A discrete quantum momentum operator

Subjects: Physics, Mathematical | Others
Contributor: Gabino Torres-Vega

We introduce finite-differences derivatives intended to be exact when applied to the real exponential function. We want to recover the known results of continuous calculus with our finite differences derivatives but in a discrete form. The purpose of this work is to have a discrete momentum operator suitable for use as an operator in discrete quantum mechanics theory.

Keywords: discrete derivative ; discrete symmetric operator, ; discrete quantum mechanics

Introduction

The subject of finite differences is an old, but useful method with wide application in science and engineering. The story starts with Newton and Leibnitz themselves with the very definition of the derivative of a function; the limit when the differences become zero, as is well known. The formal definition of the derivative $f'(x_0)$ of some function $f(x)$ of a single variable x, at x_0, is obtained from the limit $x \to x_0$ of any of the following ratios of differences

$$f'(x_0) := \lim_{x \to x_0^-} \frac{f(x_0) - f(x)}{x_0 - x}, \quad f'(x_0) := \lim_{x \to x_0^+} \frac{f(x) - f(x_0)}{x - x_0}.$$

These ratios are known as backward and forward differences, respectively.

The limit of vanishing finite differences involves variables which are continuous. However, many times it is not possible to perform such limit at all. A situation like that appears when doing numerical simulations in a computer due to the limit in how small a number can be represented in the computer. Another situation in which it is not possible to take the infinitesimal difference limit is when the independent variable is a discrete variable by nature, as is the case found in Quantum Mechanics theory regarding the spectrum of quantum operators.

Finite differences are necessary in numerical computations to approximate several quantities like derivatives and integrals of functions, as well as, differential and integral equations. Their use as a numerical tool is a well developed subject, see for instance the series of books *Numerical Recipes.*[1] An interesting development is the use of a complex finite differences to evaluate the real derivative of a function.[2]

On the other hand, the reader can learn about the calculus of finite differences from the classical works of Kopal[3], Boole[4]. Jordan[5], Richardson[6], for instance.

Another branch of the finite differences tree, is known as the exact finite differences technique. That scheme was developed by researchers like Potts,[7][8] Ronald E. Mickens[9] with the purpose of obtaining exact finite differences representations of continuous differential equations and of their solutions.

Another use of finite differences was developed by Armando Martínez-Pérez and Gabino Torres-Vega[10] with the intention of obtaining discrete operators for use in Quantum Mechanics theory. It is common that a quantum operator has a discrete spectrum and a derivative with respect to the spectrum is necessary some times. The aim is to obtain discrete operators which comply with discrete versions of the properties that a quantum operator must have.

The explicit form of the exact finite difference derivative depends on the functions that we want to consider. In this article, we discuss the use of an exact finite differences derivative when its eigenfunction is the real exponential function. This will provide with a momentum operator to be used in discrete Quantum Mechanics.

The partition

Let $\{q_i\}_{i=-N}^{N}$ be a $N+1$ points partition of the real interval $[-a,a]$, that is

$$-a = q_{-N} < q_{-N+1} < \cdots < q_{N-1} < q_N = a.$$

The separations between mesh points are

$$\Delta_j = q_{j+1} - q_j, \quad j = -N, \ldots, N-1.$$

These separations can or cannot be equal and are finite. The discrete variable q_j is the independent variable with respect to we will calculate the derivative of a function.

The exact finite differences derivative

For a given $v \in \mathbb{R}$, backward and forward finite differences derivatives, of a vector $g = (g_{-N}, g_{-N+1}, \ldots, g_{N-1}, g_N)^T$, at q_j, defined on the partition, are

$$(D_b g)_j = \frac{g_j - g_{j-1}}{\eta_j},$$

$$(D_f g)_j = \frac{g_{j+1} - g_j}{\chi_j},$$

where the denominators are defined as

$$\eta_j = \frac{2}{v}\, e^{-v\Delta_{j-1}/2} \sinh\left(\frac{v}{2}\Delta_{j-1}\right) = \Delta_{j-1} + \frac{v}{2}\Delta_{j-1}^2 + \mathcal{O}(\Delta_j^3),$$

$$\chi_j = \frac{2}{v}\, e^{v\Delta_j/2} \sinh\left(\frac{v}{2}\Delta_j\right) = \Delta_j + \frac{v}{2}\Delta_j^2 + \mathcal{O}(\Delta_j^3).$$

The discrete variable q_j is the independent variable with respect to which we will calculate the derivative of a function. The functions in the denominators of these expressions, the functions η_j and χ_j, makes sure that the real exponential function e^{vq} be, exactly, an eigenfunction of the discrete derivative operation with real eigenvalue v,

$$(D_b e^{vq})_j = (D_f e^{vq})_j = v\, e^{vq_j},$$

which is the same property as the continuous variable derivative has.

