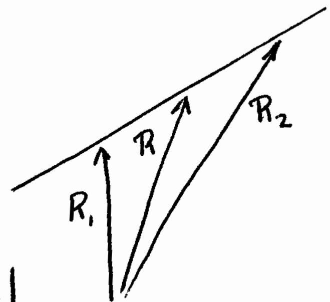
DETERMINANTS AND GEOMETRY

Basic geometry

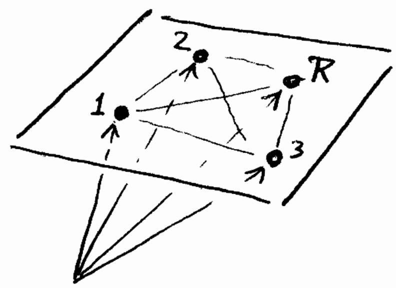
(1) Let $\vec{R}, \vec{R}_1, \vec{R}_2$ be collinear (in $\mathbb{R}^2$)



$$\begin{vmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x \\ y_1 & y_2 & y \end{vmatrix} = 0 \Rightarrow x \begin{vmatrix} 1 & 1 \\ y_1 & y_2 \end{vmatrix} - y \begin{vmatrix} 1 & 1 \\ x_1 & x_2 \end{vmatrix} = \begin{vmatrix} x_1 & x_2 \\ y_1 & y_2 \end{vmatrix}$$

Equation of line through (x_1, y_1) & (x_2, y_2)

(2) Let $\vec{R}, \vec{R}_1, \vec{R}_2, \vec{R}_3$ be coplanar (in $\mathbb{R}^3$)

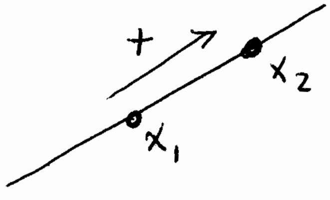


$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x \\ y_1 & y_2 & y_3 & y \\ z_1 & z_2 & z_3 & z \end{vmatrix} = 0 \Rightarrow x \begin{vmatrix} 1 & 1 & 1 \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{vmatrix} - y \begin{vmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ z_1 & z_2 & z_3 \end{vmatrix} + z \begin{vmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \end{vmatrix}$$

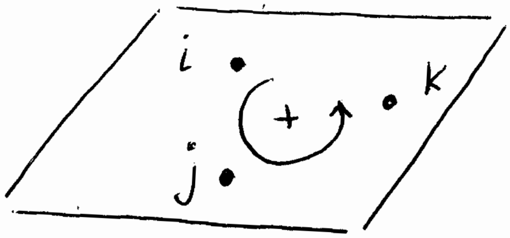
$$= \vec{R}_1 \cdot \vec{R}_2 \times \vec{R}_3 = \begin{vmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{vmatrix}$$

(3) Same goes for a hyperplane of dim. $n-1$ in $\mathbb{R}^n$.

In general, the above formulas are volume formulas, employed as necessary & sufficient conditions for the vanishing of volume: consider the expression $X_{ij} = \begin{vmatrix} 1 & 1 \\ x_i & x_j \end{vmatrix} = x_j - x_i$ giving the signed distance between points x_j, x_i on $\mathbb{R}^1$. It can also be used to define orientation on the line. Similarly



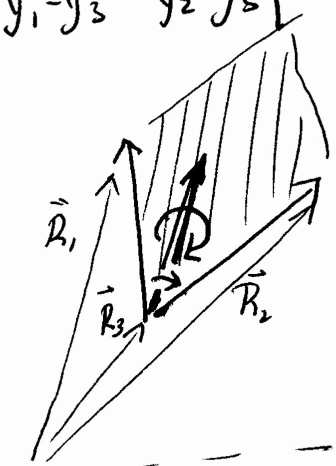
$$X_{ijk} = \begin{vmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ y_1 & y_2 & y_2 \end{vmatrix}$$



can be used to define orientation on the plane.

