Hilbert Space and Dirac notation

- An (in)finite-dimensional vector (or function) space of square-integrable vectors (or functions)
- Vectors (or functions) are denoted by "kets" $|f\rangle$
- Inner product of $|f\rangle$ with $|g\rangle$ is obtained by taking Hermitian conjugate and multiplying $|f\rangle^\dagger |g\rangle$
- There is also a dual Hermitian-conjugate Hilbert space of "bras" $\langle g |$. Inner products can therefore be written

$$|f\rangle^\dagger |g\rangle = \langle f | g \rangle$$

This works for finite-dimensional vectors, or functions etc. functions of $x$

$$\langle f | g \rangle = \int_{-\infty}^{\infty} f^*(x) g(x) \, dx$$
\[ \langle \psi | \psi \rangle \text{ is real and non-negative} \]

- Orthonormal basis set \( \{|f_n\rangle, n = 1, 2, 3, \ldots\} \)
  \[ \langle f_n | f_m \rangle = \delta_{nm} \]

- Basis set is complete if any vector (or function) in Hilbert space can be expressed as a linear combination of basis vectors (or functions)
  \[ |f\rangle = \sum_n c_n |f_n\rangle \]
  Then, \[ \langle f_m | f \rangle = \sum_n c_n \langle f_m | f_n \rangle = \sum_n c_n \delta_{nm} = c_m \]
  So \[ c_n = \langle f_n | f \rangle \]

Note:
\[ |f\rangle = \sum_n |f_n\rangle \langle f_n | f \rangle = \left( \sum_n |f_n\rangle \langle f_n | \right) |f\rangle \]
\[ \sum_n |f_n\rangle \langle f_n | = \hat{1} \quad \text{(identity)} \]
Observables are Hermitian operators

- They have real eigenvalues and orthonormal eigenvectors (or eigenfunctions)
- Commute w/ vectors in Hilbert space

\[ \langle f | Q | f \rangle = \langle f | Q f \rangle = (\langle f | Q f \rangle)^\dagger = \langle Q^\dagger f | f \rangle = \langle Q f | f \rangle \]

- The matrix elements of \( Q \) in the \( |f_n\rangle \) basis are

\[ \langle f_n | Q | f_m \rangle \]

Example: \( Q = H \) → \( \langle \psi_m | H | \psi_n \rangle = \langle \psi_m | E_n | \psi_n \rangle = E_n \langle \psi_m | \psi_n \rangle = E_n \delta_{mn} \)

\[
\begin{bmatrix}
E_1 & 0 & 0 & \cdots \\
0 & E_2 & 0 & \cdots \\
0 & 0 & E_3 & \cdots \\
\vdots & \vdots & \vdots & \ddots \\
\end{bmatrix}
\]

(a diagonal matrix)

→ The eigenfunctions/vectors of an operator "diagonalize" that operator!
Example

\[ \hat{A} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \] (in basis \( |x\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \) and \( |y\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \))

1. Show that \( \langle n | \hat{A} | m \rangle \) is the \( n^{th} \) row, \( m^{th} \) column element of \( \hat{A} \):

\[ H_n = \langle x | H | x \rangle = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0, \quad H_{12} = \langle x | H | y \rangle = H_{21}^\dagger = 1 \]

\[ H_{21} = \langle y | H | x \rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 1, \quad H_{22} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0 \]

2. What are the eigenvalues of \( \hat{A} \)?

\[ \hat{A} | \psi \rangle = E | \psi \rangle \] (Schrödinger equation)

\[ (\hat{A} - E \mathbb{1}) | \psi \rangle = 0 \]

\[ \begin{vmatrix} -E & 1 \\ 1 & -E \end{vmatrix} = 0 \quad E^2 - 1 = 0 \]

\[ E = \pm 1 \]

\[ E_+ = +1, \quad E_- = -1 \]
3. What are the eigenvectors of $A$?

$$(\hat{A} - E_{+} \hat{1}) |+\rangle = 0$$

$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = 0$$

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$(\hat{A} - E_{-} \hat{1}) |-\rangle = 0$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = 0$$

$$|-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

4. Show that $\sum_{n} |\Psi_{n}\rangle \langle \Psi_{n}| = \hat{1}$

$$|+\rangle = |+1\rangle + |-2\rangle$$

$$\frac{1}{2} \left( \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \right) = \frac{1}{2} \left( \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \right) = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \hat{1}$$
A random complex-valued Hermitian matrix:

\[
H = 
\begin{bmatrix}
0.53427 + 0.00000i & 1.55496 - 0.48363i & 0.98593 + 0.41434i & 1.04617 - 0.08737i \\
1.55496 + 0.48363i & 1.17180 + 0.00000i & 0.69207 - 0.14460i & 1.38173 + 0.10256i \\
0.98593 - 0.41434i & 0.69207 + 0.14460i & 0.12701 + 0.00000i & 1.28715 + 0.40134i \\
1.04617 + 0.08737i & 1.38173 - 0.10256i & 1.28715 - 0.40134i & 1.66651 + 0.00000i \\
\end{bmatrix}
\]

Notice that the outer product (column vector times row vector) of eigenvectors is a matrix:

\[
\text{ans} = 
\begin{bmatrix}
0.41404 + 0.00000i & -0.23109 + 0.10564i & -0.25090 - 0.30816i & 0.03233 + 0.13815i \\
-0.23109 - 0.10564i & 0.15593 + 0.00000i & 0.06141 + 0.23601i & 0.01720 - 0.08536i \\
-0.25090 - 0.30816i & 0.06141 - 0.23601i & 0.38141 + 0.00000i & -0.12242 - 0.05965i \\
0.03233 - 0.13815i & 0.01720 + 0.08536i & -0.12242 + 0.05965i & 0.04862 + 0.00000i \\
\end{bmatrix}
\]

when we sum the outer products of eigenvectors, we get the identity to within machine precision

\[
C = 
\begin{bmatrix}
1.00000 + 0.00000i & 0.00000 + 0.00000i & 0.00000 - 0.00000i & -0.00000 - 0.00000i \\
0.00000 - 0.00000i & 1.00000 + 0.00000i & 0.00000 - 0.00000i & -0.00000 + 0.00000i \\
0.00000 + 0.00000i & 0.00000 + 0.00000i & 1.00000 + 0.00000i & -0.00000 - 0.00000i \\
-0.00000 + 0.00000i & -0.00000 - 0.00000i & -0.00000 + 0.00000i & 1.00000 + 0.00000i \\
\end{bmatrix}
\]

the maximum error for the elements of this random matrix is:

1.3878e-016 ± 2.0817e-016

whereas machine precision on this computer is 2.2204e-016