When $|\eta_j - \Delta_j|$ and $|\chi_j - \Delta_j|$ are less than some small ϵ, our method and the usual finite-differences derivative give similar results for any vector defined on the mesh. Note that the denominators η_j and χ_j become Δ_j when $v=0$.

Properties of the finite-differences derivative

Some properties of the exact finite-differences derivative are

The *connection between forward and backward discrete derivatives.* The equality $\eta_{j+1} = e^{-v\Delta_j}\chi_j$ implies that

$$(D_f g)_j = e^{-v\Delta_j}\,(D_b g)_{j+1}.$$

The summation of the derivative. The finite differences versions of $\int_a^x dy\, g'(y) = g(x) - g(a)$ are

$$\sum_{j=-N}^{n} \Delta_j (D_f g)_j = -\frac{\Delta_{-N}}{\chi_{-N}} g_{-N} + \sum_{j=-N+1}^{n} \left(\frac{\Delta_{j-1}}{\chi_{j-1}} - \frac{\Delta_j}{\chi_j}\right) g_j + \frac{\Delta_n}{\chi_n} g_{n+1},$$

and $\sum_{j=-N+1}^{n} \Delta_{j-1}(D_b g)_j = -\frac{\Delta_{-N}}{\eta_{-N+1}} g_{-N} + \sum_{j=-N+1}^{n-1} \left(\frac{\Delta_{j-1}}{\eta_j} - \frac{\Delta_j}{\eta_{j+1}}\right) g_j + \frac{\Delta_{n-1}}{\eta_n} g_n,$

where $n<N$. The summation term at the right hand side of these equalities involve asymmetry terms that vanish when the

separation between mesh points is the same.

The eigenfunction of the summation. The finite differences versions of $\int_a^x dx\, v\, e^{vx} = e^{vx} - e^{va}$ are

$$\sum_{j=-N}^{n} \Delta_j v\, e^{vq_j} = \sum_{j=-N}^{n} \Delta_j (D_f\, e^{vq})_j = -\frac{\Delta_{-N}}{\chi_{-N}} e^{vq_{-N}} + \sum_{-N+1}^{n} \left(\frac{\Delta_{j-1}}{\chi_{j-1}} - \frac{\Delta_j}{\chi_j} \right) e^{vq_j} + \frac{\Delta_n}{\chi_n} e^{vq_{n+1}},$$

and

$$\sum_{j=-N+1}^{n} \Delta_{j-1} v\, e^{vq_j} = \sum_{j=-N+1}^{n} \Delta_{j-1} (D_b\, e^{vq})_j = -\frac{\Delta_{-N}}{\eta_{-N+1}} e^{vq_{-N}} + \sum_{j=-N+1}^{n-1} \left(\frac{\Delta_{j-1}}{\eta_j} - \frac{\Delta_j}{\eta_{j+1}} \right) e^{vq_j} + \frac{\Delta_{n-1}}{\eta_n} e^{vq_n},$$

where $-N<n<N$.

The derivative of a constant function c.

$$(D_f\, c)_j = 0, \quad \text{and} \quad (D_b\, c)_j = 0.$$

The derivatives of q.

$$(D_f\, q)_j = \frac{q_{j+1} - q_j}{\chi_j} = \frac{\Delta_j}{\chi_j}, \quad \text{and} \quad (D_b\, q)_j = \frac{q_j - q_{j-1}}{\eta_j} = \frac{\Delta_{j-1}}{\eta_j}.$$

These derivatives will approach to one in the limit of small Δ_j. In particular, both $(D_f\, q)_j$ and $(D_b\, q)_j$ are equal to one when $v = 0$.

