VI-2-2. Multi-dimensional Scaling method; MDS
VI-2-2-1. What is MDS

Purpose of Multi-dimensional Scaling method (MDS) is similar as that of Principle Component Analysis (PCA). MDS and PCA put data in multi-dimensional space for observation of relationship among data. However, forms of given data are different between MDS and PCA. A datum is composed from more than two measurement items in PCA. When we consider average vectors of each measurement item, length of vector is standard deviation, angle between vectors is arccosine, and data can be expressed by linear combinations in multi-dimensional space. Given data in MDS are distance between survey points. Rhetorically, distance means not only physical distance in Euclidean space (orthogonal space). All difference can be recognized as "distance" when it satisfies definition of distance. The definition is

1. Distance from A to B is equal to Distance from B to A
2. Distance from A to C is no longer than sum of distance from A to B and distance from B to C.

However, we consider the distances is Euclidean distance in this explanation for simplification. We learned congruency of triangle in junior high school. We can allocate 3 point on two-dimensional flat. We can add another point in three-dimensional space if we know the distance from the new point to all of the three points on the flat. Generally, the points form delta corn. Of course, they sometimes form plane locus in particular cases. Similarly, 5 points can allocate in 4-dimansional space. Theoretically, we can allocate all data in n-1-dimensional space at most, when the size of data is n. In reality, obtainable data include limited number of components and most of the dimensions come into the space by error and the space is depressed in the directions of vectors of the component made by error. Neglecting such dimensions, we can allocate all data in limited dimensional space, ideally 2 or 3-dimension. This is a simplest explanation of MDS. A datum has a number of observed measurement items in PCA. We can estimate angle between two vectors of observed value from the correlation efficiency. From the lengths of vectors (standard deviation) and angles among vectors, we can frame multi-dimensional space. This is comparable to proof of congruence of triangles by two lengths and an angle between the sides. For this reason, maximum dimension of the space is p when number of observed measurement items is p. Comparatively, space is fremed only by distance in MDS. This is comparable to proof of congruence of triangle by length of three side. Data form and calculation procedure are different, though purposes of the analyses are the same between MDS and PCA.

MDS is used widely in ecological survey, because we can identify structure of data depending on the difference among data when the difference satisfies the definition of distance.   However, we can use MDS in other disciplines.

VI-2-2-1. Calculation of MDS
VI-2-2-1-1. Problem setting of MDS

We regularly see result of MDS expressed by 2-dimensional or 3-dimentional plots in MDS to express differences of species composition among sampling site or differences of sampling site among species in studies of distribution ecology. These results are often used for categorization of sampling site or species.

Table 45. Species composition of each site (Original data).

	Species 1	Species 2	$\cdots$	Species m
Site 1	x_{11}	x_{12}	$\cdots$	x_{1m}
Site 2	x_{21}	x_{22}	$\cdots$	x_{2m}
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
Site n	x_{n1}	x_{n2}	$\cdots$	x_{nm}

We need to make table of coordinate as shown in Table 46 to express the distribution of the site in two-dimensional space.

Table 46. Coordinate table of sites.

	$Y_1(\text{axis } 1)$	$Y_2(\text{axis } 2)$
Site 1	y_{11}	y_{12}
Site 2	y_{21}	y_{22}
$\vdots$	$\vdots$	$\vdots$
Site n	y_{n1}	y_{n2}

This is already form of matrix

$$X = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nm} \end{pmatrix}, \quad Y = \begin{pmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \\ \vdots & \vdots \\ y_{n1} & y_{n2} \end{pmatrix}$$

We want to get Y from X by transformation A.

Mathematic equation is as follow、

$$XA = Y$$

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ \vdots & \vdots \\ a_{m1} & a_{m2} \end{pmatrix}$$

The equation is question of optimization of irregular simultaneous equation.

Theoretically, we could obtain optimum solution of A, when we knew Y. However, we do not know Y actually.

When we presume that Y is expressing the points expressed by 2-dimensional coordinate such as latitude and longitude and we are requested to a table expressing distances among sites, even students in junior high school can calculate the distances using the differences using Phythagorean theorem. (This is an approximate treatment. We cannot calculate distances on the surface of the earth without curvature of the earth. The author is presuming approximate flatness of surface of the earth in short distance.)

Table 47. Round robin table of distances

	Site 1	Site 2	$\cdots$	Site n
Site1	d_{11}	d_{12}	$\cdots$	d_{1n}
Site 2	d_{21}	d_{22}	$\cdots$	d_{2n}
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
Site n	d_{n1}	d_{n2}	$\cdots$	d_{nn}

$d_{ii} = 0, because\ d_{ii}$ is distance between the same site, and $d_{ij} = d_{ji}$.

Matrix expressing all distances is as follow.

$$D = \begin{pmatrix} 0 & d_{12} & \cdots & d_{1n} \\ d_{21} & 0 & \cdots & d_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ d_{n1} & d_{n2} & \cdots & 0 \end{pmatrix}$$

Matrix D is symmetric and diagonal matrix elements of D is 0. Classical metric MDS is inverse operation of this calculation in which we estimate Y from given D. Some may think that is very easy procedure. They draw a line segment corresponding to the distance of a pair of sites on a flat. Then they draw a circles of which radius are corresponding to the distance to third point from an end of the line segment and draw another circle from the other end of the line segment of which radius is is the same as the other end of the line segment. The third point is existing at the inter section of the circles. Then draw three spheres from the three points on a flat in 3-dimensional space. The 4th point is existing at the intersection of the three spheres. Repeating this we can allocate all points in (n-1)-dimensional space. This is correct. However, we have to make (n-1)-dimensional compasses for drawing distribution. There is no such a convenient tool. I think that it is possible to draw distribution using mathematical calculation. However, if the data include measurement errors, we could not fix the points clearly and last point will have huge error range. For this reason, we cannot discuss statistical significance of the result. However, it not so bad idea to find our direction to establish adequate method. I will try this innocent idea in next paragraph.

It is not necessary to perform following operation logically. However, it is simplest example of MDS and we can learn meaning of each step of MDS.

The most famous example of Phythagorean theorem is following equation.

$$3^2 + 4^2 = 5^2$$

We use this as a simple example

This is right triangle. Everyone notices a method to allocate rectangle angle at origin and allocate the other angles on vertical and horizontal axes.

$$\alpha(0,0), \quad \beta(4,0), \quad \gamma(3,0)$$

We express this in a matrix as follow

$$Y = \begin{pmatrix} 0 & 0 \\ 4 & 0 \\ 0 & 3 \end{pmatrix}$$

We do not need to use our brain to find this solution. However, this is not only one solution. This is one of the possible solution. We call this solution as solution 1.

$$\alpha'(-2,-1), \quad \beta'(2,-1), \quad \gamma'(-2.\ 2)$$

is another possible solution

For the confirmation, we calculate the distances

$$d_{\alpha'\beta'} = (2 - (-2), -1 - (-1)) = (4,0)$$
$$d_{\beta'\gamma'} = (-2 - 2, 2 - (-1)) = (-4,3)$$
$$d_{\gamma'\alpha'} = (-2 - (-2), -1 - 2) = (0,-3)$$
$$d_{\alpha'\beta'}{}^2 = 4^2$$
$$d_{\beta'\gamma'}{}^2 = (-4)^2 + 3^2 = 25 = 5^2$$
$$d_{\gamma'\alpha'}{}^2 = (-3)^2 = 3^2$$

We call this solution as solution 2.

