a derivation

Let us consider a partition, $P(N):=\{q_i\}_1^N$, $q_i \in \mathbb{R}$, of N equally spaced points q_i of the interval $[a,b] \in \mathbb{R}$, $a < b$, with the same separation $\Delta = (b-a)/(N-1)$ between them.

The rows of the result of the multiplication of the derivative matrix $\mathbf{D}_N$ and a vector $\mathbf{g}:=(g_1, g_2, \ldots, g_n)^T$ are

$$(\mathbf{D}_N \mathbf{g})_j = \frac{g_{j+1} - g_{j-1}}{2\chi(v,\Delta)}, \quad j = 1, 2, \ldots, N, \tag{21}$$

where $g_0:=e^{-v\Delta}g_1$ and $g_{N+1}:=e^{v\Delta}g_N$. We recognize these expressions as the second order derivatives of the function $g(x)$ at the mesh points, but instead of dividing by twice the separation Δ between the mesh points, there is the function $\chi(v,\Delta)$ in the denominator. This function makes it possible that the exponential function be an eigenvector of the matrix $\mathbf{D}_N$.

The values $g_0 = e^{-v\Delta}g_1$ and $g_{N+1} = e^{v\Delta}g_N$ extend the original interval $[a,b]$ to $[a-\Delta, b+\Delta]$ so that we have well defined the second order derivatives at all the points of the initial partition, including the edges of the interval. When $g(x)$ is the exponential function, we have $g_0 = e^{v(x_1-\Delta)}$ and $g_{N+1} = e^{v(x_N+\Delta)}$, i.e., they are the values of the exponential function evaluated at the points of the extension.

Thus, we define finite differences derivatives for any function $g(x)$ defined on the partition as

$$(\mathrm{D}g)_1 = \frac{g_2 - e^{-v\Delta}g_1}{2\chi(v,\Delta)}, \tag{22}$$

$$(\mathrm{D}g)_j = \frac{g_{j+1} - g_{j-1}}{2\chi(v,\Delta)}, \tag{23}$$

$$(\mathrm{D}g)_N = \frac{e^{v\Delta}g_N - g_{N-1}}{2\chi(v,\Delta)}, \tag{24}$$

to be used on the first, central, and last points of the partition.

The determinant of the derivative matrix is not always zero, and in fact, it is [see Eqs. (4) and (9)]

$$|\overline{\mathbf{D}}_N| = 2\sinh(v\Delta)F_N(0). \tag{25}$$

But, since $F_{2j+1} = 1$, and $F_{2j} = 0$, then

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$$|\overline{\mathbf{D}}_{2j}| = 0, \quad |\overline{\mathbf{D}}_{2j+1}| = 2\sinh(v\Delta). \tag{26}$$

Hence, only the matrices with an odd dimension have an inverse.

Next, we will derive some properties of these finite differences derivatives.

3.1. The derivative of a product of vectors

There are two equivalent expressions for the finite differences derivative of a product of vectors defined on the partition. A set of such expressions is

$$\begin{aligned}(\mathrm{D}gh)_1 &= \frac{g_2h_2 - e^{-v\Delta}g_1h_1}{2\chi(v,\Delta)}\\ &= \frac{g_2h_2 - e^{-v\Delta}g_1h_2}{2\chi(v,\Delta)} + g_1\frac{e^{-v\Delta}h_2 - h_2 + h_2 - e^{-v\Delta}h_1}{2\chi(v,\Delta)}\\ &= h_2(\mathrm{D}g)_1 + g_1(\mathrm{D}h)_1 + g_1h_2\frac{e^{-v\Delta}-1}{2\chi(v,\Delta)}\\ &= h_2(\mathrm{D}g)_1 + g_1(\mathrm{D}h)_1 + g_1h_2\left[-\frac{v}{2} + \frac{v^2}{4}\Delta + O\left(\Delta^3\right)\right],\end{aligned} \tag{27}$$

$$(\mathrm{D}gh)_j = h_{j+1}(\mathrm{D}g)_j + g_{j-1}(\mathrm{D}h)_j, \tag{28}$$

$$\begin{aligned}(\mathrm{D}gh)_N &= h_N(\mathrm{D}g)_N + g_{N-1}(\mathrm{D}h)_N + \frac{1-e^{v\Delta}}{2\chi(v,\Delta)}g_{N-1}h_N\\ &\approx h_N(\mathrm{D}g)_N + g_{N-1}(\mathrm{D}h)_N + g_{N-1}h_N\left[-\frac{v}{2} - \frac{v^2}{4}\Delta + O\left(\Delta^3\right)\right].\end{aligned} \tag{29}$$

