Infinite matrices may violate the associative law

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Abstract. The momentum operator for a particle in a box is represented by an infinite-order Hermitian matrix P. Its square P^2 is well-defined (and diagonal), but its cube P^3 is ill-defined, because $P P^2 \neq P^2 P$. Truncating these matrices to a finite order restores the associative law, but leads to other curious results.

Matrices of infinite order are used in quantum mechanics for representing dynamical variables. It is commonly assumed that these matrices obey the usual laws valid for finite matrices. However, it is obvious that difficulties may occasionally arise because of divergent infinite sums. We give here a very simple example of a Hermitian matrix P such that P^2 is well-defined, but P^3 is not, because $P P^2 \neq P^2 P$.

Related ambiguities may also arise in numerical calculations when infinite matrices are truncated to finite size (because there are no infinite computers). While the associative law is obviously fulfilled, the difficulty emerges in some other way. In particular, we sometimes encounter in quantum mechanics operators which are symmetric, but not self-adjoint (for example, the radial momentum operator). The representation of these operators by Hermitian matrices conceals their lack of self-adjointness and leads to curious results, as in the following example.

Consider the Hilbert space of functions $f(x)$, with $0 \leqslant x \leqslant \pi$, and inner product

$$\langle f, g \rangle = \int_0^\pi f^*(x)\, g(x)\, \mathrm{d}x. \tag{1}$$

In that space, the set of functions $u_m(x) = (2/\pi)^{1/2} \sin mx$, for all positive integers m, can be taken as a complete orthonormal basis (namely, any square integrable function of x can be written as a linear combination of the u_m, except at a finite number of isolated points). The operator $p = -\mathrm{i}\,\mathrm{d}/\mathrm{d}x$ has matrix elements

$$
\begin{aligned}
P_{mn} &= \int_0^\pi u_m\,(-\mathrm{i}\,\mathrm{d}/\mathrm{d}x)\,u_n\,\mathrm{d}x \\[6pt]
&= \begin{cases} -4\mathrm{i}mn/\pi(m^2 - n^2) & \text{if } m + n \text{ is odd} \\[4pt] 0 & \text{if } m + n \text{ is even}. \end{cases}
\end{aligned} \tag{2}
$$

This operator, currently defined only on functions which vanish at $x = 0$ and $x = \pi$, has the physical meaning of the linear momentum of a particle in a rigid one-dimensional box. It can be directly verified by algebraic methods [1] that

$$\sum_{s=1}^\infty P_{ms}\,P_{sn} = mn\,\delta_{mn} \tag{3}$$

as could be expected from

$$(P^2)_{mn} = \int_0^\pi u_m \, (-\mathrm{i}\mathrm{d}/\mathrm{d}x)^2 \, u_n \, \mathrm{d}x \, . \tag{4}$$

However, difficulties occur if we likewise try to define

$$(P^3)_{mn} \stackrel{?}{=} \int_0^\pi u_m \, (-\mathrm{i}\mathrm{d}/\mathrm{d}x)^3 \, u_n \, \mathrm{d}x \, . \tag{5}$$

The result is not Hermitian. This should not be a surprise, because, with the above boundary conditions, the operator $-\mathrm{i}\mathrm{d}/\mathrm{d}x$ is not self-adjoint [2, 3]. The matrices P_{mn} and $(P^2)_{mn}$ in (2) and (4) were Hermitian, because it was then possible to perform integrations by parts, in which the boundary terms vanished. However, if we attempt to do the same with (5), we obtain

$$\int_0^\pi u_m' \, u_n'' \, \mathrm{d}x = -\int_0^\pi u_m'' \, u_n' \, \mathrm{d}x + \left[u_m' \, u_n'\right]_0^\pi \tag{6}$$

and the last term does not vanish.

The source of the difficulty is that the domain of P consists of functions on the interval $[0, \pi]$ which vanish at the interval end-points. However, Pu_n does not vanish at these end-points, and therefore does not belong to the domain of P: the expression $P(Pu_n)$ is not mathematically defined. This does not contradict the fact that $(-\mathrm{d}^2/\mathrm{d}x^2)u_n = n^2 u_n$. The point is that, when P is defined as above, P^2 is not the same as $(-\mathrm{d}^2/\mathrm{d}x^2)$, notwithstanding equation (4). These two operators coincide in the common part of their domains of definition, but the domain of definition of P^2 is smaller.

