Further Review

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Physics Cafe

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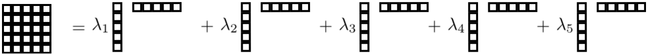
Outline

Projection Operators

- Recall from the Spectral Decomposition Theorem that we are able to diagonalize Hermitian operators into a weighted sum of rank one outer products,

$$A = \sum_i \lambda_i |i\rangle\langle i|, \tag{1}$$



- The set of eigenvectors, $|i\rangle$, are orthonormal and span the entire vector space. They form a convenient coordinate system for the vector space.

- So for any vector $|\psi\rangle$ we can write it as,

$$|\psi\rangle = \sum_i \psi_i |i\rangle \qquad \text{Usual basis expansion.} \tag{2}$$

$$= \sum_i |i\rangle \cdot \underbrace{\langle i|\psi\rangle}_{\psi_i} \qquad \text{Writing components as inner product projections.} \tag{3}$$

$$= \sum_i |i\rangle\langle i| \cdot |\psi\rangle \qquad \text{Shifted the order of multiplication by associativity.} \tag{4}$$

- The quantity on rhs of the first line is a ket multiplied by a scalar (it's an inner product).

- The quantity on the last line is a linear operator multiplying a ket.
- But these two quantities are equal: $\psi_i|i\rangle = |i\rangle\langle i| \cdot |\psi\rangle$
- The operators $|i\rangle\langle i|$ are special operators — they are rank-one *projection* operators that project onto the one-dimensional subspaces spanned by the $|i\rangle$.
- If we take a collection of these projectors, the first k, for example,

$$P \equiv \sum_{i=1}^{k} |i\rangle\langle i|, \tag{5}$$

  it will be the projector onto the k-dimensional linear subspace spanned by the first k eigenvectors, $|1\rangle, \ldots, |k\rangle$.
- The orthogonal complement of P is $Q \equiv I - P$. It is a projector onto the vector space spanned by $|k+1\rangle, \ldots, |n\rangle$. Why?
- Also, $|v\rangle\langle v| = (|v\rangle\langle v|)^\dagger$. Why? This implies P is Hermitian.
- Note, too, that $P^2 = P$. Why?

- The projection operation can be visualized like this.

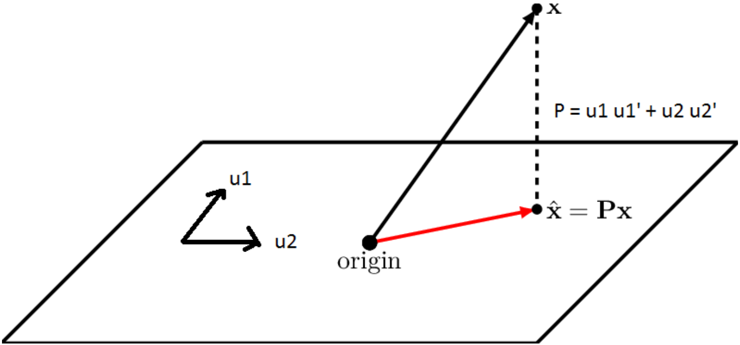


Figure: Example of projection into a two-dimensional linear subspace.

The Trace

- Previously the trace of a matrix was defined as the sum of its diagonal elements,

$$\mathrm{tr}(A) = \sum_i a_{ii}. \tag{6}$$

- It's important to understand we are really evaluating a property, that we call the trace, of the *linear operator* that the matrix represents.

- It's intrinsic to the operator and
does not depend on the particular orthonormal coordinate system we are using to represent the operator as as a matrix.

- This is the same as the norm (or length) of a geometric vector. The numbers in the column matrix we use to represent that vector will change with the coordinate system chosen. But it's *norm* is invariant. It's intrinsic to that vector.

Example (1. The length (Euclidean norm) of a vector is invariant.)