A second set of equalities is

$$\begin{aligned}(\mathrm{D}gh)_1 &= g_2(\mathrm{D}h)_1 + h_1(\mathrm{D}g)_1 + g_2h_1\frac{e^{-v\Delta}-1}{2\chi(v,\Delta)}\\ &= g_2(\mathrm{D}h)_1 + h_1(\mathrm{D}g)_1 + g_2h_1\left[-\frac{v}{2} + \frac{v^2}{4}\Delta + O\left(\Delta^3\right)\right],\end{aligned} \tag{30}$$

$$(\mathrm{D}gh)_j = g_{j+1}(\mathrm{D}h)_j + h_{j-1}(\mathrm{D}g)_j, \tag{31}$$

$$\begin{aligned}(\mathrm{D}gh)_N &= g_N(\mathrm{D}h)_N + h_{N-1}(\mathrm{D}g)_N + g_Nh_{N-1}\frac{1-e^{v\Delta}}{2\chi(v,\Delta)}\\ &\approx g_N(\mathrm{D}h)_N + h_{N-1}(\mathrm{D}g)_N + g_Nh_{N-1}\left[-\frac{v}{2} - \frac{v^2}{4}\Delta + O\left(\Delta^3\right)\right],\end{aligned} \tag{32}$$

3.2. Summation by parts

The sum of Eqs. (28) or (31), with weights $2\chi(v,\Delta)$, results in

$$\begin{aligned}&\sum_{j=n}^{m}2\chi(v,\Delta)h_{j+1}(\mathrm{D}g)_j+\sum_{j=n}^{m}2\chi(v,\Delta)g_{j-1}(\mathrm{D}h)_j\\&=\sum_{j=n}^{m}2\chi(v,\Delta)(\mathrm{D}gh)_j\\&=g_{m+1}h_{m+1}+g_mh_m-g_nh_n-g_{n-1}h_{n-1},\end{aligned}\tag{33}$$

or

$$\begin{aligned}&\sum_{j=n}^{m}2\chi(v,\Delta)g_{j+1}(\mathrm{D}h)_j+\sum_{j=n}^{m}2\chi(v,\Delta)h_{j-1}(\mathrm{D}g)_j\\&=g_{m+1}h_{m+1}+g_mh_m-g_nh_n-g_{n-1}h_{n-1}.\end{aligned}\tag{34}$$

This is the discrete version of the integration by parts theorem for continuous variable functions, a very useful result.

3.3. Second derivatives

Expressions for higher order derivatives are obtained through the powers of $\mathbf{D}_N$. For instance, for the first two points, the second derivative is

$$\left(\mathrm{D}^2g\right)_1=\frac{\left(e^{-2v\Delta}-1\right)g_1-e^{-v\Delta}g_2+g_3}{4\chi^2(v,\Delta)}=\frac{(\mathrm{D}g)_2-e^{-v\Delta}(\mathrm{D}g)_1}{2\chi(v,\Delta)},\tag{35}$$

$$\left(\mathrm{D}^2g\right)_2=\frac{e^{-v\Delta}g_1-2g_2+g_4}{4\chi^2(v,\Delta)}=\frac{(\mathrm{D}g)_3-(\mathrm{D}g)_1}{2\chi(v,\Delta)},\tag{36}$$