How about next.

$$\alpha''\left(\frac{1}{2} - \sqrt{3}, -1 - \frac{\sqrt{3}}{2}\right), \quad \beta''\left(\sqrt{3} + \frac{1}{2}, 1 - \frac{\sqrt{3}}{2}\right), \quad \gamma''(-\sqrt{3} - 1, -1 + \sqrt{3})$$

Confirmation

$$d_{\alpha'\beta'}{}^2 = \left(\frac{1}{2} - \sqrt{3} - \left(\sqrt{3} + \frac{1}{2}\right)\right)^2 + \left(-1 - \frac{\sqrt{3}}{2} - \left(1 - \frac{\sqrt{3}}{2}\right)\right)^2 = 12 + 4 = 4^2$$

$$d_{\beta'\gamma'}{}^2 = \left(\sqrt{3} + \frac{1}{2} - (-\sqrt{3} - 1)\right)^2 + \left(1 - \frac{\sqrt{3}}{2} - (-1 + \sqrt{3})\right)^2 = \left(2\sqrt{3} + \frac{3}{2}\right)^2 + \left(2 - \frac{3\sqrt{3}}{2}\right)^2$$

$$= 4 \times 3 + 2 \times 3\sqrt{3} + \frac{9}{4} + 4 - 2 \times 3\sqrt{3} + \frac{9 \times 3}{4} = 12 + \frac{9}{4} + 4 + \frac{9 \times 3}{4} = 25 = 5^2$$

$$d_{\gamma'\alpha'}{}^2 = \left(-\sqrt{3} - 1 - \left(\frac{1}{2} - \sqrt{3}\right)\right)^2 + \left(-1 + \sqrt{3} - \left(-1 - \frac{\sqrt{3}}{2}\right)\right)^2 = \left(-\frac{3}{2}\right)^2 + \left(\frac{3\sqrt{3}}{2}\right)^2$$

$$= \frac{9}{4} + \frac{9 \times 3}{4} = 9 = 3^2$$

This is also one of the solutions. There are infinite number of solutions.

Solution 2: triangle $\alpha'\beta'\gamma'$ is obtained by parallel translation of triangle $\alpha\beta\gamma$ by 2 to the left and by 1 to the bottom. Triangle $\alpha''\beta''\gamma''$ is obtained by rotating $\frac{\pi}{6}$ anticlockwise.

Confirmation

Matrix of rotation anticlockwise is as follow

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

$$\begin{pmatrix} \cos\frac{\pi}{6} & \sin\frac{\pi}{6} \\ -\sin\frac{\pi}{6} & \cos\frac{\pi}{6} \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix}$$

$$\begin{pmatrix} -2 & -1 \\ 2 & -1 \\ -2 & 2 \end{pmatrix} \begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} - \sqrt{3} & -1 - \frac{\sqrt{3}}{2} \\ \sqrt{3} + \frac{1}{2} & 1 - \frac{\sqrt{3}}{2} \\ -\sqrt{3} - 1 & -1 + \sqrt{3} \end{pmatrix}$$

It is trivial that parallel translation and rotation cause no change in relative positional relationship. The implication obtained in this trial is that we can fix the shape and size of triangle from the information of distances among 3 points, though we need to consider appropriate position and angle of the viewing point by ourselves.

Question to obtain shape and size of triangle from length of three sides is typical question in elementary geometry called sine theorem and cosine theorem. Mathematically this question is essential question to obtain circumcircle of the triangle as showing in figure 79.
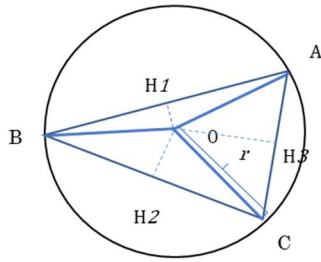
Fig. 79. Circumcircle of triangle

Here, O is center of circumcircle, and r is length of radius.

We assume lengths of each side as follow.

$$[AB] = a, \qquad [BC] = b, \qquad [CA] = c$$

Point $H_1,$ H_2, and H_3 are foots of perpendicular form center of the circle, and

$$\angle OHA = \angle OHB = \angle OHC = \frac{\pi}{2}$$

$\varDelta OAB, \varDelta OBC$ and $\varDelta OCA$ are isosceles triangle.

$$\varDelta OH_1 A \equiv \varDelta OH_1 aB 、 \varDelta OH_2 B \equiv \varDelta OH_2 C 、 \varDelta OH_3 C \equiv \varDelta OH_3 A$$

Most seplest proof of sine thoerem and cosine theorem is as follow

At first, we make following figure

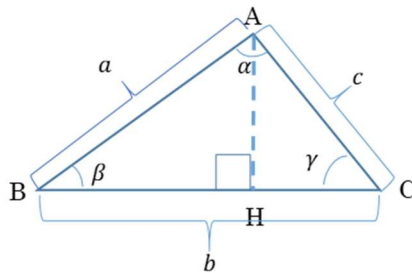

Fig.80. Sine theorem 1.

H is the foot of perpendicular from A to side BC.

$$[AH] = a \sin \beta = c \sin \gamma$$

Concerning H', the foot from C to side AB

$$c \sin \alpha = b \sin \beta$$

Concerning H", the foot from B to side AC

$$b \sin \gamma = a \sin \alpha$$

This is sine theorem

For cosine theorem,

$$[BH] = a \cos \beta$$
$$[HC] = c \cos \gamma$$
$$[BH] + [HC] = [BH] = b$$

⊿AHC is rectangle triangle. Using Pythagorean theorem,
$$[AH]^2 + [HC]^2 = [AC]^2$$
$$a^2\sin^2\beta + (b - a\cos\beta)^2 = c^2$$
$$a^2\sin^2\beta + b^2 - 2ab\cos\beta + a^2\cos^2\beta = c^2$$
$$a^2\sin^2\beta + a^2\cos^2\beta + b^2 - 2ab\cos\beta = c^2$$
$$a^2(\sin^2\beta + \cos^2\beta) + b^2 - 2ab\cos\beta = c^2$$
$$a^2 + b^2 - c^2 = 2ab\cos\beta$$
$$\cos\beta = \frac{a^2 + b^2 - c^2}{2ab}$$

Similarly,

$$\cos\alpha = \frac{a^2 + c^2 - b^2}{2ac}$$

$$\cos\gamma = \frac{b^2 + c^2 - a^2}{2bc}$$

This is enough as a proof, though we cannot understand the relation between r and length of sides. We transform sine theorem to another form.

The relation between radius r and angles is as follow.