- Recall that the norm squared of a vector equals its inner product with itself,

$$|v|^2 = \langle v \,|\, v \rangle = v^\dagger v. \tag{7}$$

- Recall the change of basis on slide 13 from the previous talk.
  Given a matrix U with orthonormal columns containing the basis vectors of the new coordinate system, the new vector is given by,

$$v' = U^\dagger v. \tag{8}$$

- But the norm squared in the new coordinate system is just

$$\begin{aligned} v'^\dagger v' &= v^\dagger U U^\dagger v && (9) \\ &= v^\dagger I v && (10) \\ &= v^\dagger v. && (11) \end{aligned}$$

- Recall that the (i, j) element of a matrix representation of a linear operator is given by,

$$a_{ij} = \langle i|A|j\rangle. \tag{12}$$

- We can then write the trace as,

$$\operatorname{tr} A = \sum_i \langle i|A|i\rangle. \tag{13}$$

- Note that it is linear. Why?

- Next we show two useful and properties of the trace:

Properties of the trace

- The trace is independent of the coordinate system used.

- The trace equals the sum of the operator's eigenvalues.

(Proof) 1. The Trace is Independent of the Coordinate System.

- The trick is using the completion of unity from last slides,

$$I = \sum_i |i\rangle\langle i| \tag{14}$$

$$\begin{aligned}
\mathrm{tr}\, A &= \sum_i \langle i | A | i \rangle && (15)\\
&= \sum_i \langle i | A \left(\sum_j |\phi_j\rangle\langle\phi_j| \right) |i\rangle && (16)\\
&= \sum_i \sum_j \langle i | A | \phi_j \rangle \langle \phi_j | i \rangle && (17)\\
&= \sum_i \sum_j \langle \phi_j | i \rangle \langle i | A | \phi_j \rangle && (18)\\
&= \sum_j \langle \phi_j | \left(\sum_i |i\rangle\langle i| \right) A |\phi_j\rangle && (19)\\
&= \sum_j \langle \phi_j | A | \phi_j \rangle && (20)
\end{aligned}$$

(Proof) 2. The Trace is the Sum of the Eigenvalues.

- Recall the trace of A is given by the sum of its diagonal elements,

$$\operatorname{tr} A = \sum_i a_{ii} = \sum_i \langle i \,|\, A \,|\, i \rangle \tag{21}$$

- But in the same basis (just using a different index variable, j) we can expand A as,

$$A = \sum_j \lambda_j |j\rangle\langle j| \tag{22}$$

- Substituting this expansion into the trace definition,

$$\operatorname{tr} A = \sum_i \langle i| \cdot \sum_j \lambda_j |j\rangle\langle j| \cdot |i\rangle \tag{23}$$

$$= \sum_i \sum_j \lambda_j \langle i \,|\, j\rangle \langle j \,|\, i\rangle \tag{24}$$

$$= \sum_{ij} \lambda_j \delta_{ij} \delta_{ji} \tag{25}$$

$$\Longrightarrow \operatorname{tr} A = \sum_i \lambda_i \tag{26}$$

□

Matrix Functions

- In quantum mechanics scalar quantities that we measure classically, such as position, energy, etc., become linear operators represented by matrices in a particular coordinate system.
- So in the classical case where we might have a function of position or energy, we now have to consider functions with matrix arguments.
- In reality these are functions whose arguments are linear operators and return new linear operators.
- We are used to functions of scalar values, such as $f(x) = \sin(x)$ or $f(x) = e^x$.
- From first year we know functions can generally be expanded in a Taylor Series,

$$f(x) = \sum_{i=0}^{\infty} a_i x^i. \tag{27}$$

- For example, the exponential function,

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \tag{28}$$

- So we simply *define* matrix functions based on their scalar Taylor series.

- So we now have,

$$f(X) = \sum_i a_i X^i, \tag{29}$$

- For example,

$$e^X = I + \frac{X^2}{2!} + \frac{X^3}{3!} + \cdots \tag{30}$$

- In principle we may have hundreds of terms, requiring raising a matrix to a hundreth power by repeated multiplication. These matrices may be of dimensions of thousands or millions, again in principle.
$\Longrightarrow$ See the Cayley-Hamilton Theorem for more details. E.g., wikipedia.

- There is a remarkable fact that we can write this matrix function strictly in terms of the eigenvalues of X!