So, $X_{ij} = 0 \Leftrightarrow x_i = x_j$ while $X_{ij} \gtrless 0$ implies x_j is to the $\left\{\begin{matrix}\text{right}\\ \text{left}\end{matrix}\right.$ of x_i. In the latter cases X_{ij} gives the distance bet. x_i, x_j. Similarly $X_{ijk} = 0$ implies collinearity of points (0 volume) while X_{ijk} in general gives the oriented area of the parallelogram defined by vectors $R_1 - R_3, R_2 - R_3$:

$$\begin{vmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \end{vmatrix} = \begin{vmatrix} 0 & 0 & 1 \\ x_1 - x_3 & x_2 - x_3 & x_3 \\ y_1 - y_3 & y_2 - y_3 & y_3 \end{vmatrix} = \begin{vmatrix} x_1 - x_3 & x_2 - x_3 \\ y_1 - y_3 & y_2 - y_3 \end{vmatrix}$$



In general, given the vectors $\vec R_0, \vec R_1, \ldots, \vec R_n$ in $\mathbb{R}^n$, the volume of the ~~rectangle~~ parallelopiped they define is given by

(swap)

$$\hat{V}_n = \det(R_1 - R_0, R_2 - R_0, \ldots, R_n - R_0) = \left|\begin{array}{cccc|c} 0 & 0 & \cdots & 0 & 1 \\ (R_1 - R_0)_1 & (R_2 - R_0)_1 & & (R_n - R_0)_1 & R_{0,1} \\ \vdots & \vdots & & \vdots & \vdots \\ (R_1 - R_0)_n & (R_2 - R_0)_n & & (R_n - R_0)_n & R_{0n} \end{array}\right|$$

It turns out that the volume of the $(n+1)$-**simlex** formed by joining each point to the other n (i.e. triangle in $\mathbb{R}^2$, tetrahedron in $\mathbb{R}^3$ etc) is

$$V_n = \frac{1}{n!} \hat{V}_n = \frac{1}{n!} \begin{vmatrix} 1 & 1 & \cdots & 1 \\ x_{0,1} & x_{1,1} & & x_{n,1} \\ \vdots & \vdots & & \vdots \\ x_{0,n} & x_{1,n} & & x_{n,n} \end{vmatrix}$$

Distance Geometry. Given a set of points $\{R_i\}_1^N$ consider $d_{ij}^2 = \|R_i - R_j\|^2$. The matrix

$$D = \left(d_{ij}^2\right)$$

is called the distance matrix of these points. An interesting mathematical problem arises if we attempt to determine the points $\{R_i\}_1^N$ from their distance matrix. This problem has important application in molecular physics / biochemistry where some experimental techniques (NMR) determine distances between specific atoms and it is desired to determine the structure of the molecule from that information.

Here we use determinants to examine the distance matrix: consider the formula for the volume of a $(n+1)$-simplex in $\mathbb{R}^n$:

$$V_n = \frac{1}{n!}\begin{vmatrix} 1 & 1 & \cdots & 1 \\ x_{0,1} & x_{1,1} & & x_{n,1} \\ \vdots & \vdots & & \vdots \\ x_{0,n} & x_{1,n} & & x_{n,n} \end{vmatrix}$$

We have:

$$V_n^2 = \frac{(-1)^{n+1}}{2^n (n!)^2}\begin{vmatrix} 0 & 1 & \cdots & \cdots & 1 \\ 1 & 0 & d_{01}^2 & \cdots & d_{0n}^2 \\ 1 & d_{01}^2 & 0 & d_{12}^2 \cdots & d_{1n}^2 \\ \vdots & \vdots & & \ddots & \vdots \\ 1 & d_{0n}^2 & \cdots & \cdots & 0 \end{vmatrix} \qquad (1)$$

Determinants of this form built from the distance matrix by adding a row/column of 1's are called Cayley-Menger determinants.

Proof of formula (1)

Clearly

$$V = \frac{1}{n!}\begin{vmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 1 \\ \vdots & x_{0,1} & & x_{n,1} \\ & \vdots & & \vdots \\ 0 & x_{0,n} & & x_{n,n} \end{vmatrix} = -\frac{1}{n!}\begin{vmatrix} 0 & 1 & \cdots & 1 \\ 1 & 0 & \cdots & 0 \\ 0 & x_{0,1} & \cdots & x_{n,1} \\ \vdots & \vdots & & \\ 0 & x_{0,n} & \cdots & x_{n,n} \end{vmatrix}$$

$$\Rightarrow V^2 = -\frac{1}{(n!)^2}\begin{vmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & x_{0,1} & & x_{0,n} \\ \vdots & \vdots & & & \\ 1 & 0 & x_{n,1} & & x_{n,n} \end{vmatrix}\begin{vmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 1 \\ \vdots & x_{0,1} & & x_{n,1} \\ & \vdots & & \\ 0 & x_{0,n} & & x_{n,n} \end{vmatrix}$$

$$= -\frac{1}{(n!)^2}\begin{vmatrix} 0 & 1 & \cdots & 1 \\ 1 & \langle x_0,x_0\rangle & & \langle x_0,x_n\rangle \\ \vdots & & & \\ 1 & \langle x_n,x_0\rangle & & \langle x_n,x_n\rangle \end{vmatrix} \qquad (2)$$