For inner points we get

$$\left(\mathrm{D}^2g\right)_j=\frac{g_{j-2}-2g_j+g_{j+2}}{4\chi^2(v,\Delta)}=\frac{(\mathrm{D}g)_{j+1}-(\mathrm{D}g)_{j-1}}{2\chi(v,\Delta)},\quad 3\le j\le N-3,\tag{37}$$

and for the last two points of the mesh, we find

$$\left(\mathrm{D}^2g\right)_{N-1}=\frac{g_{N-3}-2g_{N-1}+e^{v\Delta}g_N}{4\chi^2(v,\Delta)}=\frac{(\mathrm{D}g)_N-(\mathrm{D}g)_{N-2}}{2\chi(v,\Delta)},\tag{38}$$

$$\begin{aligned}\left(\mathrm{D}^2g\right)_N&=\frac{g_{N-2}-e^{v\Delta}g_{N-1}+\left(e^{2v\Delta}-1\right)g_N}{4\chi^2(v,\Delta)}\\&=\frac{e^{v\Delta}(\mathrm{D}g)_N-(\mathrm{D}g)_{N-1}}{\chi_2(v,2\Delta)}.\end{aligned}\tag{39}$$

These derivatives also have the exponential function as one of their eigenvectors, and we can generate expressions for higher derivatives with higher powers of the derivative matrix.

3.4. The derivative of the inverse of functions

It is possible to give an expression for the derivative of $h^{-1}(q)$, including the edge points. For the first point, we have

$$\begin{aligned}\left(\mathrm{D}\frac{1}{h}\right)_1 &= \frac{1}{2\chi(v,\Delta)}\left(\frac{1}{h_2}-\frac{e^{-v\Delta}}{h_1}\right)\\ &= \frac{1}{2\chi(v,\Delta)}\left(-\frac{h_2-h_1}{h_1h_2}+\frac{1-e^{-v\Delta}}{h_1}\right)\\ &= -\frac{(\mathrm{D}h)_1}{h_1h_2}+\frac{1-e^{-v\Delta}}{2\chi(v,\Delta)}\left(\frac{1}{h_1}+\frac{1}{h_2}\right).\end{aligned} \tag{40}$$

For central and last points, we find that

$$\left(\mathrm{D}\frac{1}{h}\right)_j = -\frac{(\mathrm{D}h)_j}{h_{j-1}h_{j+1}}, \tag{41}$$

$$\left(\mathrm{D}\frac{1}{h}\right)_N = -\frac{(\mathrm{D}h)_N}{h_{N-1}h_N}+\frac{e^{v\Delta}-1}{2\chi(v,\Delta)}\left(\frac{1}{h_{N-1}}+\frac{1}{h_N}\right). \tag{42}$$

The derivatives for the first and last points coincide with the derivative for central points when $\Delta = 0$.

3.5. The derivative of the ratio of functions

Now, we take advantage of the derivative for the inverse of a function and the derivative of a product of functions and obtain what the derivative of a ratio of functions is

$$\begin{aligned}\left(\mathrm{D}\frac{g}{h}\right)_1 &= \frac{1}{h_2}(\mathrm{D}g)_1+g_1\left(\mathrm{D}\frac{1}{h}\right)_1+\frac{g_1}{h_2}\frac{e^{-v\Delta}-1}{2\chi(v,\Delta)}\\ &= \frac{1}{h_2}(\mathrm{D}g)_1+g_1\left[-\frac{(\mathrm{D}h)_1}{h_1h_2}+\frac{1}{2\chi(v,\Delta)}\left(\frac{1}{h_1}+\frac{1-e^{-v\Delta}}{h_2}\right)\right]+\frac{g_1}{h_2}\frac{e^{-v\Delta}-1}{2\chi(v,\Delta)}\\ &= \frac{1}{h_2}(\mathrm{D}g)_1-\frac{g_1}{h_1h_2}(\mathrm{D}h)_1+\frac{g_1}{h_1}\frac{1-e^{-v\Delta}}{2\chi(v,\Delta)},\end{aligned} \tag{43}$$

$$\left(\mathrm{D}\frac{g}{h}\right)_j = \frac{(\mathrm{D}g)_j}{h_{j-1}}-g_{j+1}\frac{(\mathrm{D}h)_j}{h_{j+1}h_{j-1}}, \tag{44}$$

$$\left(\mathrm{D}\frac{g}{h}\right)_N = \frac{1}{h_N}(\mathrm{D}g)_N-\frac{g_{N-1}}{h_{N-1}h_N}(\mathrm{D}h)_N+\frac{g_{N-1}}{h_{N-1}}\frac{e^{v\Delta}-1}{2\chi(v,\Delta)}, \tag{45}$$

expressions which are very similar to the continuous variable results. Again, these expressions coincide in the limit $\Delta \to 0$, and they reduce to the corresponding expressions for continuous variables.

