Appendix D: Numerical Tensor Products

This appendix discusses how tensor products are handled in numerical linear algebra software. We will focus on Python with the Numeric Python (numpy) module. The discussion is also applicable, with minor modifications, to GNU Octave or Matlab. We assume the reader is familiar with the basics of Python/Numpy, e.g. how vectors can be represented by 1D arrays, linear operators (matrices) can be represented by 2D arrays, etc.

Tensor products are implemented by the `numpy.kron` function, which performs an operation called a **Kronecker product**. The function takes two inputs, which can be 1D arrays, 2D arrays, or even higher-dimensional arrays (which we won't discuss). It returns a new array representing the tensor product of the inputs, whose dimensionality depends on that of the inputs. The function can be used to compute products of vectors ($|a\rangle \otimes |b\rangle$), products of operators ($\hat{O}_A \otimes \hat{O}_B$), etc. It can even compute "mixed" products like $|a\rangle \otimes \hat{O}_B$, which is useful for calculating partial projections and partial traces.

In the next few sections, we will prove that the various tensor products of bras, kets, and operators can be represented using the following Numpy expressions involving `numpy.kron`:

$$
\begin{aligned}
|a\rangle \otimes |b\rangle \;&\leftrightarrow\; \texttt{kron(a, b)} & \langle a| \otimes \langle b| \;&\leftrightarrow\; \texttt{kron(a.conj(), b.conj())} \\
\hat{A} \otimes \hat{B} \;&\leftrightarrow\; \texttt{kron(A, B)} \\
|a\rangle \otimes \hat{B} \;&\leftrightarrow\; \texttt{kron(a, B.T).T} & \langle a| \otimes \hat{B} \;&\leftrightarrow\; \texttt{kron(a.conj(), B)} \\
\hat{A} \otimes |b\rangle \;&\leftrightarrow\; \texttt{kron(A.T, b).T} & \hat{A} \otimes \langle b| \;&\leftrightarrow\; \texttt{kron(A, b.conj())}
\end{aligned}
$$

D.1. PRODUCTS OF VECTORS

Suppose a and b are both 1D arrays, of length M and N respectively; let their components be $(a_0, a_1, \ldots, a_{M-1})$ and $(b_0, b_1, \ldots, b_{N-1})$. Following Numpy conventions, we do not explicitly distinguish between "row vectors" and "column vectors", and component indices start from 0. The Kronecker product between a and b generates the following 1D array:

$$
\texttt{kron}(a, b) = \Big(a_0 b_0, \ldots, a_0 b_{N-1}, a_1 b_0, \ldots, a_1 b_{N-1}, \ldots, a_{M-1} b_{N-1}\Big). \tag{D.1}
$$

We can think of this as *taking each component of a, and multiplying it by the entire b array*:

$$
\texttt{kron}(a, b) = \Big(a_0 b, \; a_1 b, \; \ldots, \; a_{M-1} b\Big). \tag{D.2}
$$

As we shall see, this description of the Kronecker product extends to higher-dimensional arrays as well. In the present case, a and b are both 1D, and the result is a 1D array of MN components, which can be described compactly in index notation by

$$
\big[\texttt{kron}(a, b)\big]_\mu = a_m b_n \quad \text{where} \quad \mu = mN + n. \tag{D.3}
$$

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The index μ is defined so that as we sweep through $m = 0, \ldots, M - 1$ and $n = 0, \ldots, N - 1$, μ runs through the values $0, 1, \ldots, MN - 1$ without duplication. Note, by the way, that the order of inputs into `kron` is important: `kron(a,b)` is not the same as `kron(b,a)`! The asymmetry between a and b is apparent in the definitions (D.1) and (D.2).