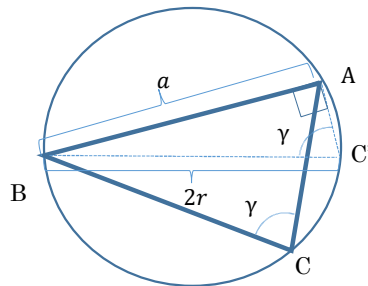Fig. 81. Sine theorem 2

We move C to C′ along the circle. At C′,
$$[BC'] = 2r$$
∠ACB and ∠AC′B are sharing the same chord AB.
$$\angle ACB = \angle AC'B = \gamma$$
Line segment BC′ is diameter of the circle.
$$\angle C'AB = \frac{\pi}{2}$$

From this,

$$\frac{a}{2r} = \sin\gamma$$

Similarly,

$$\frac{b}{2r} = \sin\alpha$$

$$\frac{c}{2r} = \sin\beta$$

This is sine theorem. Following equation is mathematically more beautiful.

$$\frac{a}{\sin\gamma} = \frac{b}{\sin\alpha} = \frac{c}{\sin\beta} = 2r$$

Frim this, we can obtain r.

$$\sin\gamma = \sqrt{1 - \cos^2\gamma} = \sqrt{1 - \left(\frac{b^2 + c^2 - a^2}{2bc}\right)^2} = \frac{1}{2bc}\sqrt{(4b^2c^2 - (b^2 + c^2 - a^2)^2)}$$

$$(b^2 + c^2 - a^2)^2 = (b^2 + c^2)^2 - 2(b^2 + c^2)a^2 + a^4$$
$$= b^4 + 2b^2c^2 + c^4 - 2a^2b^2 - 2c^2a^2 + a^4$$
$$4b^2c^2 - (b^2 + c^2 - a^2)^2 = 4b^2c^2 - b^4 - 2b^2c^2 - c^4 + 2a^2b^2 + 2c^2a^2 - a^4$$
$$= -a^4 - b^4 - c^4 + 2b^2c^2 + 2a^2b^2 + 2c^2a^2 - a^4$$
$$= a^2b^2 - \frac{1}{2}(a^2 - b^2)^2 + b^2c^2 - \frac{1}{2}(b^2 - c^2)^2 + c^2a^2 - \frac{1}{2}(c^2 - a^2)^2$$

$$\sin\gamma = = \frac{1}{2bc}\sqrt{a^2b^2 - \frac{1}{2}(a^2 - b^2)^2 + b^2c^2 - \frac{1}{2}(b^2 - c^2)^2 + c^2a^2 - \frac{1}{2}(c^2 - a^2)^2}$$

$$2r = \frac{a}{\sin\gamma} = \frac{2abc}{\sqrt{a^2b^2 - \frac{1}{2}(a^2 - b^2)^2 + b^2c^2 - \frac{1}{2}(b^2 - c^2)^2 + c^2a^2 - \frac{1}{2}(c^2 - a^2)^2}}$$

$$r = \frac{abc}{\sqrt{a^2b^2 - \frac{1}{2}(a^2 - b^2)^2 + b^2c^2 - \frac{1}{2}(b^2 - c^2)^2 + c^2a^2 - \frac{1}{2}(c^2 - a^2)^2}}$$

Using sine theorem and cosine theorem, we could obtain shape and size of triangle. The size can be expressed by r of circumcircle.

Let us go back to first figure of circumcircle (Fig.79). Central angle ∠AOB is sharing the same chord AB with angle of circumference ∠ACB. Central angle is twice of circumference angle. Therefor,

$$\angle AOB = 2\gamma$$

Similarly,

$$\angle BOC = 2\alpha$$

$$\angle COA = 2\beta$$

We have to decide the rotation of the triangle.

The author thinks that easiest calculation is the best. We allocate vector $\overrightarrow{OA}$ on horizontal axis. Vector $\overrightarrow{OB}$ is obtained by rotating vector $\overrightarrow{OA}$ 2γ anticlockwise, and vector $\overrightarrow{OC}$ is obtained by rotating vector $\overrightarrow{OA}$ 2β clockwise.

Formula of rotation anticlockwise is following matrix.

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

Conclusively,

$$OB = (r \quad 0)\begin{pmatrix} \cos 2\gamma & \sin 2\gamma \\ -\sin 2\gamma & \cos 2\gamma \end{pmatrix}$$

$$OB = (r \quad 0)\begin{pmatrix} \cos 2\gamma & \sin 2\gamma \\ -\sin 2\gamma & \cos 2\gamma \end{pmatrix}$$

$$= (r\cos 2\gamma \quad r\sin 2\gamma) = (r(1 - 2\sin^2\gamma) \quad 2r\sin\gamma\cos\gamma)$$

$$= \left(r(1 - 2\left(\frac{a}{2}\right)^2) \quad 2r\left(\frac{a}{2}\right)\left(\frac{b^2 + c^2 - a^2}{2bc}\right) \right)$$

$$= \left(r(1 - \frac{a^2}{2}) \quad ra\left(\frac{b^2 + c^2 - a^2}{2bc}\right) \right)$$

$$OC = (r \quad 0)\begin{pmatrix} \cos -2\beta & \sin -2\beta \\ -\sin -2\beta & \cos -2\beta \end{pmatrix} = (r \quad 0)\begin{pmatrix} \cos 2\beta & -\sin 2\beta \\ \sin 2\beta & \cos 2\beta \end{pmatrix} = (r\cos 2\beta \quad -r\sin 2\beta)$$

$$= \left(r(1 - \frac{c^2}{2}) \quad ra\left(\frac{b^2 + a^2 - c^2}{2ab}\right) \right)$$

The author does this calculation for the first time in 50yeas after graduation of junior high school. We cannot expand this method to higher dimensional space directly. For this reason, we can say that we did meaningless trial. However, when we can make triangle as a flat, we can make multi-dimensional polyhedron in multi-dimensional space by connecting triangle. Following is an example of 4 points in 3-dimensional space.
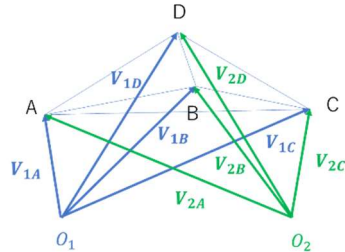

Fig.82. Cubic diagram of 4 points and origin.

When distances between A and B, A and C, A and D, B and C, B and D and D and C are

given correctly, we can make tetrahedron. When we fix the origin of the coordinate, we can express the distance as follow.

$$\overline{AB} = [V_A - V_B]$$
$$\overline{AC} = [V_A - V_C]$$
$$\overline{AD} = [V_A - V_D]$$
$$\overline{BC} = [V_B - V_C]$$
$$\overline{BD} = [V_B - V_D]$$
$$\overline{CD} = [V_C - V_D]$$

This relation is stable when we move the origin of vectors to the other points as shown in figure 82. In the case there are more than 5 points, if all distances are measured correctly and they have only 3-dimensional elements. We can make more complex polyhedron in 3-dimensional space. As shown in the figure 82, we can allocate the origin of the space in any point in the space.

VI-2-2-1-3. Classical MDS (Metric MDS)

Given data is following distance matrix.

$$D = \begin{pmatrix} 0 & D_{12} & \cdots & D_{1n} \\ D_{21} & 0 & \cdots & D_{2n} \\ \cdots & \cdots & \ddots & \vdots \\ D_{n1} & D_{n2} & \cdots & 0 \end{pmatrix}$$

We define matrix of square of distances as follow.

$$D^2 = \begin{pmatrix} 0 & D_{12}{}^2 & \cdots & D_{1n}{}^3 \\ D_{21}{}^2 & 0 & \cdots & D_{2n}{}^2 \\ \cdots & \cdots & \ddots & \vdots \\ D_{n1}{}^2 & D_{n2}{}^2 & \cdots & 0 \end{pmatrix}$$

In this chapter, D^2 is not square of D.

We want to know the vectors from origin to each point. The matrix of vector is as follow.

$$V = \begin{pmatrix} V_1 \\ V_2 \\ \vdots \\ V_n \end{pmatrix}$$

$$D_{ij2} = [V_i - V_j]$$

When the Vectors have m-dimension

$$V = \begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1m} \\ v_{21} & v_{22} & \cdots & v_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nm} \end{pmatrix}$$

From trial of our innocent idea, we could make clear the procedure of calculation of MDS, and we understood that we have to allocate origin of coordinate by ourselves considering visual effects. This is essential, as coordinate and viewing direction are strongly affect

our recognition of phenomena. Most general idea is allocating coordinate on the median point of the data. Median point is representative of all data. When we select origine of coordinate on median point of the data, that means we treat all data in even weight. This makes easier the calculation statistical calculations.

