We have computed the eigenvalues of the rotation matrix

$$A = \begin{bmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{bmatrix}$$

We have seen that the eigenvalues are $e^{i\alpha} = \cos(\alpha) + i\sin(\alpha)$, the eigenvectors are $\frac{\pm i}{1}$. The eigenvectors are the same for every rotation-dilation matrix. With

$$A = \begin{bmatrix} a & -b \\ b & a \end{bmatrix}, \quad S = \begin{bmatrix} i & -i \\ 1 & 1 \end{bmatrix}$$

we have

$$S^{-1}AS = \begin{bmatrix} a + ib & 0 \\ 0 & a - ib \end{bmatrix}.$$
Cayley Hamilton theorem

For any polynomial $p$, we can form the matrix $p(A)$. For example, for $p(x) = x^2 + 2x + 3$, we have $p(A) = A^2 + 2A + 3$.

If $f_A$ is the characteristic polynomial, we can form $f_A(A)$

If $A$ is diagonalizable, then $f_A(A) = 0$.

The matrix $B = S^{-1}AS$ 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.

An application in chemistry

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 tetrahedral shape or methan $CH_4$ the simplest organic compound or freon, $CF_2Cl_2$ which is used in refrigerants.

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 inter-atomar forces bonding the atoms is modeled by springs. The first atom feels a force $x_3 - x_1 + x_4 - x_1 + x_4 - x_4$ and is accelerated in the same amount. Let’s just chose units so that the force is equal to the acceleration. Then

$$\ddot{x}_1 = (x_2 - x_1) + (x_3 - x_1) + (x_4 - x_1)$$

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

$A = \begin{bmatrix}
-3 & 1 & 1 & 1 \\
1 & -3 & 1 & 1 \\
1 & 1 & -3 & 1 \\
1 & 1 & 1 & -3
\end{bmatrix}$

are the eigenvectors to the eigenvalues $\lambda_1 = 0, \lambda_2 = -4, \lambda_3 = -4, \lambda_4 = -4$. With $S = [v_1, v_2, v_3, v_4]$, the matrix $B = S^{-1}AS$ is diagonal with entries $0, -4, -4, -4$. The coordinates $y_i$ satisfy $y_i = 0, y_2 = -4y_3, y_3 = -4y_4, y_4 = -4y_0$ which we can solve $y_0$ which is the center of mass satisfies $y_0 = x + b \dot{t}$ (move molecule with constant speed). The motions $y_i = a \cos(2t) + b \sin(2t)$ of the other eigenvectors are oscillations, called normal modes. The general motion of the molecule is a superposition of these modes.

Homework due April 20, 2011

1. What is the probability that an upper triangular $3 \times 3$ matrix with entries 0 and 1 is diagonalizable?

2. Which of the following matrices are similar?

$A = \begin{bmatrix}
1 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 1 \\
0 & 0 & 0 & 1
\end{bmatrix}$, $B = \begin{bmatrix}
1 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}$, $C = \begin{bmatrix}
1 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 \\
0 & 0 & 1 & 1 \\
0 & 0 & 0 & 1
\end{bmatrix}$, $D = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 1 & 0 \\
0 & 0 & 1 & 1 \\
0 & 0 & 0 & 1
\end{bmatrix}$.

3. Diagonalize the following matrix in the complex:

$A = \begin{bmatrix}
2 & -3 & 0 & 0 \\
3 & 2 & 0 & 0 \\
0 & 0 & 5 & 6 \\
0 & 0 & 6 & 5
\end{bmatrix}$.

1We grabbed the pdb Molecule files from http://www.sci.ouc.bc.ca, translated them with "povchem" from .pdb to .pov rendered them under Povray.