In terms of abstract linear algebra (as used in quantum theory), let $\mathscr{H}_A$ be an M-dimensional space with basis $\{|m\rangle\}$, and $\mathscr{H}_B$ be an N-dimensional space with basis $\{|n\rangle\}$. Any two vectors $|a\rangle \in \mathscr{H}_A$ and $|b\rangle \in \mathscr{H}_B$ can be written as

$$|a\rangle = \sum_{m=0}^{M-1} a_m|m\rangle, \quad |b\rangle = \sum_{n=0}^{N-1} b_n|n\rangle. \tag{D.4}$$

A natural basis for the product space $\mathscr{H}_A \otimes \mathscr{H}_B$ is

$$\left\{|\mu\rangle \equiv |m\rangle|n\rangle\right\} \quad \text{where} \quad \begin{cases} \mu &= mN + n \\ m &= 0, 1, \ldots, M - 1 \\ n &= 0, 1, \ldots, N - 1. \end{cases} \tag{D.5}$$

Using Eq. (D.3), we can show that

$$|a\rangle \otimes |b\rangle = \sum_{mn} a_m b_n|m\rangle|n\rangle = \sum_{\mu=0}^{MN-1} \left[\texttt{kron}(a,b)\right]_\mu |\mu\rangle. \tag{D.6}$$

Therefore, we need only remember that the tensor product of two kets is represented by

$$|a\rangle \otimes |b\rangle \quad \leftrightarrow \quad \texttt{kron}(a,b). \tag{D.7}$$

Likewise, for bras,

$$\langle a| \otimes \langle b| \quad \leftrightarrow \quad \texttt{kron}(a^*, b^*). \tag{D.8}$$

D.2. PRODUCTS OF MATRICES

Let A and B be 2D arrays of size $M \times M$ and $N \times N$ respectively:

$$A = \begin{bmatrix} A_{00} & \cdots & A_{0,M-1} \\ \vdots & \ddots & \vdots \\ A_{M-1,0} & \cdots & A_{M-1,M-1} \end{bmatrix}, \quad B = \begin{bmatrix} B_{00} & \cdots & B_{0,N-1} \\ \vdots & \ddots & \vdots \\ B_{N-1,0} & \cdots & B_{N-1,N-1} \end{bmatrix}. \tag{D.9}$$

Then the Kronecker product of A and B is an $MN \times MN$ array of the form

$$\texttt{kron}(A, B) = \begin{bmatrix} A_{00}B & \cdots & A_{0,M-1}B \\ \vdots & \ddots & \vdots \\ A_{M-1,0}B & \cdots & A_{M-1,M-1}B \end{bmatrix}. \tag{D.10}$$

As before, this can be interpreted as taking each component of A, and multiplying it by B. The result can be written using index notation as

$$\left[\texttt{kron}(A, B)\right]_{\mu\mu'} = A_{mm'}B_{nn'} \quad \text{where} \quad \mu = mN + n, \ \mu' = m'N + n'. \tag{D.11}$$

In the language of abstract linear algebra, let $\mathscr{H}_A$ and $\mathscr{H}_B$ again be spaces with bases $\{|m\rangle\}$ and $\{|n\rangle\}$. Consider two linear operators $\hat{A}$ and $\hat{B}$ acting respectively on these spaces:

$$\hat{A} = \sum_{m,m'=0}^{M-1} |m\rangle A_{mm'} \langle m'|, \quad \hat{B} = \sum_{n,n'=0}^{N-1} |n\rangle B_{nn'} \langle n'|. \tag{D.12}$$

Then we can show using Eq. (D.11) that

$$\hat{A} \otimes \hat{B} = \sum_{mm'nn'} |m\rangle|n\rangle \, A_{mm'} B_{nn'} \, \langle m'|\langle n'| \tag{D.13}$$

$$= \sum_{\mu,\mu'} |\mu\rangle \, \big[\, \texttt{kron}(A,B) \,\big]_{\mu\mu'} \, \langle \mu'|, \tag{D.14}$$

where $\{|\mu\rangle\}$ is the basis for $\mathscr{H}_A \otimes \mathscr{H}_B$ previously defined in Eq. (D.5). Thus,

$$\hat{A} \otimes \hat{B} \ \leftrightarrow \ \texttt{kron}(A,B). \tag{D.15}$$

This result, like Eq. (D.7), is nice because it means that we can relegate the handling of tensor product components entirely to the $\texttt{kron}$ function. So long as we make a particular basis choice for the spaces $\mathscr{H}_A$ and $\mathscr{H}_B$, and keep to that choice, $\texttt{kron}$ will return the vector products and operator products expressed using an appropriate and natural basis for $\mathscr{H}_A \otimes \mathscr{H}_B$ [i.e., the basis defined in Eq. (D.5)].