Grabbing vertex of triangle formed by two vectors at origin putting the distance on the base of triangle. Making tetrahedron from 3 triangles. Lining the tetrahedrons in all the direction of the space. This procedure is analogical image of MDS. For this, we use centralization matrix. Generally, we use parallel translation for this procedure. We can express the procedure in a formula by using centralization matrix.

It is too hastily to show the formula. The author explains the function of centralization matrix step by step from single parallel translation.

Translation of coordination to median point is subtraction of average coordinate from each coordinate datum. This is expressed as follow.

$$v_{ij} - \frac{1}{n}\sum_{k=1}^{n} v_{kj}$$

Second term of the equation means average (median point).

When we expand sign of sum, it expressed as follow.

$$v_{ij} - \frac{1}{n}v_{1j} - \frac{1}{n}v_{2j} - \cdots \frac{1}{n}v_{2j}$$

Then we transform this as follow

$$-\frac{1}{n}v_{1j} - \frac{1}{n}v_{2j} - \cdots + \left(1 - \frac{1}{n}\right)v_{ij} - \cdots - \frac{1}{n}v_{nj}$$

This can be expressed by following inner product of two vectors.

$$\left(-\frac{1}{n}v_{1j} - \frac{1}{n}v_{2j} - \cdots + \left(1 - \frac{1}{n}\right)v_{ij} - \cdots - \frac{1}{n}v_{nj}\right) = \left(-\frac{1}{n} \quad -\frac{1}{n} \quad \cdots 1 - \frac{1}{n} \cdots -\frac{1}{n}\right)\begin{pmatrix} v_{1j} \\ v_{2j} \\ \vdots \\ v_{ij} \\ \vdots \\ v_{nj} \end{pmatrix}$$

We can expressed all translation by following multiplication of matrixes.

$$V = \begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1m} \\ v_{21} & v_{22} & \cdots & v_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nm} \end{pmatrix}$$

$$V' = \begin{pmatrix} 1 - \frac{1}{n} & -\frac{1}{n} & \cdots & -\frac{1}{n} \\ -\frac{1}{n} & 1 - \frac{1}{n} & \cdots & -\frac{1}{n} \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{n} & -\frac{1}{n} & \cdots & 1 - \frac{1}{n} \end{pmatrix}\begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1m} \\ v_{21} & v_{22} & \cdots & v_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nm} \end{pmatrix}$$

We call following matrix as centralizing matrix.

$$
G = \begin{pmatrix}
1 - \dfrac{1}{n} & -\dfrac{1}{n} & \cdots & -\dfrac{1}{n} \\
-\dfrac{1}{n} & 1 - \dfrac{1}{n} & \cdots & -\dfrac{1}{n} \\
\vdots & \vdots & \ddots & \vdots \\
-\dfrac{1}{n} & -\dfrac{1}{n} & \cdots & 1 - \dfrac{1}{n}
\end{pmatrix}
$$

Formula 76

General expression of the matrix is as follow

$$
G_n = I_n - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n{}^{\mathrm{T}}
$$

I_n is $n \times n$ unit vector.

$$
\mathbf{1}_n = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}
$$

$$
\mathbf{1}_n{}^{\mathrm{T}} = (1 \quad 1 \quad \cdots \quad 1)
$$

From this,

$$
\mathbf{1}_n \mathbf{1}_n{}^{\mathrm{T}} = \begin{pmatrix}
1 & 1 & \cdots & 1 \\
1 & 1 & \cdots & 1 \\
\vdots & \vdots & \ddots & \vdots \\
1 & 1 & \cdots & 1
\end{pmatrix}
$$

$$
\left(\mathbf{1}_n \mathbf{1}_n{}^{\mathrm{T}}\right)^2 = \begin{pmatrix}
n & n & \cdots & n \\
n & n & \cdots & n \\
\vdots & \vdots & \ddots & \vdots \\
n & n & \cdots & n
\end{pmatrix} = n \begin{pmatrix}
1 & 1 & \cdots & 1 \\
1 & 1 & \cdots & 1 \\
\vdots & \vdots & \ddots & \vdots \\
1 & 1 & \cdots & 1
\end{pmatrix} = n \mathbf{1}_n \mathbf{1}_n{}^{\mathrm{T}}
$$

Centralizing matrix G_n has unique and convenient characteristics.

First,

$$
G_n{}^k = G_n
$$

Confirmation

$$
G_n{}^2 = \left(I_n - \frac{1}{n}\mathbf{1}_n\mathbf{1}_n{}^{\mathrm{T}}\right)\left(I_n - \frac{1}{n}\mathbf{1}_n\mathbf{1}_n{}^{\mathrm{T}}\right)
$$

$$
= I_n I_n - 2 I_n \frac{1}{n}\mathbf{1}_n\mathbf{1}_n{}^{\mathrm{T}} + \frac{1}{n^2}\left(\mathbf{1}_n\mathbf{1}_n{}^{\mathrm{T}}\right)^2
$$

$$
= I_n - \frac{1}{n}\mathbf{1}_n\mathbf{1}_n{}^{\mathrm{T}} = G_n
$$

$$
\because I_n I_n = I_n, \; I_n \mathbf{1}_n\mathbf{1}_n{}^{\mathrm{T}} = \mathbf{1}_n\mathbf{1}_n{}^{\mathrm{T}}, \left(\mathbf{1}_n\mathbf{1}_n{}^{\mathrm{T}}\right)^2 = n\mathbf{1}_n\mathbf{1}_n{}^{\mathrm{T}}
$$

This is logically trivial. Because, center is only one. When we centralize data, we cannot centralize any more. However, this character is important in the calculation. As an

example, we centralize $\mathbf{A} = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$ by $\boldsymbol{G}_n$.

This is the inverse operation of the operation in which we make centralizing matrix.

$$\boldsymbol{G}_4\boldsymbol{A} = \left(\boldsymbol{I}_4 - \frac{1}{4}\boldsymbol{1}_4\boldsymbol{1}_4{}^{\mathrm{T}}\right)\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} - \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$$

$$= \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} - \frac{1}{4}\begin{pmatrix} a+b+c+d \\ a+b+c+d \\ a+b+c+d \\ a+b+c+d \end{pmatrix}$$

$$= \begin{pmatrix} a - \dfrac{a+b+c+d}{4} \\ b - \dfrac{a+b+c+d}{4} \\ c - \dfrac{a+b+c+d}{4} \\ d - \dfrac{a+b+c+d}{4} \end{pmatrix}$$

Second term in each factor is written by fraction. The fraction means average.

