Chapter 19 – Matrix Eigenvalue Problem

Motivation: Our entire semester of quantum is based on the Schrödinger's equation which is an eigenvalue problem in and of itself. We will not necessarily be using matrix notation in lecture but nonetheless this will be a good exercise so that you will have an opportunity to see this problem from a different viewpoint.

* 19.1 Systems of Linear equations

- as we say in the last chapter we can write:

$$\begin{matrix} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = y_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = y_2 \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = y_n \end{matrix} \quad \text{or} \quad \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \rightarrow \mathbf{Ax} = \mathbf{y}$$

- if **A** is nonsingular with a nonzero determinant then:

$$\mathbf{A}^{-1}(\mathbf{Ax}) = (\mathbf{A}^{-1}\mathbf{A})\mathbf{x} = \mathbf{Ix} = \mathbf{x}$$

- this means that $\mathbf{A}^{-1}\mathbf{Ax} = \mathbf{A}^{-1}\mathbf{y} \rightarrow \mathbf{x} = \mathbf{A}^{-1}\mathbf{y}$ and so we can use the inverse to solve systems possessing nonsingular matrices
- how do we get $\mathbf{A}^{-1}$
  - -- we need to get the cofactor, C_{ij}, for each matrix element
  - -- we then replace all the elements in the matrix with their cofactors
  - -- next, we transpose the matrix of cofactors which is called the adjoint of the matrix
  - -- finally we the adjoint by the determinant
  - -- Example: Find the inverse of the matrix below.

$$\mathbf{A} = \begin{pmatrix} 2 & 1 & 3 \\ 4 & -2 & 0 \\ -1 & 1 & 0 \end{pmatrix}$$

The cofactor matrix:

$$\mathbf{C} = \begin{pmatrix} 0 & 0 & 2 \\ 3 & 3 & -3 \\ 6 & 12 & -8 \end{pmatrix} \rightarrow \mathbf{C}^T = \begin{pmatrix} 0 & 3 & 6 \\ 0 & 3 & 12 \\ 2 & -3 & -8 \end{pmatrix}$$

If the determinant is $\frac{1}{6}$ then

$$\mathbf{A}^{-1} = \frac{1}{6}\begin{pmatrix} 0 & 3 & 6 \\ 0 & 3 & 12 \\ 2 & -3 & -8 \end{pmatrix}$$

We can verify by checking the product of the matrix & its inverse

$$\mathbf{A}^{-1}\mathbf{A} = \frac{1}{6}\begin{pmatrix} 0 & 0 & 2 \\ 3 & 3 & -3 \\ 6 & 12 & -8 \end{pmatrix}\begin{pmatrix} 2 & 1 & 3 \\ 4 & -2 & 0 \\ -1 & 1 & 0 \end{pmatrix} = \frac{1}{6}\begin{pmatrix} 6 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 6 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

- Great, so how will this help us solve an equation? Say we look at our previous matrix as an example.

$$\begin{aligned} 2x+y+3z&=4 \\ 4x-2y&=2 \\ -x+y&=1 \end{aligned} \rightarrow \begin{pmatrix} 2 & 1 & 3 \\ 4 & -2 & 0 \\ -1 & 1 & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 4 \\ 2 \\ 1 \end{pmatrix} \rightarrow \mathbf{Ax}=\mathbf{y}$$

$$\mathbf{x}=\mathbf{A}^{-1}\mathbf{y} \rightarrow \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \frac{1}{6}\begin{pmatrix} 0 & 3 & 6 \\ 0 & 3 & 12 \\ 2 & -3 & -8 \end{pmatrix}\begin{pmatrix} 4 \\ 2 \\ 1 \end{pmatrix} = \frac{1}{6}\begin{pmatrix} 0\bullet 4+3\bullet 2+6\bullet 1 \\ 0\bullet 4+3\bullet 2+12\bullet 1 \\ 2\bullet 4-3\bullet 2-8\bullet 1 \end{pmatrix} = \frac{1}{6}\begin{pmatrix} 12 \\ 18 \\ -6 \end{pmatrix} = \begin{pmatrix} 2 \\ 3 \\ -1 \end{pmatrix}$$

*19.2 The Eigenvalue Problem

- we introduced the secular equation in Chapter 17 which was used to solve the roots of the characteristic determinant or $\det\left(\mathbf{A}-\lambda\mathbf{I}\right)=0$
- these roots are eigenvalues of the set of linear equations from which they come from
- furthermore, we can get corresponding eigenvectors for each of these values

  $\mathbf{A}x_k=\lambda x_k \quad k=1,2,...,n$
- if each eigenvalue is unique (which is the case with our QM models) then there will be n different eigenvectors

Properties of Eigenvectors

1. If x is an eigenvector corresponding to eigenvalue, λ, then kx is also an eigenvector corresponding to the same eigenvalue for any nonzero value of k:

   if $\mathbf{A}x=\lambda x$ then $\mathbf{A}\left(kx\right)=k\left(\mathbf{A}x\right)=k\left(\lambda x\right)=\lambda\left(kx\right)$

   -- in other words, eigenvectors which differ only by a scalar are indistinct

   -- it is for this reason we often make k the normalization constant

   -- matrix definition of normalization: $\mathbf{C}^T\mathbf{C}=1$

$$v=\begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} \rightarrow N^2\begin{pmatrix} 1 & 2 & 3 & 4 \end{pmatrix}\begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix}=1 \rightarrow N^2(1+4+9+16)=1 \rightarrow N^2=\frac{1}{30} \rightarrow N=\frac{1}{\sqrt{30}}$$

This is very similar to our normalization : $\int_{all\ space} \psi^*(x)\psi(x)dx=1$

2. If $\mathbf{A}$ is a real symmetric matrix, the eigenvectors corresponding to distinct eigenvalues are orthogonal.
3. For a symmetric matrix, the eigenvectors corresponding to the same eigenvalue are either orthogonal or can be made so.

Putting it all together we get the Kronecker delta: The n eigenvalues of a real symmetric matrix of order n form a system of n orthogonal unit (orthonormal) vectors:

$$x_k^T x_l=\delta_{kl}=\begin{cases} 1 & if\ k=l \\ 0 & if\ k\neq l \end{cases}$$

*19.3-19.4 Skip

*19.5 Complex matrices

- The complex conjugate in matrix notation:
  - if $\mathbf{A} = \left(a_{ij}\right)$ then $\mathbf{A}^* = \left(a_{ij}^*\right)$
  - -- for $\mathbf{A} = \mathbf{B} + i\mathbf{C}$ then $\mathbf{A}^* = \mathbf{B} - i\mathbf{C}$
  - -- for a real matrix: $\mathbf{A} = \mathbf{A}$ & $\mathbf{C} = 0$
- The Hermitian conjugate matrix, $\mathbf{A}^\dagger$
  - -- defn: $\mathbf{A}^\dagger = \left(\mathbf{A}^*\right)^T = \left(\mathbf{A}^T\right)^*$
  - -- this matrix plays the same role for complex matrices that the transpose does for real Matrices
- Hermitian matrices
  - -- defn: $\mathbf{A}^\dagger = \mathbf{A}$
  - -- you have heard this in terms of operators (which matrices are) from Chapter 4 in quantum you were told Hermitian operators are those which when applied to one of their eigenfunctions are real regardless of whether the operator and the eigenfunction is complex.
- Unitary matrices
  - -- defn: $\mathbf{A}^\dagger = \mathbf{A}^{-1}$
  - -- the columns and rows of such a matrix form a system of orthogonal vectors