Homework for Thursday April 18: Section 8.1, Numbers 2,10,12,16,26*,36

**Symmetric Matrices.** A matrix $A$ with real entries is symmetric, if $A^T = A$.

**Examples.** $A = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix}$ is symmetric, $A = \begin{bmatrix} 1 & 1 \\ 0 & 3 \end{bmatrix}$ is not symmetric.

**Eigenvalues of Symmetric Matrices.** Symmetric matrices $A$ have real eigenvalues.

**Proof.** The dot product is extended to complex vectors as $(v, w) = \sum_i v_i w_i$. For real vectors it satisfies $(v, w) = v \cdot w$ and has the property $(Av, w) = (v, A^T w)$ for real matrices $A$ and $(\lambda v, w) = \lambda (v, w)$ as well as $(v, \lambda w) = \lambda (v, w)$. Now $\lambda (v, v) = (\lambda v, v) = (Av, v) = (v, A^T v) = (v, Av) = (v, \lambda v) = \lambda (v, v)$ shows that $\lambda \neq 0$ because $(v, v) \neq 0$ for $v \neq 0$.

**Example.** $A = \begin{bmatrix} p & -q \\ q & p \end{bmatrix}$ has eigenvalues $p + iq$ which are real if and only if $q = 0$.

**Eigenvectors of Symmetric Matrices.** If $A$ is symmetric, then the eigenvectors to different eigenvalues are orthogonal.

**Proof.** If $Av = \lambda v$ and $Aw = \mu w$. The relation $\lambda (v, w) = (Av, w) = (v, A^T w) = (v, Aw) = (v, \mu w) = \mu (v, w)$ is only possible if $(v, w) = 0$ if $\lambda \neq \mu$.

**Why Are Symmetric Matrices Important?** In applications, matrices are often symmetric. For example in geometry as generalized dot products $v \cdot Av$, or in statistics as correlation matrices $\text{Cov}[X_i, X_i]$ or in quantum mechanics as observables or in neural networks as learning maps $x \mapsto \text{sign}(Wx)$ or in graph theory as adjacency matrices etc. etc. Symmetric matrices play the same role as real numbers do among the complex numbers. Their eigenvalues often have physical or geometrical interpretations. One can also calculate with symmetric matrices like with numbers: for example, we can solve $B^2 = A$ (one calls such a $B$ square root of $A$.) Try to find a matrix $B$ such that $B^2 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$.

**Recall.** We have seen when an eigenbasis exists, a matrix $A$ can be transformed to a diagonal matrix $B = S^{-1} AS$, where $S = [v_1, \ldots, v_n]$. The matrices $A$ and $B$ are similar. $B$ is called the diagonalisation of $A$. Similar matrices have the same characteristic polynomial $\det(B - \lambda) = \det(S^{-1}(A - \lambda)S) = \det(A - \lambda)$ and have therefore the same determinant, trace and eigenvalues. Physics who call the set of eigenvalues also the spectrum, say, that they are isospectral. The spectrum is what you ”see” (etymologically the name origins from the fact that in quantum mechanics the spectrum of radiation is associated with eigenvalues of matrices.)

**Spectral Theorem.** Symmetric matrices $A$ can be diagonalized $B = S^{-1} AS$ with an orthogonal $S$. The diagonal entries of $B$ are the eigenvalues of $A$.

**Proof.** If all eigenvalues are different, there is an eigenbasis and diagonalisation is possible. The eigenvectors are all orthogonal and $B = S^{-1} AS$ is diagonal containing the eigenvalues. In general, we can change the matrix $A$ to $A = A + (C - A)t$ where $C$ is a matrix with pairwise different eigenvalues. Then the eigenvalues are different for most $t$ different from 0. (If $\lambda_i(t) - \lambda_j(t)$ were zero for $t$ on some interval, then we had $\lambda_i(t) = \lambda_j(t)$ for all $t$ which would contradict in the case $t = 1$.) The orthogonal matrices $S_t$ converge for $t \to 0$ to an orthogonal matrix $S$.

**Wait a Second ...** We could also perturb a general matrix $A_t$ to have disjoint eigenvalues and $A_t$ could be diagonalized: $S_t^{-1} A_t S_t = B_t$? THE PROBLEM IS THAT $S_t$ might blow up for $t \to 0$.

**Example 1.** The matrix $A = \begin{bmatrix} a & b \\ b & a \end{bmatrix}$ has the eigenvalues $a + b, a - b$ and the eigenvectors $v_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} / \sqrt{2}$ and $v_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix} / \sqrt{2}$. They are orthogonal. The orthogonal matrix $S = \begin{bmatrix} v_1 & v_2 \end{bmatrix}$ diagonalized $A$. 

EXAMPLE 2. The $3 \times 3$ matrix $A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$ has 2 eigenvalues 0 to the eigenvectors $[1 \ -1 \ 0]$, $[1\ 0 \ -1]$ and one eigenvalue 3 to the eigenvector $[1 \ 1 \ 1]$. All these vectors can be made orthogonal and a diagonalisation is possible even so the eigenvalues have multiplicities.