$$\boldsymbol{G}_4(\boldsymbol{G}_4\boldsymbol{A}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} a - \dfrac{a+b+c+d}{4} \\ b - \dfrac{a+b+c+d}{4} \\ c - \dfrac{a+b+c+d}{4} \\ d - \dfrac{a+b+c+d}{4} \end{pmatrix} - \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} a - \dfrac{a+b+c+d}{4} \\ b - \dfrac{a+b+c+d}{4} \\ c - \dfrac{a+b+c+d}{4} \\ d - \dfrac{a+b+c+d}{4} \end{pmatrix}$$

$$= \begin{pmatrix} a - \dfrac{a+b+c+d}{4} \\ b - \dfrac{a+b+c+d}{4} \\ c - \dfrac{a+b+c+d}{4} \\ d - \dfrac{a+b+c+d}{4} \end{pmatrix} - \frac{1}{4}\begin{pmatrix} a+b+c+d-(a+b+c+d) \\ a+b+c+d-(a+b+c+d) \\ a+b+c+d-(a+b+c+d) \\ a+b+c+d-(a+b+c+d) \end{pmatrix}$$

$$= \begin{pmatrix} a - \dfrac{a+b+c+d}{4} \\ b - \dfrac{a+b+c+d}{4} \\ c - \dfrac{a+b+c+d}{4} \\ d - \dfrac{a+b+c+d}{4} \end{pmatrix} - 0 = \begin{pmatrix} a - \dfrac{a+b+c+d}{4} \\ b - \dfrac{a+b+c+d}{4} \\ c - \dfrac{a+b+c+d}{4} \\ d - \dfrac{a+b+c+d}{4} \end{pmatrix} = \boldsymbol{G_4 A}$$

We confirmed

$$\boldsymbol{G_n(G_n A)} = \boldsymbol{(G_n G_n)^2 A} = \boldsymbol{G_n A}$$

Secondly, $\boldsymbol{G_n}$ has following character.

$$\boldsymbol{G_n 1_n} = \boldsymbol{1_n}^{\mathrm{T}} \boldsymbol{G_n} = 0$$

Confirmation

$$\boldsymbol{G_n 1_n} = \left(\boldsymbol{I_n} - \frac{1}{n} \boldsymbol{1_n 1_n}^{\mathrm{T}} \right) \boldsymbol{1_n} = \boldsymbol{I_n 1_n} - \frac{1}{n} \boldsymbol{1_n} (\boldsymbol{1_n}^{\mathrm{T}} \boldsymbol{1_n}) = \boldsymbol{1_n} - \frac{1}{n} n \boldsymbol{1_n} = 0$$

$$\boldsymbol{G_n 1_n} = \boldsymbol{1_n}^{\mathrm{T}} \left(\boldsymbol{I_n} - \frac{1}{n} \boldsymbol{1_n 1_n}^{\mathrm{T}} \right) = \boldsymbol{1_n}^{\mathrm{T}} \boldsymbol{I_n} - \frac{1}{n} (\boldsymbol{1_n}^{\mathrm{T}} \boldsymbol{1_n}) \boldsymbol{1_n}^{\mathrm{T}} = \boldsymbol{1_n}^{\mathrm{T}} - \frac{1}{n} n \boldsymbol{1_n}^{\mathrm{T}} = 0$$

We go back to matrix $\boldsymbol{V}$.

This is a matrixed obtained by lining up row vectors vertically as follow.

$$\boldsymbol{V} = \begin{pmatrix} \boldsymbol{V_1} \\ \boldsymbol{V_2} \\ \vdots \\ \boldsymbol{V_n} \end{pmatrix} = \begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1m} \\ v_{21} & v_{22} & \cdots & v_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nm} \end{pmatrix}$$

We consider matrix $\boldsymbol{VV}^{\mathrm{T}}$.

The author calls the matrix "matrix of inner products" personally. Because we call $\boldsymbol{V^{\mathrm{T}}V}$ of which factors are composed from variance and covariance of elements of data as variance-covariance matrix, and factors of $\boldsymbol{VV^{\mathrm{T}}}$ are inner products of vector. Actually, this naming is not used generally. This naming may make confusion because matrix is a kind of vector, because we can consider inner product between matrixes, $\boldsymbol{V \cdot V^{\mathrm{T}}}$. We call this inner product of matrix. Inner product of matrix is a scalar and name of inner product of matrix is authorized. It is better not to use "matrix of inner products" in other places in order prevent confusion. However, we call $\boldsymbol{VV^{\mathrm{T}}}$ as "matrix of inner products" here. It is important to confirm $\boldsymbol{VV^{\mathrm{T}}} \neq \boldsymbol{V \cdot V^{\mathrm{T}}}$

$$\boldsymbol{VV}^{\mathrm{T}} = \begin{pmatrix} \boldsymbol{V_1} \\ \boldsymbol{V_2} \\ \vdots \\ \boldsymbol{V_n} \end{pmatrix} (\boldsymbol{V_1} \quad \boldsymbol{V_2} \quad \cdots \quad \boldsymbol{V_n}) = \begin{pmatrix} \boldsymbol{V_1 \cdot V_1}^{\mathrm{T}} & \boldsymbol{V_1 \cdot V_2}^{\mathrm{T}} & \cdots & \boldsymbol{V_1 \cdot V_n}^{\mathrm{T}} \\ \boldsymbol{V_2 \cdot V_1}^{\mathrm{T}} & \boldsymbol{V_2 \cdot V_2}^{\mathrm{T}} & \cdots & \boldsymbol{V_2 \cdot V_n}^{\mathrm{T}} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{V_n V_1}^{\mathrm{T}} & \boldsymbol{V_n V_2}^{\mathrm{T}} & \cdots & \boldsymbol{V_n V_n}^{\mathrm{T}} \end{pmatrix}$$

$V_i \cdot V_j^{\mathrm{T}}$ is inner product of vector V_i and V_j

$$V_i \cdot V_j^{\mathrm{T}} = (v_{i1} \quad \cdots \quad v_{in}) \begin{pmatrix} v_{j1} \\ \vdots \\ v_{jn} \end{pmatrix}$$

Then we consider matrix of inner product of centralized matrix.

$$V' = G_m V$$

From cosine theorem, we can express the relation among vectors as follow.

$$2V'_i \cdot V'_j = [V'_i]^2 + [V'_j]^2 - [V'_i - V'_j]^2$$

The last term of the right side is square of distance between arrow heads of both vectors.

$$[V'_i - V'_j]^2 = d_{ij}^2$$
$$2V'_i \cdot V'_j = [V'_i]^2 + [V'_j]^2 - d_{ij}^2$$

This is relation in each factor of matrix. We express this in the form of matrix.

$$2V'V'^T = 1n1n^{\mathrm{T}} diag(V'V'^T) + diag V'V'^T 1n1n^{\mathrm{T}} - D^2$$

In this, $diag A$ is matrix composed only from diagonal factor of matrix A.

Expansion of this calculation is as follow.

$$2V'V'^T = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix} \begin{pmatrix} V'_1{}^2 & 0 & \cdots & 0 \\ 0 & V'_2{}^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & V'_n{}^2 \end{pmatrix} + \begin{pmatrix} V'_1{}^2 & 0 & \cdots & 0 \\ 0 & V'_2{}^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & V'_n{}^2 \end{pmatrix} \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix} - D^2$$

We transform left side by

$$V'V'^T = G_n V(G_n V)^T = G_n VV^{\mathrm{T}} G_n{}^{\mathrm{T}} = G_n VV^{\mathrm{T}} G_n$$

$$2G_n VV^{\mathrm{T}} G_n = \begin{pmatrix} V'_1{}^2 & V'_2{}^2 & \cdots & V'_n{}^2 \\ V'_1{}^2 & V'_2{}^2 & \cdots & V'_n{}^2 \\ \vdots & \vdots & \ddots & \vdots \\ V'_1{}^2 & V'_2{}^2 & \cdots & V'_n{}^2 \end{pmatrix} + \begin{pmatrix} V'_1{}^2 & V'_1{}^2 & \cdots & V'_1{}^2 \\ V'_2{}^2 & V'_2{}^2 & \cdots & V'_2{}^2 \\ \vdots & \vdots & \ddots & \vdots \\ V'_n{}^2 & V'_n{}^2 & \cdots & V'_n{}^2 \end{pmatrix} - D^2$$

