Coordinates 4/11/2001 **Math 21b, O. Knill**

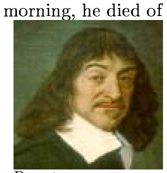
Homework for Friday April 13: Section 7.1, 2,4,6,12,22,24

COORDINATES. In this section we reconsider the question "What are coordinates?" Cartesian geometry was introduced by Fermat and Descartes (1596-1650) around 1636, it had a large influence on mathematics and introduced algebraic methods into geometry. The beginning of the vector concept came only later at the beginning of the 19th Century with the work of Bolzano (1781-1848). The full power of coordinates however is possible only if we allow to chose our coordinate system to adapt to the situation.

From Decartes biography. (A part which shows how far can dedication to teaching of mathematics go ...)

(...) In 1649 Queen Christina of Sweden persuaded Descartes to go to Stockholm. However the Queen wanted to draw tangents at 5 a.m. in the morning and Descartes broke the habit of his lifetime of getting up at 11 o'clock. After only a few months in the cold northern climate, walking to the palace at 5 o'clock every morning, he died of pneumonia.


Fermat


Decartes


Bolzano

VECTOR IN NEW COORDINATES. If a vector v is written as a linear combination $v = \sum_i x_i v_i$ of vectors in a basis $\mathcal{B} = \{v_1, \dots, v_n\}$. Define $S = \begin{bmatrix} v_1 & \cdots & v_2 \end{bmatrix}$. The solution of $v = Sx = \sum_i v_i x_i$ is of course $x = S^{-1}v$. We write $[v]_{\mathcal{B}} = x = \begin{bmatrix} x_1 \\ \cdots \\ x_n \end{bmatrix}$ and call x_i the **coordinates** of v with respect to the basis $\mathcal{B}$.

EXAMPLE. Find the coordinates of $v = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$ with respect to the basis $\mathcal{B} = \{v_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, v_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}\}$.

We have $S = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$ and $S^{-1} = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix}$. Therefore $[v]_{\mathcal{B}} = S^{-1}v = \begin{bmatrix} -1 \\ 3 \end{bmatrix}$. Indeed $-1v_1 + 3v_2 = v$.

LINEAR TRANSFORMATION IN NEW COORDINATES. The transformation S^{-1} maps the coordinates from the standard basis into the coordinates of the new basis. In order to see what a transformation A does in the new coordinates, we map it back to the old coordinates, apply A and then map it back again to the new coordinates: $B = S^{-1}AS$.

The transformation in "bad" coordinates.

$$\begin{array}{ccc} v & \overset{S}{\leftarrow} & w \\ A\downarrow & & \downarrow B \\ Av & \overset{S^{-1}}{\rightarrow} & Bw \end{array}$$

The transformation in "good" coordinates.

IN OTHER WORDS. In a basis $\mathcal{B} : v_1, \dots, v_n$, the coordinates of a transformation T from $\mathbf{R}^n$ to $\mathbf{R}^n$ is the matrix B with columns $[T(v_i)]_{\mathcal{B}}$. In the standard basis, we have the matrix A with columns $T(v_i) = TSe_i$ and $[T(v_i)]_{\mathcal{B}} = S^{-1}TSe_i = Be_i$.

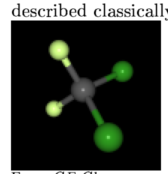
BASIS IS EIGENBASIS. If v_i are eigenvectors of A with eigenvalues λ_i then $Be_i = S^{-1}ASe_i = S^{-1}Av_i = S^{-1}\lambda_i v_i = \lambda_i e_i$. (Note that $Se_i = v_i$ implies $S^{-1}v_i = e_i$.) The matrix B is diagonal in that basis.

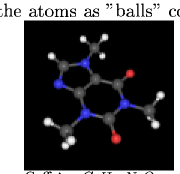
APPLICATION: SOLVING LINEAR DIFFERENTIAL EQUATIONS. A differential equation $\dot{x} = Ax$ is solved by $x(t) = e^{At}x(0)$, where $e^{At} = 1 + At + A^2t^2/2! + A^3t^3/3!...)x(0)$. (Differentiate this sum with respect to t to get $Ae^{At}x(0) = Ax(t)$.) If we write this in an eigenbasis of A, then $y(t) = e^{Bt}y(0)$ 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.

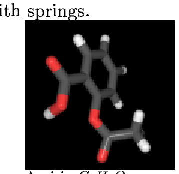
APPLICATION: FUNCTIONAL CALCULUS. If $p(x) = 1 + x + x^2 + x^3/3! + x^4/4!$ be a polynomial and A is a matrix, then $p(A) = 1 + A + A^2/2! + A^3/3! + A^4/4!$ is a matrix. If $B = S^{-1}AS$ is diagonal with diagonal entries λ_i, then $p(B)$ is diagonal with diagonal entries $p(\lambda_i)$. And $p(A) = S\,p(B)S^{-1}$. 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.

EXAMPLE. Find e^A, where $A = \begin{bmatrix} 0 & -\phi \\ \phi & 0 \end{bmatrix}$. Since A is a rotation dilation matrix, we know its eigenvalues are $\lambda_\pm = \pm i\phi$, and the eigenvectors are $v_\pm = \begin{bmatrix} \pm i \\ 1 \end{bmatrix}$. The matrix S is $\begin{bmatrix} i & -i \\ 1 & 1 \end{bmatrix}$ and $S^{-1} = \begin{bmatrix} -i & 1 \\ i & 1 \end{bmatrix}/2$. Therefore $e^A = S^{-1}\begin{bmatrix} \exp(i\phi) & 0 \\ 0 & \exp(-i\phi) \end{bmatrix} S = \begin{bmatrix} \cos(\phi) & -\sin(\phi) \\ \sin(\phi) & \cos(\phi) \end{bmatrix}$.
We could have got that easier: A corresponds to multiplication with $i\phi$. e^A corresponds to a multiplication with $e^{i\phi} = \cos(\phi) + i\sin(\phi)$ which is a rotation matrix with diagonal elements $\cos(\phi)$ and side diagonal elements $\pm\sin(\phi)$.

MOLECULAR VIBRATIONS. White phosphorus P_4 is a platonic molecule in the shape of a tetrahedron. A platonic molecule with a center atom is the **methan molecule** CH_4 which is the simplest organic compound. Another example is **freon**, CF_2Cl_2 (used in refrigerants), which can be destroyed by ultraviolet light. The freed chlorine atoms Cl then react with **ozone** O_3. The **caffeine** or **aspirin** molecules are examples of more complicated molecules. While quantum mechanics describes the behaviour of these molecules, the molecular vibrations can roughly be described classically, treating the atoms as "balls" connected with springs.


Freon CF_2Cl_2


Caffeine $C_8H_{10}N_4O_2$


Aspirin $C_9H_8O_4$

WHITE PHOSPHORUS VIBRATIONS. Let x_1, x_2, x_3, x_4 be the positions of the four phosphorus atoms (each of them is a 3-vector but we don't need to incorporate this into the notation). Simplifying the interatomar forces bonding the atoms together, we assume they are connected 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

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

has the eigenvectors

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

to the eigenvalues $\lambda_1 = 0, \lambda_2 = -4, \lambda_3 = -4, \lambda_3 = -4$. With $S = [v_1 v_2 v_3 v_4]$, 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 satisifies $y_0 = a + bt$ (motion with constant speed). The motion $y_i = a_i\cos(4t) + b_i\sin(4t)$ are oscillations, called **normal modes**. The general motion of the molecule is a superposition of these motions, (translations and oscillations).