The chain rule. For the forward scheme this rule turns to be

$$(D_f g(h(q)))_j = (\mathcal{D}_f g(h))_j\, (D_f h)_j,$$

where

$$(\mathcal{D}_f g(h))_j = \frac{g(h(q_{j+1})) - g(h(q_j))}{h(q_{j+1}) - h(q_j)}.$$

For the backward finite differences we have

$$(D_b g(h(q)))_j = (\mathcal{D}_b g(h))_j\, (D_b h)_j,$$

where

$$(\mathcal{D}_b g(h))_j = \frac{g(h(q_j)) - g(h(q_{j-1}))}{h(q_j) - h(q_{j-1})}.$$

The derivative of a product of vectors. There are four equalities

$$\begin{aligned}
(D_f\, gh)_j &= g_{j+1}(D_f h)_j + (D_f g)_j h_j.\,, \\
(D_f\, gh)_j &= (D_f g)_j h_{j+1} + g_j (D_f h)_j, \\
(D_b\, gh)_j &= g_j (D_b h)_j + (D_b g)_j h_{j-1}, \\
(D_b\, gh)_j &= (D_b g)_j h_j + g_{j-1} (D_b h)_j.
\end{aligned}$$

The derivative of a vector of inverses.

$$\left(D_f\, \frac{1}{h} \right)_j = -\frac{(D_f h)_j}{h_j h_{j+1}}, \quad \text{and} \quad \left(D_b\, \frac{1}{h} \right)_j = -\frac{(D_b h)_j}{h_j h_{j-1}},$$

provided $h_j, h_{j\pm 1} \neq 0$.

The derivative of a vector of ratios. There are four versions of this property

$$\left(D_f\, \frac{g}{h} \right)_j = \frac{(D_f\, g)_j}{h_j} - \frac{(D_f h)_j}{h_j h_{j+1}} g_{j+1},$$

$$\left(D_f\, \frac{g}{h} \right)_j = \frac{(D_f\, g)_j}{h_{j+1}} - \frac{(D_f h)_j}{h_j h_{j+1}} g_j,$$

$$\left(D_b\,\frac{g}{h}\right)_j = \frac{(D_b\,g)_j}{h_{j-1}} - \frac{(D_b h)_j}{h_j h_{j-1}} g_j,$$

$$\left(D_b\,\frac{g}{h}\right)_j = \frac{(D_b\,g)_j}{h_j} - \frac{(D_b h)_j}{h_j h_{j-1}} g_{j-1}.$$

Summation by parts.

$$\sum_{j=-N}^{N-1} \Delta_j g_{j+1} (D_f h)_j + \sum_{j=-N}^{N-1} \Delta_j (D_f g)_j h_j = \mathcal{I}_1,$$

where $\mathcal{I}_1 = \sum_{j=-N}^{N-1} \Delta_j (D_f\, gh)_j = -\frac{\Delta_{-N}}{\chi_{-N}} g_{-N} h_{-N} + \sum_{-N+1}^{N-1} \left(\frac{\Delta_{j-1}}{\chi_{j-1}} - \frac{\Delta_j}{\chi_j}\right) h_j g_j + \frac{\Delta_{N-1}}{\chi_{N-1}} h_N g_N$.The terms in the summation vanish when $\Delta_j \to 0$, i.e. when the separation between the mesh points is the same. But we can chose the vectors $\mathbf{h}$ and $\mathbf{g}$ is such a way that the last sum vanishes. Also

$$\sum_{j=-N+1}^{n} \Delta_{j-1} g_j (D_b h)_j + \sum_{j=-N+1}^{n} \Delta_{j-1} (D_b g)_j h_{j-1} = \mathcal{I}_2,$$

$$\mathcal{I}_2 = -\frac{\Delta_{-\mathcal{N}}}{\chi_{b,-\mathcal{N}+1}} g_{-\mathcal{N}} h_{-\mathcal{N}} + \sum_{j=-\mathcal{N}+1}^{\mathcal{N}-1} \left(\frac{\Delta_{j-1}}{\chi_{b,j}} - \frac{\Delta_j}{\chi_{b,j+1}}\right) g_j h_j + \frac{\Delta_{\mathcal{N}-1}}{\chi_{b,\mathcal{N}}} g_{\mathcal{N}} h_{\mathcal{N}}.$$