We multiply G_n from left and right to both sides.

$$2G_n{}^2 VV^{\mathrm{T}} G_n{}^2 = G_n \begin{pmatrix} V'_1{}^2 & V'_2{}^2 & \cdots & V'_n{}^2 \\ V'_1{}^2 & V'_2{}^2 & \cdots & V'_n{}^2 \\ \vdots & \vdots & \ddots & \vdots \\ V'_1{}^2 & V'_2{}^2 & \cdots & V'_n{}^2 \end{pmatrix} G_n + G_n \begin{pmatrix} V'_1{}^2 & V'_1{}^2 & \cdots & V'_1{}^2 \\ V'_2{}^2 & V'_2{}^2 & \cdots & V'_2{}^2 \\ \vdots & \vdots & \ddots & \vdots \\ V'_n{}^2 & V'_n{}^2 & \cdots & V'_n{}^2 \end{pmatrix} G_n - G_n D^2 G_n$$

From the characteristic of Centralizing matrix.

$$G_n{}^2 = G_n$$

Left size is

$$G_n{}^2 VV^{\mathrm{T}} G_n{}^2 = G_n VV^{\mathrm{T}} G_n$$

Concerning right side, first and second term are 0. Confirmation is as follow.

$$G_n \begin{pmatrix} {V'}_1{}^2 & {V'}_2{}^2 & \cdots & {V'}_n{}^2 \\ {V'}_1{}^2 & {V'}_2{}^2 & \cdots & {V'}_n{}^2 \\ \vdots & \vdots & \ddots & \vdots \\ {V'}_1{}^2 & {V'}_2{}^2 & \cdots & {V'}_n{}^2 \end{pmatrix}$$

When we focus on first column of second vector. First column is lining up of square of the same vector as follow. This means that first row of first column of obtainable matrix is as follow.

$$G_n \begin{pmatrix} {V'}_1{}^2 \\ {V'}_1{}^2 \\ \vdots \\ {V'}_1{}^2 \end{pmatrix} = {V'}_1{}^2 G_n \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} = 0$$

$$\therefore G_n \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} = 0 \text{ from character of centralizing matrix}$$

Similarly, all the other factors in obtainable matrix are 0. Consequently,

$$G_n \begin{pmatrix} {V'}_1{}^2 & {V'}_2{}^2 & \cdots & {V'}_n{}^2 \\ {V'}_1{}^2 & {V'}_2{}^2 & \cdots & {V'}_n{}^2 \\ \vdots & \vdots & \ddots & \vdots \\ {V'}_1{}^2 & {V'}_2{}^2 & \cdots & {V'}_n{}^2 \end{pmatrix} = 0$$

Similarly, concerning second term,

$$\begin{pmatrix} {V'}_1{}^2 & {V'}_1{}^2 & \cdots & {V'}_1{}^2 \\ {V'}_2{}^2 & {V'}_2{}^2 & \cdots & {V'}_2{}^2 \\ \vdots & \vdots & \ddots & \vdots \\ {V'}_{1n}{}^2 & {V'}_n{}^2 & \cdots & {V'}_n{}^2 \end{pmatrix} G_n$$

First row of obtainable matrix is as follow

$$\begin{pmatrix} {V_1}^2 & {V_1}^2 & \cdots & {V_1}^2 \end{pmatrix} G_n = {V_1}^2 \begin{pmatrix} 1 & 1 & \cdots & 1 \end{pmatrix} G_n = 0$$

Similarly, other factors in obtainable matrix is 0, and

$$\begin{pmatrix} {V'}_1{}^2 & {V'}_1{}^2 & \cdots & {V'}_1{}^2 \\ {V'}_2{}^2 & {V'}_2{}^2 & \cdots & {V'}_2{}^2 \\ \vdots & \vdots & \ddots & \vdots \\ {V'}_n{}^2 & {V'}_n{}^2 & \cdots & {V'}_n{}^2 \end{pmatrix} G_n = 0$$

Conclusively,

$$2G_n V V^{\mathrm{T}} G_n = -G_n D^2 G_n$$

By this transformation, right side distances matrix can be explained by "matrix of inner products".

We can give position in a space to D^2 which was roving in inanity by folding G_n. The author can give safe refuge to Hebrews. The author is brushing brisk breeze doing good.

We want to know $G_n V$

$$Y = G_n V$$

$$Y^{\mathrm{T}} = (G_n V)^{\mathrm{T}} = V^{\mathrm{T}} G_n$$

$$YY^{\mathrm{T}} = G_n V V^{\mathrm{T}} G_n = -\frac{1}{2} G_n D^2 G_n$$

At first, we calculate,

$$Z = -\frac{1}{2} G_n D^2 G_n$$

Then we do spectral decomposition of Z

$$Z = P \Lambda P^{-1} = P \Lambda^{\frac{1}{2}} \Lambda^{\frac{1}{2}} P^{-1} = P \Lambda^{\frac{1}{2}} \Lambda^{\frac{1}{2}} P^{\mathrm{T}} = P \Lambda^{\frac{1}{2}} \left(P \Lambda^{\frac{1}{2}} \right)^{\mathrm{T}}$$

$$-\frac{1}{2} G_n D^2 G_n = P \Lambda^{\frac{1}{2}} \left(P \Lambda^{\frac{1}{2}} \right)^{\mathrm{T}}$$

Then

$$Y = P \Lambda^{\frac{1}{2}}$$

Formula 77

VI-2-2-2. Theoretical discussions about classical MDS

There is a data X which obtained by observation. Each datum of X is composed from m elements. X is expressed by n data which has m elements as following matrix.

$$X = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nm} \end{pmatrix}$$

It is difficult to understand structure of distribution of all data and relationship among data, when a lot of elements is existing. We want to summarize the data combining several elements to reduce the number of elements from m to $l\,(l < m)$. This is motivation of MDS and PCA. Most extreme case we want reduce the number to only one $(l = 1)$.

$$\tilde{y}_1 = a_1 x_{11} + a_2 x_{12} + \cdots + a_n x_{1n}$$

As matrix calculation

$$\tilde{Y} = X A^{\mathrm{T}}$$

$$A = (a_1 \quad a_2 \quad \cdots \quad a_n)$$

In the case $l > 1$,

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \vdots & \vdots & \cdots & \vdots \\ a_{l1} & a_{l2} & & a_{ln} \end{pmatrix}$$

$$\widetilde{Y} = XA^{\mathrm{T}} = \begin{pmatrix} \tilde{y}_{11} & \cdots & \tilde{y}_{1l} \\ \vdots & \ddots & \vdots \\ \tilde{y}_{n1} & \cdots & \tilde{y}_{nl} \end{pmatrix}$$

When number of data (n) is larger than number of elements (p), the simultaneous equation is irregular, and data include error generally. For this reason, we optimize A by minimizing differences between observed data and expected values.

$$\|Y - \widetilde{Y}\|$$

$\|Y - \widetilde{Y}\|$ is norm expressing the magnitude of difference between two vectors. We consider Euclidian norm in orthogonal space.

$$\|Y - \widetilde{Y}\|^2 = \left(\left[Y - \widetilde{Y}\right]\right)^2$$

In the MDS which express the data in plotting data in 2-dimensinal flat is summarizing the all elements to two representative elements. In this meaning, MDS is a kind of approximation by least square method. However, the data are given as form of the difference of among elements. Thus, we have to make "matrix of inner products after centralization of the given data as follow.

$$Z = -\frac{1}{2} G_n D^2 G_n$$

Then, we implement diagonalization of this matrix in order to make form of $P\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}}P^{\mathrm{T}}$.。

$$P\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}}P^{\mathrm{T}} = \left(P\Lambda^{\frac{1}{2}}\right)\left(P\Lambda^{\frac{1}{2}}\right)^{\mathrm{T}}$$

Right side is form of "matrix of inner products" XX^{T}, when we consider

$$X = P\Lambda^{\frac{1}{2}}$$

In singular value decomposition, we made variance-covariance matrix $X^{\mathrm{T}}X$ and "matrix of inner products" XX^{T}, and then we diagonalize both matrixes.

$$XX^{\mathrm{T}} = P\Lambda P^{\mathrm{T}}$$
$$X^{\mathrm{T}}X = Q\Lambda Q^{\mathrm{T}}$$
$$P = U$$
$$Q = V$$
$$X = U\Sigma V^{\mathrm{T}} = U\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}}V^{\mathrm{T}}$$

In MDS, we are not given vector data which has direction. We cannot make variance-covariance matrix and matrix of inner products directly.