D.3. MIXED PRODUCTS

For "mixed" products of operators with bras or kets, the representation using $\texttt{kron}$ is more complicated, but only slightly. First, consider the 1D array a and 2D array B:

$$a = (a_0, \ldots, a_{M-1}), \quad B = \begin{bmatrix} B_{00} & \cdots & B_{0,N-1} \\ \vdots & \ddots & \vdots \\ B_{N-1,0} & \cdots & B_{N-1,N-1} \end{bmatrix}. \tag{D.16}$$

Then the Kronecker product between the two is

$$\texttt{kron}(a,B) = (a_0 B, a_1 B, \ldots, a_{M-1} B). \tag{D.17}$$

Note that a is explicitly treated as a row vector. In component terms,

$$[\texttt{kron}(a,B)]_{n\mu'} = a_{m'} B_{nn'}, \quad \text{where} \quad \mu' = m'N + n'. \tag{D.18}$$

In linear algebraic terms, let

$$|a\rangle = \sum_m a_m |m\rangle, \quad \hat{B} = \sum_{nn'} |n\rangle B_{nn'} \langle n'|. \tag{D.19}$$

Then

$$|a\rangle \otimes \hat{B} = \sum_{\mu n'} |\mu\rangle \, a_m B_{nn'} \, \langle n'|, \qquad \mu = mN + n. \tag{D.20}$$

This does not quite match Eq. (D.18)! The basic problem is that the Kronecker product treats a a row vector. However, we can patch things up by massaging Eq. (D.18) a bit:

$$
\begin{aligned}
[\, \texttt{kron}(a, B^T)^T]_{\mu n'} &= [\texttt{kron}(a, B^T)]_{n' \mu} \\
&= a_m (B^T)_{n'n} \quad \text{where} \ \ \mu' = m'N + n' \\
&= a_m B_{nn'}.
\end{aligned}
\tag{D.21}
$$

This is an appropriate match for Eq. (D.20), so we conclude that

$$
|a\rangle \otimes \hat{B} \ \leftrightarrow \ \texttt{kron}(a, B^T)^T.
\tag{D.22}
$$

To take the product using the bra $\langle a|$, we replace Eq. (D.20) by

$$
\langle a| \otimes \hat{B} = \sum_{n\mu'} |n\rangle \, a^*_{m'} B_{nn'} \, \langle \mu'|, \qquad \mu' = m'N + n'.
\tag{D.23}
$$

Comparing this to Eq. (D.18) yields

$$
\langle a| \otimes \hat{B} \ \leftrightarrow \ \texttt{kron}(a^*, B).
\tag{D.24}
$$

Likewise, consider the 2D array A and 1D array b:

$$
A = \begin{bmatrix} A_{00} & \cdots & A_{0,M-1} \\ \vdots & \ddots & \vdots \\ A_{M-1,0} & \cdots & A_{M-1,M-1} \end{bmatrix}, \quad b = (b_0, \ldots, b_{N-1}).
\tag{D.25}
$$

Then the Kronecker product is

$$
\texttt{kron}(A, b) = \begin{bmatrix} A_{00}b & \cdots & A_{0,M-1}b \\ \vdots & \ddots & \vdots \\ A_{M-1,0}b & \cdots & A_{M-1,M-1}b \end{bmatrix}.
\tag{D.26}
$$

Similar to before, b is treated as a row vector. In component terms,

$$
[\texttt{kron}(A, b)]_{m\mu'} = A_{mm'} b_{n'}, \quad \text{where} \ \ \mu' = m'N + n'.
\tag{D.27}
$$

Using the same procedure as before, we can straightforwardly show that

$$
\hat{A} \otimes |b\rangle = \sum_{\mu m'} |\mu\rangle \, [\texttt{kron}(A^T, b)^T]_{\mu m'} \, \langle m'| \qquad \leftrightarrow \quad \texttt{kron}(A^T, b)^T
\tag{D.28}
$$

$$
\hat{A} \otimes \langle b| = \sum_{m\mu'} |m\rangle \, [\texttt{kron}(A, b^*)]_{m\mu'} \, \langle \mu'| \qquad \leftrightarrow \quad \texttt{kron}(A, b^*).
\tag{D.29}
$$