DIAGONALIZATION — Math 21b, O.Knill

HOMEWORK: Section 7.4: 14,20,26,36,54,58*,56*

SUMMARY. A $n \times n$ matrix, $A\vec{v} = \lambda\vec{v}$ with eigenvalue λ and eigenvector $\vec{v}$. The eigenvalues are the roots of the characteristic polynomial $f_A(\lambda) = \det(\lambda - A) = \lambda^n - \mathrm{tr}(A)\lambda^{n-1} + ... + (-1)^n\det(A)$. The eigenvectors to the eigenvalue λ are in $\ker(\lambda - A)$. The number of times, an eigenvalue λ occurs in the full list of n roots of $f_A(\lambda)$ is called algebraic multiplicity. It is bigger or equal than the geometric multiplicity: $\dim(\ker(\lambda - A)$.
EXAMPLE. The eigenvalues of $\begin{bmatrix} a & b \\ c & d \end{bmatrix}$ are $\lambda_\pm = T/2 + \sqrt{T^2/4 - D}$, where $T = a + d$ is the trace and $D = ad - bc$ is the determinant of A. If $c \neq 0$, the eigenvectors are $v_\pm = \begin{bmatrix} \lambda_\pm - d \\ c \end{bmatrix}$. If $c = 0$, then a, d are eigenvalues to the eigenvectors $\begin{bmatrix} a \\ 0 \end{bmatrix}$ and $\begin{bmatrix} -b \\ a - d \end{bmatrix}$. If $a = d$, then the second eigenvector is parallel to the first and the geometric multiplicity of the eigenvalue $a = d$ is 1.

EIGENBASIS. If A has n different eigenvalues, then A has an eigenbasis, consisting of eigenvectors of A.

DIAGONALIZATION. How does the matrix A look in an eigenbasis? If S is the matrix with the eigenvectors as columns, then we know $\boxed{B = S^{-1}AS}$. We have $S\vec{e}_i = \vec{v}_i$ and $AS\vec{e}_i = \lambda_i\vec{v}_i$ we know $S^{-1}AS\vec{e}_i = \lambda_i\vec{e}_i$. Therefore, B is diagonal with diagonal entries λ_i.

EXAMPLE. $A = \begin{bmatrix} 2 & 3 \\ 1 & 2 \end{bmatrix}$ has the eigenvalues $\lambda_1 = 2 + \sqrt{3}$ with eigenvector $\vec{v}_1 = [\sqrt{3}, 1]$ and the eigenvalues $\lambda_2 = 2 - \sqrt{3}$ with eigenvector $\vec{v}_2 = [-\sqrt{3}, 1]$. Form $S = \begin{bmatrix} \sqrt{3} & -\sqrt{3} \\ 1 & 1 \end{bmatrix}$ and check $S^{-1}AS = D$ is diagonal.

APPLICATION: FUNCTIONAL CALCULUS. Let A be the matrix in the above example. What is $A^{100} + A^{37} - 1$? The trick is to diagonalize A: $B = S^{-1}AS$, then $B^k = S^{-1}A^kS$ and We can compute $A^{100} + A^{37} - 1 = S(B^{100} + B^{37} - 1)S^{-1}$.

APPLICATION: SOLVING LINEAR SYSTEMS. $x(t+1) = Ax(t)$ has the solution $x(n) = A^nx(0)$. To compute A^n, we diagonalize A and get $x(n) = SB^nS^{-1}x(0)$. This is an explicit formula.

SIMILAR MATRICES HAVE THE SAME EIGENVALUES.
One can see this in two ways:

1) If $B = S^{-1}AS$ and $\vec{v}$ is an eigenvector of B to the eigenvalue λ, then $S\vec{v}$ is an eigenvector of A to the eigenvalue λ.

2) From $\det(S^{-1}AS) = \det(A)$, we know that the characteristic polynomials $f_B(\lambda) = \det(\lambda - B) = \det(\lambda - S^{-1}AS) = \det(S^{-1}(\lambda - AS) = \det((\lambda - A) = f_A(\lambda)$ are the same.

CONSEQUENCES.
1) Because the characteristic polynomials of similar matrices agree, the trace $\mathrm{tr}(A)$ of similar matrices agrees.
2) The trace is the sum of the eigenvalues of A. (Compare the trace of A with the trace of the diagonalize matrix.)

THE CAYLEY HAMILTON THEOREM. If A is diagonalizable, then $f_A(A) = 0$.
PROOF. The DIAGONALIZATION $B = S^{-1}AS$ has the eigenvalues in the diagonal. So $f_A(B)$, which contains $f_A(\lambda_i)$ in the diagonal is zero. From $f_A(B) = 0$ we get $Sf_A(B)S^{-1} = f_A(A) = 0$.

The theorem holds for all matrices: the coefficients of a general matrix can be changed a tiny bit so that all eigenvalues are different. For any such perturbations one has $f_A(A) = 0$. Because the coefficients of $f_A(A)$ depend continuously on A, they are zero in general.