Theorem (1. Cayley-Hamilton Theorem (sort of))

- *A function of an $n \times n$ Hermitian matrix can be written in terms of n scalar functions of its eigenvalues.*
- *If X has the eigendecomposition $X = U\Lambda U^\dagger$, where $\Lambda = diag(\lambda_1, \lambda_2, \ldots, \lambda_n)$, then $f(X)$ can be written as,*

$$f(X) = U \begin{pmatrix} f(\lambda_1) & 0 & \cdots & 0 \\ 0 & f(\lambda_2) & \cdots & 0 \\ \vdots & & \ddots & 0 \\ 0 & \cdots & \cdots & f(\lambda_n) \end{pmatrix} U^\dagger \tag{31}$$

- Why is this such a big deal?
  For example, what is X^{100}?

$$X^{100} = U \begin{pmatrix} \lambda_1^{100} & 0 & \cdots & 0 \\ 0 & \lambda_2^{100} & \cdots & 0 \\ \vdots & & \ddots & 0 \\ 0 & \cdots & \cdots & \lambda_n^{100} \end{pmatrix} U^\dagger \tag{32}$$

Example (1. Examples of Matrix Functions)

- Some matrix functions,

$$e^{X} = U \begin{pmatrix} e^{\lambda_1} & 0 & \cdots & 0 \\ 0 & e^{\lambda_2} & \cdots & 0 \\ \vdots & & \ddots & 0 \\ 0 & \cdots & \cdots & e^{\lambda_n} \end{pmatrix} U^{\dagger} \tag{33}$$

$$\sin(X) = U \begin{pmatrix} \sin(\lambda_1) & 0 & \cdots & 0 \\ 0 & \sin(\lambda_2) & \cdots & 0 \\ \vdots & & \ddots & 0 \\ 0 & \cdots & \cdots & \sin(\lambda_n) \end{pmatrix} U^{\dagger} \tag{34}$$

$$X^{-1} = U \begin{pmatrix} \frac{1}{\lambda_1} & 0 & \cdots & 0 \\ 0 & \frac{1}{\lambda_2} & \cdots & 0 \\ \vdots & & \ddots & 0 \\ 0 & \cdots & \cdots & \frac{1}{\lambda_n} \end{pmatrix} U^{\dagger} \tag{35}$$

1. Proof (Cayley-Hamilton Theorem (sort of).

- Define the function $f(x) = \sum_i a_i X^i$ where $X = U\Lambda U^\dagger$
- The i'th power of X is then,

$$X^i = \left(U\Lambda U^\dagger\right)^i \tag{36}$$

$$= U\Lambda U^\dagger \cdot U\Lambda U^\dagger \cdots U\Lambda U^\dagger \cdot U\Lambda U^\dagger \tag{37}$$

$$= U\Lambda^i U^\dagger \tag{38}$$

- So carrying the a_i coefficients into the diagonal eigenvalue matrix,

$$f(x) = \sum_i a_i U\Lambda^i U^\dagger \tag{39}$$

$$= \sum_i U \begin{pmatrix} a_i\lambda_1^i & & \\ & a_i\lambda_2^i & \\ & & \ddots \end{pmatrix} U^\dagger \tag{40}$$

$$= U \begin{pmatrix} \sum_i a_i\lambda_1^i & & \\ & \sum_i a_i\lambda_2^i & \\ & & \ddots \end{pmatrix} \tag{41}$$

1. Proof (Cayley-Hamilton Theorem (sort of), cont'd.

- And so we have,

$$f(X) = U \begin{pmatrix} f(\lambda_1) & & \\ & f(\lambda_2) & \\ & & \ddots \end{pmatrix} U^\dagger \tag{43}$$

$$= Uf(\Lambda)U^\dagger. \tag{44}$$

- So the function is applied element-wise to the *eigenvalues* of X. Not the elements of X.

$\square$

Example (2. Examples of Matrix Functions)

- There are interesting analytical results from this.
- Suppose we exponentiate the antisymmetric (not Hermitian here!) matrix multiplied by a parameter θ,

$$A = \theta \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{45}$$

  So we have e^A.