Now: $\langle x_i,x_j\rangle = \frac{1}{2}\left(\langle x_i,x_i\rangle + \langle x_j,x_j\rangle - d_{ij}^2\right)$ (3)

$\left(\text{since } d_{ij}^2 = \langle x_j - x_i, x_j - x_i\rangle = \langle x_j,x_j\rangle + \langle x_i,x_i\rangle - 2\langle x_i,x_j\rangle\right)$

Consider the i-th row of the above determinant:

$[1, \langle x_i,x_0\rangle, \langle x_i,x_1\rangle, \ldots, \langle x_i,x_n\rangle] =$

$[1, \frac{1}{2}\langle x_i,x_i\rangle + \frac{1}{2}\langle x_0,x_0\rangle - \frac{1}{2}d_{i0}^2, \ldots, \frac{1}{2}\langle x_i,x_i\rangle + \frac{1}{2}\langle x_n,x_n\rangle - d_{in}^2]$ (4)

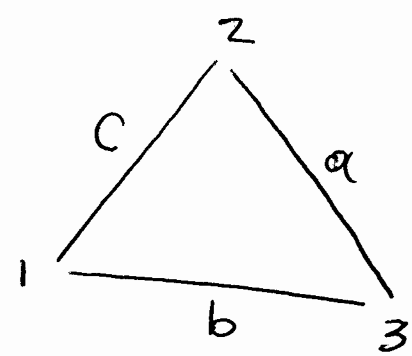
By subtracting from the i-th row an appropriate multiple of the first row $[0,1,\ldots,1]$

We can eliminate the term $\frac{1}{2}\langle x_i, x_i \rangle$ from the ith row. Similarly, the other term can be also eliminated by subtracting from the j-th column an appropriate ~~...~~ multiple of the first column. In this way we can show

$$V_n^2 = -\frac{1}{(n!)^2}\begin{vmatrix} 0 & 1 & \cdots & \cdots & 1 \\ 1 & 0 & -\frac{1}{2}d_{01}^2 & \cdots & -\frac{1}{2}d_{0n}^2 \\ \vdots & -\frac{1}{2}d_{01}^2 & 0 & & -\frac{1}{2}d_{2n}^2 \\ \vdots & \vdots & & \ddots & \vdots \\ 1 & -\frac{1}{2}d_{0n}^2 & \cdots & \cdots & 0 \end{vmatrix} \tag{5}$$

from which formula (1) follows.

For example, for the area of the triangle we have



$$V_2^2 = \frac{(-1)^3}{2^2(2!)^2}\begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & d_{12}^2 & d_{13}^2 \\ 1 & d_{12}^2 & 0 & d_{23}^2 \\ 1 & d_{13}^2 & d_{23}^2 & 0 \end{vmatrix}$$

$$= \cancel{4}\,\cancel{\frac{(-1)^3}{2^2(2!)}}\ \frac{-1}{16}\begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & c^2 & b^2 \\ 1 & c^2 & 0 & a^2 \\ 1 & b^2 & a^2 & 0 \end{vmatrix}$$

$$= \cancel{4}\,(a+b+c)(a+b-c)(a-b+c)(-a+b+c) \tag{6}$$

Problems

(1) Complete ~~Carry out~~ the details in the proof of formula (1).

(a) Show that (2) implies (5) by adding appropriate multiples of the first row and column to each row/column in the matrix.

(b) Show that (5) implies (1) by noting that multiplying a single row (or column) by a number results in the determinant being multiplied by the same number.

(2) Prove formula (6) (Heron's formula) for the area of a triangle in terms of the lengths of its sides.

References

(1) M.J. Sippl & H.A. Scheraga, Cayley-Menger coordinates, PNAS, 83(8), 1986, 2283-2287

(2) T.F. Havel, I.D. Kuntz & G.M. Crippen, The theory and practice of distance geometry, Bull. Math. Biology, 45(5), 1983, 665-720.