However, we can give direction to the data by centralization, and we can diagonalize $G_n D^2 G_n$ considering $X = G_n D$

$$XX^{\mathrm{T}} = P\Lambda P^{\mathrm{T}}$$

When we consider that "matrix of inner products" is reverse of variance-covariance matrix, we can say that MDS is reverse of PCA. We are expecting that components which have higher contribution rate are concentrated in 2 or 3 directions in PCA and MDS and make 2-dimensional plot or 3-dimensional plot. Most interesting function of MDS is plotting data of which dimension we do not know on 2 or 3dimensional space. However, components do not always concentrate to seldom direction. Analyzers who know that MDS is selecting several representative axes from orthogonal axes can understand importance of confirmation of cumulative contribution ratio in analysis. The author personally interested in drawing plotts using miner importance axis. We may discover new findings from minor relation. PCA and MDS are methods to see phenomena from various viewing points. Knowing mathematical meaning of MDS, you can use this tool for unique and interesting findings.

VI-2-2-3. Several examples of calculation of MDS.

The author perform calculation of MDS of simple examples in this paragraph aiming deepening the calculation and meaning of MDS and PCA.

Example 1 (equilateral triangle)

We allocate of vertexes of equilateral triangle which length of sides is 1 in a space. It is easy to understand direction of viewing point, because, three points make triangle on a flat naturally. We confirm whether the triangle can be drawn on 2-dimensional flat from the information of distances among vertexes.

Round robin square of distance matrix is as follow

$$D^2 = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

Centralization

$$GnD^2Gn = \begin{pmatrix} 1-\dfrac{1}{3} & -\dfrac{1}{3} & -\dfrac{1}{3} \\ -\dfrac{1}{3} & 1-\dfrac{1}{3} & -\dfrac{1}{3} \\ -\dfrac{1}{3} & -\dfrac{1}{3} & 1-\dfrac{1}{3} \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1-\dfrac{1}{3} & -\dfrac{1}{3} & -\dfrac{1}{3} \\ -\dfrac{1}{3} & 1-\dfrac{1}{3} & -\dfrac{1}{3} \\ -\dfrac{1}{3} & -\dfrac{1}{3} & 1-\dfrac{1}{3} \end{pmatrix}$$

$$\begin{pmatrix} \dfrac{2}{3} & -\dfrac{1}{3} & -\dfrac{1}{3} \\ -\dfrac{1}{3} & \dfrac{2}{3} & -\dfrac{1}{3} \\ -\dfrac{1}{3} & -\dfrac{1}{3} & \dfrac{2}{3} \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} \dfrac{2}{3} & -\dfrac{1}{3} & -\dfrac{1}{3} \\ -\dfrac{1}{3} & \dfrac{2}{3} & -\dfrac{1}{3} \\ -\dfrac{1}{3} & -\dfrac{1}{3} & \dfrac{2}{3} \end{pmatrix}$$

$$\begin{pmatrix} -\dfrac{2}{3} & \dfrac{1}{3} & \dfrac{1}{3} \\ \dfrac{1}{3} & -\dfrac{2}{3} & \dfrac{1}{3} \\ \dfrac{1}{3} & \dfrac{1}{3} & -\dfrac{2}{3} \end{pmatrix} \begin{pmatrix} \dfrac{2}{3} & -\dfrac{1}{3} & -\dfrac{1}{3} \\ -\dfrac{1}{3} & \dfrac{2}{3} & -\dfrac{1}{3} \\ -\dfrac{1}{3} & -\dfrac{1}{3} & \dfrac{2}{3} \end{pmatrix}$$

$$\begin{pmatrix} -\dfrac{6}{9} & \dfrac{3}{9} & \dfrac{3}{9} \\ \dfrac{3}{9} & -\dfrac{6}{9} & \dfrac{3}{9} \\ \dfrac{3}{9} & \dfrac{3}{9} & -\dfrac{6}{9} \end{pmatrix} = \dfrac{1}{3}\begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}$$

We diagonalize $\begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}$.

We solve eigen equation to obtain eigenvalue.

○

$$\begin{vmatrix} -2-\lambda & 1 & 1 \\ 1 & -2-\lambda & 1 \\ 1 & 1 & -2-\lambda \end{vmatrix} = 0$$

$$-(2+\lambda)^3 + 2 + 3(2+\lambda)$$

$$-(\lambda^2 + 4\lambda + 4)(2+\lambda) + 2 + 3(2+\lambda)$$

$$-\lambda^3 - 4\lambda^2 - 4\lambda - 2\lambda^2 - 8\lambda - 8 + 2 + 6 + 3\lambda$$

$$-\lambda^3 - 6\lambda^2 - 12\lambda - 8 + 2 + 6 + 3\lambda = 0$$

$$-\lambda^3 - 6\lambda^2 - 9\lambda = 0$$

$$\lambda(\lambda + 3)^2 = 0$$

$$\lambda = 0, \lambda = -3$$

We calculate eigenvector belonging to $\lambda = 0$.

$$\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$2x_1 - x_2 - x_3 = 0$$

$$-x_1 + 2x_2 - x_3 = 0$$

$$-x_1 - x_2 + 2x_3 = 0$$

From all equation we obtain

$$x_1 = x_2 = x_3$$

We select following vector as most simple eigen vector.

$$\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

Then we calculate eigenvector belonging to $\lambda = -3$.

$$\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = -3\lambda = 0$$

$$-2x_1 + x_2 + x_3 = -3x_1$$

$$x_1 - 2x_2 + x_3 = -3x_2$$

$$x_1 + x_2 - 3x_3 = -3x_3$$

From all equation

$$x_1 + x_2 + x_3 = 0$$

We select following equation.

$$\begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix}$$

We make the other eigen vector belonging to $\lambda = -3$ using orthogonality. The vector should be orthogonal to two vectors obtained in upper calculation.

$$(x_1 \quad x_2 \quad x_3)\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = 0$$

$$(x_1 \quad x_2 \quad x_3)\begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix} = 0$$

$$x_1 + x_2 + x_3 = 0$$

$$2x_1 - x_2 - x_3 = 0$$

We solve this simultaneous equation and obtain

$$x_1 = 0, x_2 = -x_3$$

We select following vector as simplest eigenvector.

$$\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$$

From upper equation we could obtain diagonalizing matrix of $\begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}$ as follow.

$$P = \begin{pmatrix} -2 & 0 & 1 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \end{pmatrix}$$