CRITERIA FOR SIMILARITY.

- If A and B have the same characteristic polynomial and diagonalizable, then they are similar.
- If A and B have a different determinant or trace, they are not similar.
- If A has an eigenvalue which is not an eigenvalue of B, then they are not similar.

WHY DO WE WANT TO DIAGONALIZE?

1) FUNCTIONAL CALCULUS. If $p(x) = 1 + x + x^2 + x^3/3! + x^4/4!$ be a polynomial and A is a matrix, then $p(A) = 1 + A + A^2/2! + A^3/3! + A^4/4!$ is a matrix. If $B = S^{-1}AS$ is diagonal with diagonal entries λ_i, then $p(B)$ is diagonal with diagonal entries $p(\lambda_i)$. And $p(A) = S\,p(B)S^{-1}$. This speeds up the calculation because matrix multiplication costs much. The matrix $p(A)$ can be written down with three matrix multiplications, because $p(B)$ is diagonal.

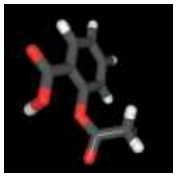
2) SOLVING LINEAR DIFFERENTIAL EQUATIONS. A differential equation $\dot{\vec{v}} = A\vec{v}$ is solved by $\vec{v}(t) = e^{At}\vec{v}(0)$, where $e^{At} = 1 + At + A^2t^2/2! + A^3t^3/3!...)x(0)$. (Differentiate this sum with respect to t to get $Ae^{At}\vec{v}(0) = A\vec{x}(t)$.) If we write this in an eigenbasis of A, then $\vec{y}(t) = e^{Bt}\vec{y}(0)$ with the diagonal matrix $B = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ 0 & 0 & \dots & \lambda_n \end{bmatrix}$. In other words, we have then explicit solutions $y_j(t) = e^{\lambda_j t}y_j(0)$. Linear differential equations later in this course. It is important motivation.

3) STOCHASTIC DYNAMICS (i.e MARKOV PROCESSES). Complicated systems can be modeled by putting probabilities on each possible event and computing the probabilities that an event switches to any other event. This defines a transition matrix. Such a matrix always has an eigenvalue 1. The corresponding eigenvector is the stable probability distribution on the states. If we want to understand, how fast things settle to this equilibrium, we need to know the other eigenvalues and eigenvectors.

MOLECULAR VIBRATIONS. While quantum mechanics describes the motion of atoms in molecules, the vibrations can be described classically, when treating the atoms as "balls" connected with springs. Such approximations are necessary when dealing with large atoms, where quantum mechanical computations would be too costly. Examples of simple molecules are white phosphorus P_4, which has tetrahedronal shape or methan CH_4 the simplest organic compound or **freon**, CF_2Cl_2 which is used in refrigerants. **Caffeine** or **aspirin** form more complicated molecules.


Freon CF_2Cl_2


Caffeine $C_8H_{10}N_4O_2$


Aspirin $C_9H_8O_4$

WHITE PHOSPHORUS VIBRATIONS. (Differential equations appear later, the context is motivation at this stage). Let x_1, x_2, x_3, x_4 be the positions of the four phosphorus atoms (each of them is a 3-vector). The interatomar forces bonding the atoms is modeled by springs. The first atom feels a force $x_2 - x_1 + x_3 - x_1 + x_4 - x_1$ and is accelerated in the same amount. Let's just chose units so that the force is equal to the acceleration. Then

$$\begin{aligned} \ddot{x}_1 &= (x_2 - x_1) + (x_3 - x_1) + (x_4 - x_1) \\ \ddot{x}_2 &= (x_3 - x_2) + (x_4 - x_2) + (x_1 - x_2) \\ \ddot{x}_3 &= (x_4 - x_3) + (x_1 - x_3) + (x_2 - x_3) \\ \ddot{x}_4 &= (x_1 - x_4) + (x_2 - x_4) + (x_3 - x_4) \end{aligned}$$

which has the form $\ddot{x} = Ax$, where the 4×4 matrix

$$A = \begin{bmatrix} -3 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 \\ 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & -3 \end{bmatrix} \qquad v_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, v_2 = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix}, v_3 = \begin{bmatrix} -1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, v_4 = \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

are the eigenvectors to the eigenvalues $\lambda_1 = 0, \lambda_2 = -4, \lambda_3 = -4, \lambda_3 = -4$. With $S = [v_1v_2v_3v_4]$, the matrix $B = S^{-1}BS$ is diagonal with entries $0, -4, -4, -4$. The coordinates $y_i = Sx_i$ satisfy $\ddot{y}_1 = 0, \ddot{y}_2 = -4y_2, \ddot{y}_3 = -4y_3, \ddot{y}_4 = -4y_4$ which we can solve y_0 which is the center of mass satisfies $y_0 = a + bt$ (move molecule with constant speed). The motions $y_i = a_i\cos(2t) + b_i\sin(2t)$ of the other eigenvectors are oscillations, called **normal modes**. The general motion of the molecule is a superposition of these modes.