The commutator between q and D. The discrete version of the relationship $\frac{d}{dq} qh(q) - q\frac{d}{dq} h(q) = h(q)$ becomes

$$(D_f\, qh)_j - q_{j+1} (D_f\, h)_j = \frac{\Delta_j}{\chi_j} q_j,$$

$$(D_b\, qh)_j - q_j (D_b\, h)_j = \frac{\Delta_j}{\eta_j} q_{j-1}.$$

Translation of the exponential function. The discrete derivative is the generator of translations of the exponential function

$$(e^{s\, D_{b,f}} e^{vq})_j = e^{v(q_j+s)}.$$

We will need of *the bounded Fourier transform* of a given function $g(v)$ which is defined as

$$\tilde{g}_j = (Fg)_j = \frac{1}{\sqrt{\mathcal{V}}} \int_{-\mathcal{V}/2}^{\mathcal{V}/2} e^{ivq_j} g(v) dv,$$

on the mesh.

We also need of the *discrete Fourier transform* of a vector h_j which is defined as

$$\tilde{h}(v) = (\mathcal{F}h)(v) = \sum_{j=-N}^{N-1} \sqrt{\frac{\Delta_j}{\mathcal{V}}}\, e^{-ivq_j} h_j.$$

These transformations preserve the norm of vectors and functions. In the equidistant case in which $q_{j+1} - q_j = 2\pi/(N-1)$ these transforms can be identified with the usual Fourier transform on $[-\mathcal{V}, \mathcal{V}]$ and with the Fourier series, respectively.

The adjoint of D. Consider the equality

$$v(\mathcal{F}h)_j = \sum_{j=-N}^{N-1} \sqrt{\frac{\Delta_j}{\mathcal{V}}}\, e^{-ivq_{j+1}} (-iD_f h)_j + i \sum_{j=-N}^{N} \sqrt{\frac{\Delta_j}{\mathcal{V}}}\, (D_f e^{-ivq} h)_j.$$

Then, there is the relationship

$$p \leftrightarrow e^{-iv\Delta_j} (-iD_f h)_j, \quad j = -N, \ldots, N-1,$$

provided that the asymmetry term

$$\sum_{j=-N}^{N-1} \sqrt{\frac{\Delta_j}{\mathcal{V}}}\, (D_f e^{-ivq} h)_j,$$

vanishes.

The conjugate of q_j. The relationship
$$q_j\tilde{g}_j = i\frac{1}{\sqrt{\mathcal{V}}}\int_{-\mathcal{V}/2}^{\mathcal{V}/2} e^{ivq_j}\frac{d\,g(v)}{dv}dv - i\frac{1}{\sqrt{\mathcal{V}}}e^{ivq_j}g(v)\Big|_{v=-\mathcal{V}/2}^{\mathcal{V}/2}$$
indicates that
$$q_j\tilde{g}_j = i\frac{1}{\sqrt{\mathcal{V}}}\int_{-\mathcal{V}/2}^{\mathcal{V}/2} e^{ivq_j}\frac{d\,g(v)}{dv}dv - i\frac{1}{\sqrt{\mathcal{V}}}e^{ivq_j}g(v)\Big|_{v=-\mathcal{V}/2}^{\mathcal{V}/2}$$
provided boundary term
$$\frac{i}{\sqrt{\mathcal{V}}}e^{ivq_j}g(v)\Big|_{v=-\mathcal{V}/2}^{\mathcal{V}/2}$$

vanish.

Eigenvetors of the coordinate operator

The normalized *eigenvector of the coordinate operator* with eigenvalue q_n in the v representation is
$$e_{q_n}(v) = \frac{e^{-ivq_n}}{\sqrt{\mathcal{V}}}.$$

These functions are *orthonormal* in a discrete sense, i.e.
$$\int_{-\mathcal{V}/2}^{\mathcal{V}/2} dv\, e^*_{q_m}(v)e_{q_n}(v) = \operatorname{sinc}\left[\frac{\mathcal{V}}{2}(q_m - q_n)\right]$$