3.6. The local inverse operation of the derivative

The inverse operation to the finite differences derivative, at a given point, is the summation with weights $2\chi(v, \Delta)$

$$\sum_{j=n}^{m} 2\chi(v,\Delta)(\mathrm{D}g)_j = \sum_{j=n}^{m} \left(g_{j+1} - g_{j-1}\right) = g_{m+1} + g_m - g_n - g_{n-1}. \tag{46}$$

This equality is the equivalent to the usual result for continuous functions, $\int_a^x dy(dg(y)/dy) = g(x) - g(a)$. Note that the inverse at the local level is a bit different from the expressions obtained by means of the inverse matrix **S** (see below) of the derivative matrix **D**. When dealing with matrices there are no boundary terms to worry about.

3.7. An eigenfunction of the summation operation

Because the exponential function is an eigenfunction of the finite differences derivative and according to Eq. (46), we can say that

$$\begin{aligned}\sum_{j=n}^{m} 2\chi(v,\Delta) v e^{vq_j} = \sum_{j=n}^{m} 2\chi(v,\Delta)(\mathrm{D}e^{vq})_j = \sum_{j=n}^{m} (e^{vq_{j+1}} - e^{vq_{j-1}}) \\ = e^{vq_{m+1}} + e^{vq_m} - e^{vq_n} - e^{vq_{n-1}},\end{aligned} \tag{47}$$

in agreement with the corresponding continuous variable equality $\int_a^x dx v e^{vx} = e^{vx} - e^{va}$. However, here, we have to deal with two values at each boundary.

3.8. The chain rule

The chain rule also has a finite differences version. That version is

$$\begin{aligned}(\mathrm{D}g(h(q)))_j &= \frac{g\left(h\left(q_{j+1}\right)\right) - g\left(h\left(q_{j-1}\right)\right)}{2\chi(v,\Delta)} \\ &= \frac{g\left(h\left(q_{j+1}\right)\right) - g\left(h\left(q_{j-1}\right)\right)}{2\chi\left(v, h\left(q_{j+1}\right) - h\left(q_j\right)\right)} \frac{2\chi\left(v, h\left(q_{j+1}\right) - h\left(q_j\right)\right)}{2\chi(v,\Delta)} \\ &= (Dg(h))_j \frac{\chi\left(v, h\left(q_{j+1}\right) - h\left(q_j\right)\right)}{\chi(v,\Delta)}\end{aligned} \tag{48}$$

where

$$(Dg(h))_j := \frac{g\left(h\left(q_{j+1}\right)\right) - g\left(h\left(q_{j-1}\right)\right)}{2\chi\left(v, h\left(q_{j+1}\right) - h\left(q_j\right)\right)} \tag{49}$$

is a finite differences derivative of $g(h)$ with respect to h, and the second factor approaches the derivative of $h(q)$ with respect to q

$$\frac{\chi\left(v, h\left(q_{j+1}\right) - h\left(q_j\right)\right)}{\chi(v,\Delta)} \approx \frac{h\left(q_{j+1}\right) - h\left(q_j\right) + O(\Delta h^2)}{\Delta + O(\Delta^2)}. \tag{50}$$

Thus, we will recover the usual chain rule for continuous variable functions in the limit $\Delta \to 0$.