The issue we are investigating here is how these curious properties appear when matrix notation is used to represent differential operators (for example in a mundane numerical analysis). If we try to use algebraic methods for defining P^3, we encounter the same difficulty in another form, namely

$$\sum_{s=1}^\infty P_{ms} \, (P^2)_{sn} \neq \sum_{s=1}^\infty (P^2)_{ms} \, P_{sn} \, . \tag{7}$$

Let us examine why the associative law fails. In the present case, the right-hand side of

$$(P^3)_{mn} \stackrel{?}{=} \sum_{r,s}^\infty P_{mr} \, P_{rs} \, P_{sn} \tag{8}$$

contains infinitely many terms with $r = s \pm 1 \gg m+n$, which behave as $\pm \sum 1/r$. Therefore the sum of positive terms diverges, the sum of negative terms diverges, and the entire sum in (8) is only conditionally convergent. Its value depends on the order of summation.

It is interesting to see how this difficulty is reflected in numerical calculations, where infinite matrices are truncated and replaced by finite matrices of order N (some large number). Instead of (8), we may try to define

$$S_{mn} = \lim_{N \to \infty} \sum_{r,s}^N P_{mr} \, P_{rs} \, P_{sn} \tag{9}$$

and the question is whether this sum indeed tends to a unique limit as $N \to \infty$. In the present case, it does, as is shown below. However, this happens only because of delicate cancellations between positive and negative terms, which would not occur in general.

Consider for definiteness the case where m and s are odd, and n, r, and N are even. The question is whether, for $N \gg m + n$, the contributions of $r = N$ and $s = N - 1$ to

the sum in (9) are vanishingly small. These contributions are, apart from an overall factor $64 \mathrm{i} m n / \pi^3$,

$$\frac{N^2}{m^2 - N^2} \sum_{s=1}^{N-1} \frac{s^2}{(N^2 - s^2)(s^2 - n^2)} + \frac{(N-1)^2}{(N-1)^2 - n^2} \sum_{r=2}^{N-2} \frac{r^2}{(m^2 - r^2)[r^2 - (N-1)^2]}. \tag{10}$$

(The second sum runs only to $r = N - 2$, in order to avoid double counting of the $r, s = N, N - 1$ matrix element.) In the above sums, the main contribution comes from terms where r and s are close to N, so that the various terms are of the order of N^{-1}, rather than N^{-2}. We therefore write $r = N - 2k$ and $s = N - 1 - 2k$, and we neglect terms with m^2 and n^2, which are much smaller than N^2. The two sums in (10) become

$$-\sum_{k=0} \frac{1}{(2k+1)(2N - 2k - 1)} + \sum_{k=1} \frac{1}{(2k-1)(2N - 2k - 1)}. \tag{11}$$

To be consistent with the preceding approximation, the sums in (11) run up to values of k which are much smaller than $N/2$ (so that both r and s are close to N). We thus obtain, approximately,

$$\frac{1}{2N}\left(-\sum_{k=0} \frac{1}{2k+1} + \sum_{k=1} \frac{1}{2k-1}\right) = \frac{1}{N}\left(\frac{1}{2} + \sum_{k=0} \frac{1}{4k^2 - 1}\right). \tag{12}$$

For large N, the sums on the left-hand side behave as $\mp \log N$. However, the sum on the right-hand side tends to $-\frac{1}{2}$ (see [1]) so that the whole expression vanishes. In summary, the total contribution of the $N - 1$ and N terms to the sum in (9) is of the order of N^{-2}, and that sum converges (for the particular matrix P_{mn} under consideration).

We have found empirically that, as N becomes much larger than m and n (which are kept fixed), the matrix elements S_{mn} tends to the Hermitian part of the right-hand side of (5), namely to

$$R_{mn} = (\mathrm{i}/2)\left[\int_0^\pi u_m\,(\mathrm{d}/\mathrm{d}x)^3\,u_n\,\mathrm{d}x - \int_0^\pi u_n\,(\mathrm{d}/\mathrm{d}x)^3\,u_m\,\mathrm{d}x\right]. \tag{13}$$

Note that the right-hand side of (13) can also be written, after integration by parts, as

$$(\mathrm{i}/2)\int_0^\pi (-u'_m\,u''_n + u'_n\,u''_m)\,\mathrm{d}x$$

$$= (\mathrm{i}/2)\int_0^\pi (n^2\,u'_m\,u_n - m^2\,u'_n\,u_m)\,\mathrm{d}x$$

$$= \frac{1}{2}(m^2\,P_{mn} - n^2\,P_{nm}) = \frac{1}{2}(m^2\,P_{mn} + P_{mn}\,n^2) \tag{14}$$

which is the average of P^2P and PP^2. The convergence was found to be of oscillatory type, as illustrated in table 1, for a few randomly chosen matrix elements.