Now, the *conjugate to the coordinate eigenvector* $e_{q_n}(v)$ is

$$e_{q_n}(m) = \frac{1}{\sqrt{\mathcal{V}}}\int_{-\mathcal{V}/2}^{\mathcal{V}/2} e^{ivq_m}\frac{e^{-ivq_n}}{\sqrt{\mathcal{V}}}dv = \sqrt{\frac{\mathcal{V}}{2a}}\operatorname{sinc}\left[\frac{\mathcal{V}}{2}(q_m - q_n)\right],$$

and the orthonormality between these vectors reads

$$\sum_{m=-N}^{N}\Delta_m e^*_{q_j}(m)e_{q_n}(m) = \sum_{m=-N}^{N}\operatorname{sinc}\left[\frac{\mathcal{V}}{2}(q_m - q_j)\right]\operatorname{sinc}\left[\frac{\mathcal{V}}{2}(q_m - q_n)\right],$$
a result which becomes the Kronecker delta δ_{jn} when $\mathcal{V}\to\infty$.

Eigenvectors of the derivative operator

Now, the normalized *eigenvector of the discrete derivative* with eigenvalue v in the coordinate representation is
$$e_v(n) = \frac{e^{ivq_n}}{\sqrt{\Delta_n(2N+1)}},$$

and the orthogonality for these states reads
$$\sum_{n=-N}^{N}\Delta_n e^*_{v'}(n)e_v(n) = \frac{1}{2N+1}\sum_{n=-N}^{N}e^{i(v-v')q_n}\underset{N\to\infty}{\longrightarrow}\delta(v-v'). \tag{31}$$

The *conjugate function to* $e_v(n) = e^{ivq_n}/\sqrt{2N+1}$ is
$$e_v(v') = \sum_{j=-N}^{N}\frac{e^{i(v'-v)q_j}}{\sqrt{\mathcal{V}(2N+1)}},$$

This function approximates a delta function with small noise in it.

Concluding remarks

This is a step more in the theory of discrete operators. It shows that it is possible to have discrete operators very similar to the usual operator of continuous variable theory. We will explore more things about this operator, Things like its inverse, its use in obtaining self-adjoint extensions, for instance.

We have discussed a local approach to the finite differences first derivative. Another point of view is obtained by collecting the finite differences at each point of the mesh in a single matrix, the subject of another a future work.

References

1. Press, W. H., Teukolsky, S. A., Vetterling, W. T. and Flannery, B. P.. Numerical recipes the Art of Numerical Computing, third edition; Cambridge University Press: Cambridge, UK, 207; pp. 1.
2. William Squire; George Trapp; Using Complex Variables to Estimate Derivatives of Real Functions. *SIAM Review* **1997**, *40*, 110-112, 10.1137/s003614459631241x.
3. Kopal, Z.. Numerical Analysis: With Emphasis on the Application of Numerical Techniques to Problems of Infinitesimal Calculus in Single Variable; John Wiley \& Sons Inc.: New York, 1961; pp. 1.
4. Boole, George. A treatise on the calculus of finite differences; Cambridge University Press: New York, 1860, 2009; pp. 1.
5. Jordan, Charles. Calculus of finite differences, 2nd ed; Chelsea Publishing Co.: New York, USA, 1950; pp. 1.
6. Richardson, C. H.. An introduction to the calculus of finite differences; Van Nostrand Co., Inc.: New York, USA, 1954; pp. 1.
7. Potts, R. B.; Differential and Difference Equations. *Am Math Monthly* **1982**, *89*, 402-407, .
8. Potts, R. B.; Ordinary and partial differences equations. *J Austral. Math. Soc. Ser. B,* **1986**, *27*, 488, .
9. Mickens, R.E.. Nonstandard finite difference models of differential equations; World Scientific: Singapore, 1994; pp. 1.
10. Martínez-Pérez, A. and Torres-Vega, G.; Exact Finite Differences. The Derivative on Non Uniformly Spaced Partitions. *Symmetry* **2017**, *9*, 217, .
11. Potts, R. B.; Differential and Difference Equations. *Am Math Monthly* **1982**, *89*, 402-407, .
12. Potts, R. B.; Ordinary and partial differences equations. *J Austral. Math. Soc. Ser. B,* **1986**, *27*, 488, .
13. Mickens, R.E.. Nonstandard finite difference models of differential equations; World Scientific: Singapore, 1994; pp. 1.
14. Martínez-Pérez, A. and Torres-Vega, G.; Exact Finite Differences. The Derivative on Non Uniformly Spaced Partitions. *Symmetry* **2017**, *9*, 217, .