4. The commutator between coordinate and derivative

Let us determine the commutator, from a local point of view first, between the coordinate—the points of the partition $P(N)$—and the finite differences derivative. We begin with the derivative of q,

$$(\mathrm{D}q)_j = \frac{q_{j+1} - q_{j-1}}{2\chi(v,\Delta)} = \frac{\Delta}{\chi(v,\Delta)} \approx 1 - \frac{v^2}{6}\Delta^2. \tag{51}$$

Hence, the finite differences derivative of the product $qg(q)$ is

$$(\mathrm{D}qg)_j = q_{j+1}(\mathrm{D}g)_j + g_{j-1}(\mathrm{D}q)_j = q_{j+1}(\mathrm{D}g)_j + g_{j-1}\frac{\Delta}{\chi(v,\Delta)}, \tag{52}$$

i.e.,

$$(\mathrm{D}_c qg)_j - q_{j+1}(\mathrm{D}_c g)_j = g_{j-1}\frac{\Delta}{\chi(v,\Delta)}. \tag{53}$$

This is the finite differences version of the commutator between the coordinate q and the finite differences derivative D. This equality will become the identity operator in the small Δ limit, as expected. An equivalent expression is

$$(\mathrm{D}qg)_j - q_{j-1}(\mathrm{D}g)_j = g_{j+1}\frac{\Delta}{\chi(v,\Delta)}. \tag{54}$$

This is the finite differences version of the commutator between coordinate and derivative; the right hand side of this equality becomes g_j in the small Δ limit, i.e., it becomes the identity operator.

4.1. The commutator between the derivative and coordinate matrices

The commutator between the partition and the finite differences derivative can also be calculated from a global point of view using the corresponding matrices. Let the diagonal matrix $[\mathbf{Q}_N]$ which will represent the coordinate partition

$$\mathbf{Q}_N{:=}\mathrm{diag}\left(q_1, q_2, \dots, q_N\right). \tag{55}$$

Then, the commutator between the derivative matrix and the coordinate matrix is

$$[\mathbf{D}_N, \mathbf{Q}_N] = \frac{\Delta}{2\chi(v,\Delta)}\begin{pmatrix} 0 & 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & \dots & 0 & 0 & 0 \\ \vdots & & & & & & & \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & \dots & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix}. \tag{56}$$

This is a kind of nearest neighbors' average operator, inside the interval. The small Δ limit is just

$$[\mathbf{D}_N, \mathbf{Q}_N] \approx I, \tag{57}$$

where $\mathbf{I}$ is the identity matrix, with the first and last elements replace with 1/2. Thus, coordinate and derivative matrices are finite differences conjugate of each other.

5. An integration matrix

Since the determinant of the derivative matrix $\mathbf{D}_N$ is not always zero, we expect that there exist an inverse of it. At a local level, the inverse of the finite differences derivation is the summation as was found in Eq. (46). In this section, we determine the inverse of the derivative matrix, and we find that it is a global finite difference integration operation.

Once we know the eigenvalues and eigenvectors of the derivative matrix $\mathbf{D}_N$, it turns out that we also know the eigenvectors and eigenvalues of the inverse matrix, when it exists. In fact, the equality $\mathbf{D}_N\mathbf{e}_m = \lambda_m\mathbf{e}_m$, with $\lambda_m \neq 0$, imply that

$$\mathbf{D}_N^{-1}\mathbf{e}_m = \lambda_m^{-1}\mathbf{e}_m. \tag{58}$$

The inverse matrix $\mathbf{S}_N = \mathbf{D}_N^{-1}$ is

$$\mathbf{S}_N = \frac{1}{z-\frac{1}{z}}\begin{pmatrix} 1 & -z & 1 & -z & 1 & \dots & -z & 1 \\ z & -1 & 1/z & -1 & 1/z & \dots & -1 & 1/z \\ 1 & -1/z & 1 & -z & 1 & \dots & -z & 1 \\ z & -1 & z & -1 & 1/z & \dots & -1 & 1/z \\ \vdots & & & & & & & \\ 1 & -1/z & 1 & -1/z & 1 & \dots & -z & 1 \\ z & -1 & z & -1 & z & \dots & -1 & 1/z \\ 1 & -1/z & 1 & -1/z & 1 & \dots & -1/z & 1 \\ z & -1 & z & -1 & z & \dots & -1 & 1/z \\ 1 & -1/z & 1 & -1/z & 1 & \dots & -1/z & 1 \end{pmatrix}, \tag{59}$$