SQUARE ROOT OF A MATRIX. How do we find a square root of a given symmetric matrix? Because $S^{-1}AS = B$ is diagonal and we know how to take a square root of the diagonal matrix $B$, we can form $C = S\sqrt{B}S^{-1}$ which satisfies $C^2 = S\sqrt{B}S^{-1}S\sqrt{B}S^{-1} = SBS^{-1} = A$.

EXHIBITION. "Where do symmetric matrices occur?" Some motivation (informal):

I) PHYSICS: In quantum mechanics a system is described with a vector $v(t)$ which depends on time $t$. The evolution is given by the Schrödinger equation $\dot{v} = i\hbar L v$, where $L$ is a symmetric matrix and $\hbar$ is a small number called the Planck constant. As for any linear differential equation, one has $v(t) = e^{i\lambda t}v(0)$. If $v(0)$ is an eigenvector to the eigenvalue $\lambda$, then $v(t) = e^{i\lambda t}v(0)$. Physical observables are given by symmetric matrices too. The matrix $L$ represents the energy. Given $v(t)$, the value of the observable $A(t)$ is $v(t) \cdot Av(t)$. For example, if $v$ is an eigenvector to an eigenvalue $\lambda$ of the energy matrix $L$, then the energy of $v(t)$ is $\lambda$.

This is called the Heisenberg picture. In order that $v \cdot A(t)v = v(t) \cdot Av(t) = S(t)v \cdot AS(t)v$ we have $A(t) = S(T)^*AS(t)$, where $S^* = \overline{S^T}$ is the correct generalization of the adjoint to complex matrices. $S(t)$ satisfies $S(t)^*S(t) = 1$ which is called unitary and the complex analogue of orthogonal. The matrix $A(t) = S(t)^*AS(t)$ has the same eigenvalues as $A$ and is similar to $A$.

II) CHEMISTRY. The adjacency matrix $A$ of a graph with $n$ vertices determines the graph: one has $A_{ij} = 1$ if the two vertices $i, j$ are connected and zero otherwise. The matrix $A$ is symmetric. The eigenvalues $\lambda_j$ are real and can be used to analyze the graph. One interesting question is to what extent the eigenvalues determine the graph.

In chemistry, one is interested in such problems because it allows to make rough computations of the electron density distribution of molecules. In this so called Hückel theory, the molecule is represented as a graph. The eigenvalues $\lambda_j$ of that graph approximate the energies an electron on the molecule. The eigenvectors describe the electron density distribution.

The Freon molecule for example has 5 atoms. The adjacency matrix is

$\begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}$

This matrix $A$ has the eigenvalue 0 with multiplicity 3 (ker($A$) is obtained immediately from the fact that 4 rows are the same) and the eigenvalues 2, -2. The eigenvector to the eigenvalue $\pm 2$ is $[\pm 2 \ 1 \ 1 \ 1 \ 1]^T$.

III) STATISTICS. If we have a random vector $X = [X_1, \ldots, X_n]$ and $E[X_k]$ denotes the expected value of $X_k$, then $|A|_{kl} = E[(X_k - E[X_k])(X_l - E[X_l])]$ is called the covariance matrix of the random vector $X$. It is a symmetric matrix. Diagonalizing this matrix $B = S^{-1}AS$ produces new random variables which are uncorrelated.

IV) MECHANICS. The Toda lattice is a particle system on the line, where neighboring particles attract each other with the force $e^{-d}$, where $d$ is the distance. If $q_n$ are the positions of the particles, then the Newton equations are $\frac{d^2}{dt^2}q_n = e^{r_{n+1} - r_n} - e^{r_n - r_{n-1}}$. A coordinate transformation $a_n^2 = e^{r_{n+1} - r_n}$, $2b_n = q_n$ brings the system into the form $\dot{a}_n = a_n(b_{n+1} - b_n)$, $\dot{b}_n = 2a_{n+1}^2 - 2a_n^2$. It can be written in matrix form as $\dot{A} = [B, A] = BA - AB$, where $A = \begin{bmatrix} b_1 & a_1 & 0 & 0 & a_n \\ b_2 & a_2 & 0 & \cdots & 0 \\ 0 & a_3 & \cdots & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & a_n & b_{n-1} & a_{n-1} \\ a_n & 0 & \cdots & b_n & a_{n-1} \end{bmatrix}$, $B = \begin{bmatrix} 0 & a_1 & 0 & \cdots & 0 & -a_n \\ -a_1 & 0 & a_2 & \cdots & 0 & 0 \\ 0 & -a_2 & \cdots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & -a_{n-2} & 0 & a_{n-1} & 0 \\ a_n & 0 & \cdots & -a_{n-2} & 0 & a_{n-1} \end{bmatrix}$.

With $\dot{S} = BS$, one has $A(t) = S^{-1}A(0)S^T$. The matrix $A(t)$ is similar to $A$. Because the eigenvalues of $A$ are preserved, one has enough conserved quantities which allow to find closed-form solutions of these differential equations. Even so nonlinear, it can be linearized. The continuum version of this system is called the KdE equation and a model for water waves.