- You can show that A has eigenvalues $\pm i\theta$ with corresponding eigenvectors $(\pm i, 1)$.
- So the eigen-decomposition of A is,

$$\Lambda = \begin{pmatrix} i\theta & 0 \\ 0 & -i\theta \end{pmatrix}, U = \begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix}, U^{-1} = \frac{1}{2i} \begin{pmatrix} 1 & i \\ -1 & i \end{pmatrix} \tag{46}$$

Example (2. Examples of Matrix Functions, cont'd)

- Recall the standard first year exponential/trig identities,

$$(e^{i\theta} + e^{-i\theta})/2 = \cos\theta \tag{47}$$
$$(e^{i\theta} - e^{-i\theta})/2i = \sin\theta \tag{48}$$

- Then expanding eigen-decompositiion and simplifying algebraically, we have,

$$e^{A} = Ue^{\Lambda}U^{-1} \tag{49}$$
$$= \begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix} \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix} \frac{1}{2i} \begin{pmatrix} 1 & i \\ -1 & i \end{pmatrix} \tag{50}$$
$$= \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \tag{51}$$

- This is the two dimensional rotation matrix and is a linear operator in its own right.

Example (3. Applcation: Solving Schrodinger's Equation)

- Suppose we have a system with a Hamiltonian $H = \hbar\omega\sigma_z$, where σ_z is the Pauli spin matrix $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.
  This is case of a constant magnetic field in the $+z$ direction.
- Recall Schrodinger's equation, which gives the time evolution of a system,

$$i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle. \tag{52}$$

- For a time independent Hamiltonian, Mike has shown it has the solution,

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(t=0)\rangle. \tag{53}$$

- This looks complicated but it's a straightforward generalization of Mike's scalar case.

Recall the d.e. $\frac{dx}{dt} = Hx$ where x and H are just scalar numbers.
Positing a solution $x = e^{Ht}$ we see it satisfies the d.e. by taking derivatives of both sides of the equation.
We have the same case here with a few constants (i and $\hbar$) thrown in and
we think of the variables being vectors and matrices now.

Example (3. Applcation: Solving Schrodinger's Equation, cont'd)

- So we need to solve to the exponential of a two by two matrix!
- Easy. Follow the steps from the previous example, modifying as appropriate.
- After a bit of algebra we find

$$e^{-iHt/\hbar} \equiv U(t) = \begin{pmatrix} \cos(\omega t) & -i\sin(\omega t) \\ -i\sin(\omega t) & \cos(\omega t) \end{pmatrix} \tag{54}$$

  where $U(t)$ is a unitary matrix.

- Suppose our initial quantum state at time $t = 0$ is $|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.
- Then the state as it evolves in time under the given Hamiltonian is,

$$|\psi(t)\rangle = U(t)\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{55}$$

$$= \begin{pmatrix} \cos(\omega t) \\ -i\sin(\omega t) \end{pmatrix} \tag{56}$$

- What is the probability of finding the particle in its original state if we make a measurement at time t?
- This will be the magnitude squared of the projection between the two vectors.
- $Prob. = |\langle\psi(0)\,|\,\psi(t)\rangle|^2 = \cos^2(\omega t)$.
- This will be the magnitude squared of the projection between the two vectors. $Prob. = |\langle\psi(0)\,|\,\psi(t)\rangle|^2 = \cos^2(\omega t)$.
- This can be seen as a prototype example of a particle with spin precessing in constant magnetic field (and so constant Hamiltonian).
- The Hamiltonian is constant in time *but* the particle state varies in time. Interesting!

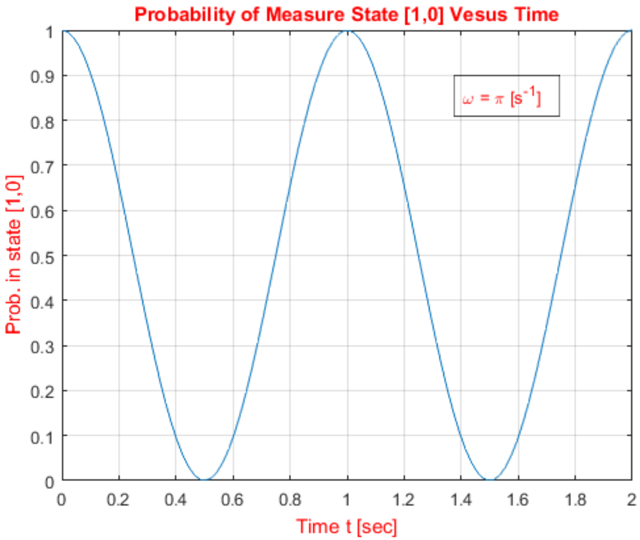


Figure: Probability of find state in $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ versus time for $\omega = \pi[s^-1]$.

End

END.