Its determinant is

$$|\mathbf{S}_N| = \sinh^{N-1}(v\Delta). \tag{60}$$

This matrix represents an integration on the partition, with an exact value when it is applied to the exponential function e^{vq} on the partition. When applied to an arbitrary vector $\mathbf{g} = (g_1, g_2, \dots, g_N)^T$, we obtain formulas for the finite differences integration, including the edge points

$$(\mathbf{S}_N\mathbf{g})_1 = \frac{1}{z-1/z}\left[g_1 + \sum_{i=1}^{M}(g_{2i+1} - zg_{2i})\right], \tag{61}$$

$$(\mathbf{S}_N\mathbf{g})_{2j} = \frac{1}{z-1/z}\left[zg_1 + \sum_{k=1}^{j-1}(zg_{2k+1} - g_{2k}) + \sum_{k=j}^{M}\left(\frac{g_{2k+1}}{z} - g_{2k}\right)\right], \tag{62}$$

$$(\mathbf{S}_N\mathbf{g})_{2j+1} = \frac{1}{z-1/z}\left[g_1 + \sum_{k=1}^{j}\left(g_{2k+1} - \frac{g_{2k}}{z}\right) + \sum_{k=j+1}^{M}(g_{2k+1} - zg_{2k})\right], \tag{63}$$

$$(\mathbf{S}_N\mathbf{g})_N = \frac{1}{z-1/z}\left[g_1 + \sum_{i=1}^{M}\left(g_{2i+1} - \frac{g_{2i}}{z}\right)\right], \tag{64}$$

where $N = 2M + 1$. These are new formulas for discrete integration for the exponential function on a partition of equally separated points with the characteristic that it is exact for the exponential function e^{vq}.

6. Transformation between coordinate and derivative representations

Since one of the eigenvalues of the derivative matrix is a continuous variable, we can talk of conjugate functions with a continuous argument v. The relationship between discrete vectors on a partition $\{q_i\}$ and functions with a continuous argument v makes use of continuous and discrete Fourier type of transformations, a wavelet [12]. If we have a function h of continuous argument v, a conjugate vector on the partition $\{q_i\}$ is defined through the type of continuous Fourier transform F as

$$(Fh)\left(q_j\right) := \frac{1}{L\sqrt{2\Delta}} \int_{-L/2}^{L/2} e^{-iq_j v} h(v) dv, \tag{65}$$

and vice-versa, a continuous variable function is defined with the help of a discrete type of Fourier transform F as

$$(\mathrm{F}g)(v) := \frac{L}{\sqrt{2\Delta}} \sum_{j=-N+1}^{N-1} 2\chi(v,\Delta) e^{iq_j v} g_j. \tag{66}$$

Assuming that the involved integrals converge absolutely, we can say that

$$\begin{aligned} F(\mathrm{F}g)\left(q_j\right) &:= \frac{1}{L\sqrt{2\Delta}} \int_{-L/2}^{L/2} e^{-iq_j v} \frac{L}{\sqrt{2\Delta}} \sum_{k=-N+1}^{N-1} 2\chi(v,\Delta) e^{iq_k v} g_k dv \\ &= \frac{1}{\Delta} \sum_{k=-N+1}^{N-1} g_k \int_{-L/2}^{L/2} e^{i\left(q_k - q_j\right)v} \sinh(v\Delta) \frac{dv}{v} \\ &= \sum_{k=-N+1}^{N-1} g_k K\left(q_k - q_j, L, \Delta\right). \end{aligned} \tag{67}$$

where

$$\begin{aligned} K\left(q_k - q_j, L, \Delta\right) &:= \frac{1}{\Delta} \int_{-L/2}^{L/2} e^{i\left(q_k - q_j\right)v} \sinh(v\Delta) \frac{dv}{v} \\ &= \frac{1}{2\Delta} \left\{ \mathrm{shi}\left[\frac{L}{2}\left(i\left(q_k - q_j\right) + \Delta\right)\right] + i\,\mathrm{shi}\left[\frac{L}{2}\left(q_k - q_j - i\Delta\right)\right] - 2i\,\mathrm{shi}\left[\frac{L}{2}\left(q_k - q_j + i\Delta\right)\right]\right\}. \end{aligned} \tag{68}$$

The function $K\left(q_k - q_j, L, \Delta\right)$ is an approximation to the Kronecker delta function $\delta_{k,j}$. The function shi is the hyperbolic sine integral $\mathrm{shi}(z) = \int_0^z dt \sinh(t)/t$. A plot of it is shown in **Figure 1**.