On the other hand, truncation may also lead to counter-intuitive results. For example, if we define

$$Q_{mn} = \begin{cases} P_{mn} & \text{if } m \text{ and } n \leqslant N \\ 0 & \text{if } m \text{ or } n > N \end{cases} \tag{15}$$

the eigenvalues of Q_{mn} appear in opposite pairs, λ and $-\lambda$ (because Q and $Q^{\mathrm{T}} = -Q$ have the same eigenvalues). The only exception occurs if N is odd: the eigenvalue 0 is non-degenerate. Therefore the eigenvalues of Q^2 are doubly degenerate (except the null

Table 1. Convergence of S_{mn} toward R_{mn} (the table lists values of $-iS_{mn}$).

m	n	$N=99$	$N=100$	$N=999$	$N=1000$	$N=1999$	$N=2000$	$-iR_{mn}$
1	2	2.156	2.088	2.127	2.117	2.125	2.120	2.122
2	3	9.828	10.032	9.918	9.945	9.924	9.939	9.931
20	31	935.67	959.59	956.05	958.89	956.77	958.31	957.56
60	91	5198.7	6667.9	8803.1	8828.4	8814.0	8827.5	8822.4

Table 2. Some eigenvalues of Q^2, for $N = 999$ and 1000.

	$N = 999$ (complete matrix)	$N = 1000$ (truncated to 999)	$N = 1000$ (complete matrix)
1	0.000 000	0.996 663	0.996 663
2	3.986 641	3.986 641	0.996 663
3	3.986 641	8.969 969	8.969 969
4	15.946 56	15.946 56	8.969 969
5	15.946 56	24.916 58	24.916 58
...	......	......	......
996	988 294.4	988 294.4	986 110.2
997	988 294.4	990 283.2	990 283.2
998	992 673.3	992 673.3	990 283.2
999	992 673.3	994 666.5	994 666.5
1000	—	—	994 666.5

eigenvalue, if N is odd). This should be contrasted with the spectrum of P^2 which is 1, 4, 9, 16, ...

We have found empirically that the eigenvalues of Q_{mn} are very close to integers with a parity *opposite* to that of N. The lowest and highest eigenvalues of Q^2 are listed in table 2, for $N = 999$ and 1000. They appear quite different from those of P^2. However, if we first compute Q^2 with $N = 1000$, and then truncate it by removing the 1000th row and column (or more rows and columns with the largest indices), the eigenvalues of the resulting matrix are non-degenerate and are very close to those of P^2.

These curious results can be explained by rearranging the rows and columns of these matrices according to the sequence 1, 3, ...,$N - 1$, 2, 4, ...,$N - 2$ or N. Since the only non-vanishing matrix elements $(Q^2)_{mn}$ are those whose m and n have the same parity, the matrices Q^2 separate into two blocks. In each matrix, these two blocks have the same eigenvalues (so that each eigenvalue appears twice, except the null eigenvalue, if N is odd). It can be seen by direct inspection that the truncated matrix also consists of two blocks. Its odd–odd block is identical to the odd–odd block of $Q^2_{(1000)}$, and its even–even block is the same as the even–even block of $Q^2_{(999)}$. This explain why the same eigenvalue appears in three different positions in table 2. We have also found empirically that removing additional rows and columns from Q^2 (those with the largest indices) improves the convergence toward the 'true' eigenvalues, given by (3).

As higher powers of P are considered, the results become curiouser and curiouser. For instance, $P^4 = P^2 P^2$ is well-defined, and has matrix elements $m^2 n^2 \delta_{mn}$, by virtue of (3). On the other hand, $P P^2 P$ is ill-defined. If we write

$$(P P^2 P)_{mn} = -\frac{16}{\pi^2} mn \sum_s \frac{s^4}{(m^2 - s^2)(s^2 - n^2)} \tag{16}$$

where s runs over all integers with a parity opposite to that of m and n, *each* term in this sum tends to -1 when $s \to \infty$, so that the sum is not even conditionally convergent. Moreover, if we introduce truncated matrices, as in (15), the sum $\sum Q_{mr} Q_{rs} Q_{st} Q_{tn}$ does *not* tend to $m^2 n^2 \delta_{mn}$. It diverges, for any finite m and n (with same parity), when $N \to \infty$. The point is that $\sum Q_{mr} Q_{rs}$ converges to $ms\delta_{ms}$ only if s is kept fixed as $N \to \infty$, and likewise for $\sum Q_{st} Q_{tn}$. On the other hand, when we sum over s to obtain $(Q^4)_{mn}$, that sum includes terms where s is of the order of N and the latter have a divergent contribution.

The conclusion to be drawn from these results is that truncation methods, which are common practice in quantum mechanical calculations, should be used with extreme caution when the truncated matrices represent unbounded operators. In the particular case discussed here, where the matrix P is defined by (2), the truncated matrix P^2 should be defined by squaring the truncated P and then deleting the last row and column (otherwise, the eigenvalues turn out to be completely wrong). Likewise, the truncated matrix P^3 should be defined by (9), and *not* by (5) which gives a non-Hermitian result. However, these recipes may not be valid in general, and other unbounded operators ought to be considered on a case-by-case basis.

Acknowledgments

References

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