Additionally,

$$\begin{aligned} \mathrm{F}(Fh)(v) &= \frac{L}{\sqrt{2\Delta}} \sum_{j=-N+1}^{N-1} 2\chi(v,\Delta) e^{iq_j v} \frac{1}{L\sqrt{2\Delta}} \int_{-L/2}^{L/2} e^{-iq_j u} h(u) du \\ &= \int_{-L/2}^{L/2} du\, h(u) J(v-u, N), \end{aligned} \tag{69}$$

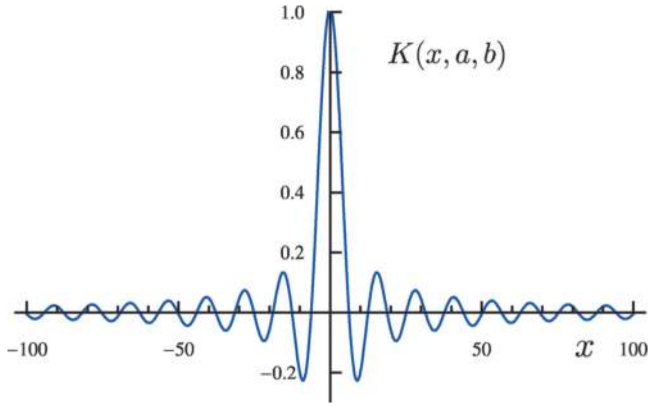

Figure 1. A plot of the kernel function $K(x, a, b)$ with $a = 1$ and $b = .1$. This function is an approximation to the Kronecker delta $\delta_{x,0}$.

where

$$J(x, N) := \frac{2\chi(v, \Delta)}{\Delta} \sum_{j=-N+1}^{N-1} e^{i q_j (v-u)} = \frac{2\chi(v, \Delta)}{\Delta} \sum_{j=-N+1}^{N-1} e^{i j (v-u)\Delta} = \frac{2\chi(v, \Delta)}{\Delta} \frac{\sin((N - 1/2)(v - u)\Delta)}{\sin((v - u)\Delta/2)}, \tag{70}$$

The ratio of sin functions, in this expression, is an approximation to a series of Dirac delta functions located at $(v - u)\Delta = k\pi$, $k \in \mathbb{N}$. Thus, the operations F and F are finite differences inverse of each other.

6.1. The discrete Fourier transform of the finite differences derivative of a vector

Next, based on Eq. (28), we find that

$$\begin{aligned} \left(\mathrm{D}e^{-iqv} g\right)_j &= g_{j+1} \left(\mathrm{D}e^{-iqv}\right)_j + e^{-iq_{j-1}v} (\mathrm{D}g)_j \\ &= -iv g_{j+1} e^{-iq_j v} + e^{-iq_{j-1}v} (\mathrm{D}g)_j. \end{aligned} \tag{71}$$

If we sum this equality, we get

$$\begin{aligned} \sum_{j=-N+1}^{N-1} 2\chi(v, \Delta) \left(De^{-iqv} g\right)_j &= -iv \sum_{j=-N+1}^{N-1} 2\chi(v, \Delta) g_{j+1} e^{-iq_j v} \\ &+ \sum_{j=-N+1}^{N-1} 2\chi(v, \Delta) e^{-iq_{j-1}v} (Dg)_j \end{aligned} \tag{72}$$

i.e.,

$$(\mathrm{F}_N(Dg))(v) = iv(\mathrm{F}_{N+1}g)(v) + e^{-iv\Delta}\left[e^{-iq_jv} g_j \Big|_{j=-N+2}^{N} + \frac{\sqrt{2}}{L} e^{-iq_jv} g_j \Big|_{j=-N+1}^{N-1} \right] \tag{73}$$

Therefore, the discrete Fourier transform of the derivative of a vector **g** is iv times the discrete Fourier transform of **g**, plus boundary terms.

The Fourier transform of the derivative of a continuous function of variable v is easily found if we consider the equality

$$\frac{d}{dv} e^{-iq_jv} = -iq_j e^{-iq_jv}. \tag{74}$$

The integration of this equality with appropriate weights gives

$$-iq_j \int_{-L/2}^{L/2} dv\, e^{-iq_jv} h(v) = -\int_{-L/2}^{L/2} dv\, e^{-iq_jv} \frac{dh(v)}{dv} + e^{-iq_jv} h(v) \Big|_{v=-L/2}^{L/2}, \tag{75}$$

i.e.,

$$(Fh')_j = iq_j (Fh)_j + \frac{1}{L\sqrt{2}} e^{-iq_jv} h(v) \Big|_{v=-L/2}^{L/2}. \tag{76}$$

Hence, as is usual, the Fourier transform of the derivative of a function $h(v)$ of continuous variable v is equal to iq_j times the Fourier transform of the function, plus boundary terms.

7. Conclusion

We proceed with a brief discussion of the relationship between the derivative matrix $\mathbf{D}_N$ and an important concept in quantum mechanics; the concept of *self-adjoint operators* [8, 9]. In particular, we focus on the momentum operator, whose continuous coordinate representation (operation) is given by $-id/dq$, i.e., a derivative times $-i$, in the case of infinite-dimensional Hilbert space.

In the finite-dimensional complex vectorial space (where each vector define a sequence $\{g_i\}_{i=1}^{N}$ of complex numbers such that $\sum_i |g_i|^2 < \infty$). A transformation **A** is usually called *Hermitian*, when its entries $a_{i,j}$ are such that $a_{i,j} = a^*_{j,i}$ (* denote the complex conjugate). Our matrix $\mathbf{D}_N$ is related to an approximation of the derivative (see Section 3) which uses second order finite differences. Therefore, we can ask if the matrix $-i\mathbf{D}_N$ is also Hermitian.

Let $\mathbf{P}_N = -i\mathbf{D}_N$ and $v = ix$ be the eigenvalue of $\mathbf{D}_N$, where $x \in \mathbb{R}$ is a free parameter, the corresponding eigenvalue of $-i\mathbf{D}_N$ is indeed the real value x; which is one of the properties of a Hermitian matrix, as is also the case of infinite-dimensional space (for the Hilbert space on a finite interval, these values are discrete, and for the Hilbert space on the real line, these values conform the continuous spectrum, instead of discrete eigenvalues). Other characteristic of $-i\mathbf{D}_N$ is that the eigenvector corresponding to x is the same exponential function which is the eigenfunction of $-id/dx$ (see Section 2).

Furthermore, let $\mathbf{P}_N^\dagger$ denote the adjoint of $\mathbf{P}_N$. Thus, if we restrict our attention to the off-diagonal entries $(\mathbf{P}_N)_{i,j} = -i(\mathbf{D}_N)_{i,j}$, it is fulfilled that $\left(\mathbf{P}_N^\dagger\right)_{i,j} = \left(-id_{j,i}\right)^* = -id_{i,j} = (\mathbf{P}_N)_{i,j}$ (noticing that, with $v = ix$ then $\chi(x, \Delta) = \sin(x, \Delta)/x \in \mathbb{R}$). Even more, if we do not care about the two entries $d_{i,i}$ for $i = 1, N$, we will have a Hermitian matrix. Finally, as it was seen in Section 4, we can say that $\mathbf{P}_N$ can be considered as a suitable approximation to the conjugate matrix to the coordinate matrix.

In conclusion, we have introduced a matrix with the properties that a Hermitian matrix should comply with, except for two of its entries. Besides, our partition provides congruency between discrete, continuous, and matrix treatments of the exponential function and of its properties.

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