It is not necessary, though the author transform this to unit vector for future convenience.

$$P = \begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & 0 & \dfrac{1}{\sqrt{3}} \\ -\dfrac{1}{\sqrt{6}} & \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \\ -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}$$

P is diagonalization matrix of symmetric matrix. Consequently,

$$P^{-1} = P^{\mathrm{T}}$$

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} = \begin{pmatrix} -3 & 0 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$$

Using these matrixes, we can diagonalize $\boldsymbol{GnD^2Gn}$ as follow.

$$\boldsymbol{GnD^2Gn = P\Lambda P^{\mathrm{T}}}$$

$$\frac{1}{3}\begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix} = \frac{1}{3}\begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & 0 & \dfrac{1}{\sqrt{3}} \\[2mm] -\dfrac{1}{\sqrt{6}} & \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \\[2mm] -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}\begin{pmatrix} -3 & 0 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{6}} \\[2mm] 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \\[2mm] \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}$$

$$= \frac{1}{3}\begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & 0 & \dfrac{1}{\sqrt{3}} \\[2mm] -\dfrac{1}{\sqrt{6}} & \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \\[2mm] -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}\begin{pmatrix} -3 & 0 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{6}} \\[2mm] 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \\[2mm] \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}$$

$$\begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & 0 & \dfrac{1}{\sqrt{3}} \\[2mm] -\dfrac{1}{\sqrt{6}} & \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \\[2mm] -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{6}} \\[2mm] 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \\[2mm] \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}$$

$$\boldsymbol{Z = \frac{GnD^2Gn}{-2}}$$

$$= \frac{1}{-2}\begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & 0 & \dfrac{1}{\sqrt{3}} \\[2mm] -\dfrac{1}{\sqrt{6}} & \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \\[2mm] -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{6}} \\[2mm] 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \\[2mm] \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}$$

$$= \begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & 0 & \dfrac{1}{\sqrt{3}} \\[2mm] -\dfrac{1}{\sqrt{6}} & \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \\[2mm] -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}\begin{pmatrix} \dfrac{1}{2} & 0 & 0 \\[2mm] 0 & \dfrac{1}{2} & 0 \\[2mm] 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{6}} \\[2mm] 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \\[2mm] \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}$$

We transform this to the form of $\boldsymbol{P\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}}P^{\mathrm{T}}}$.

$$P\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}}P^{\mathrm{T}} = \begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & 0 & \dfrac{1}{\sqrt{3}} \\ -\dfrac{1}{\sqrt{6}} & \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \\ -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \dfrac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \dfrac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{6}} \\ 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \\ \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} \end{pmatrix}$$

This is result means eigenvector $\begin{pmatrix} \dfrac{1}{\sqrt{3}} \\ \dfrac{1}{\sqrt{3}} \\ \dfrac{1}{\sqrt{3}} \end{pmatrix}$ has no expansion to its direction. We can neglect

this axis.

$$P\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}}P^{\mathrm{T}} = \begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & 0 \\ -\dfrac{1}{\sqrt{6}} & \dfrac{1}{\sqrt{2}} \\ -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 \\ 0 & \dfrac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 \\ 0 & \dfrac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{6}} \\ 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \end{pmatrix}$$

$$P\Lambda^{\frac{1}{2}} = \begin{pmatrix} \dfrac{\sqrt{2}}{\sqrt{3}} & 0 \\ -\dfrac{1}{\sqrt{6}} & \dfrac{1}{\sqrt{2}} \\ -\dfrac{1}{\sqrt{6}} & -\dfrac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 \\ 0 & \dfrac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \dfrac{1}{\sqrt{3}} & 0 \\ -\dfrac{1}{2\sqrt{3}} & \dfrac{1}{2} \\ -\dfrac{1}{2\sqrt{3}} & -\dfrac{1}{2} \end{pmatrix}$$

We can obtain the point of three vertexes as follow.

$$\left(\dfrac{1}{\sqrt{3}} \quad 0 \right), \left(-\dfrac{1}{2\sqrt{3}} \quad \dfrac{1}{2} \right), \left(-\dfrac{1}{2\sqrt{3}} \quad -\dfrac{1}{2} \right)$$
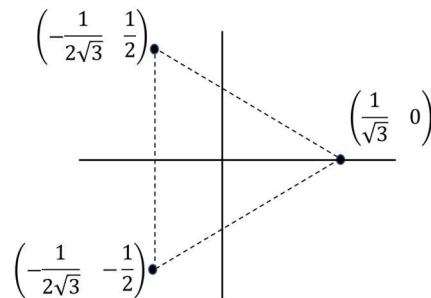
We can plot them as following figure.

Fig. 83. Two-dimensional plot of 3 points

For the confirmation, we calculate the distances.

$$\left|\left(\frac{1}{\sqrt{3}} \quad 0\right) - \left(-\frac{1}{2\sqrt{3}} \quad \frac{1}{2}\right)\right| = \sqrt{\left(\frac{\sqrt{3}}{2}\right)^2 + \left(-\frac{1}{2}\right)^2} = 1$$

$$\left|\left(\frac{1}{\sqrt{3}} \quad 0\right) - \left(-\frac{1}{2\sqrt{3}} \quad -\frac{1}{2}\right)\right| = \sqrt{\left(\frac{\sqrt{3}}{2}\right)^2 + \left(\frac{1}{2}\right)^2} = 1$$

$$\left|\left(-\frac{1}{2\sqrt{3}} \quad \frac{1}{2}\right) - \left(-\frac{1}{2\sqrt{3}} \quad -\frac{1}{2}\right)\right| = \sqrt{(0)^2 + (1)^2} = 1$$

We could obtain equilateral triangle without any loss of information.

As a result of selection of $\begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix}$ as one of eigenvector, a vertex exists on vertical axis.

We can understand the three points form a flat from the result that one of the eigenvalue is 0.

Example 2 (quadrate)

Several cynics may say that it is trivial 3 points make a flat. We try to calculate the case of quadrate of which side is 1 in length.

Distance matrix is as follow.

$$D = \begin{pmatrix} 0 & 1 & \sqrt{2} & 1 \\ 1 & 0 & 1 & \sqrt{2} \\ \sqrt{2} & 1 & 0 & 1 \\ 1 & \sqrt{2} & 1 & 0 \end{pmatrix}$$

Square distance matrix is as follow.

$$D^2 = \begin{pmatrix} 0 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{pmatrix}$$

Centralization

$$GnD^2Gn = \begin{pmatrix} \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} \end{pmatrix} \begin{pmatrix} 0 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} \end{pmatrix}$$

$$= \begin{pmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} \dfrac{3}{4} & -\dfrac{1}{4} & -\dfrac{1}{4} & -\dfrac{1}{4} \\ -\dfrac{1}{4} & \dfrac{3}{4} & -\dfrac{1}{4} & -\dfrac{1}{4} \\ -\dfrac{1}{4} & -\dfrac{1}{4} & \dfrac{3}{4} & -\dfrac{1}{4} \\ -\dfrac{1}{4} & -\dfrac{1}{4} & -\dfrac{1}{4} & \dfrac{3}{4} \end{pmatrix}$$

$$= \begin{pmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}$$

Calculation to obtain eigenvalues from eigen equation.

$$\begin{vmatrix} -1-\lambda & 0 & 1 & 0 \\ 0 & -1-\lambda & 0 & 1 \\ 1 & 0 & -1-\lambda & 0 \\ 0 & 1 & 0 & -1-\lambda \end{vmatrix} = 0$$

$$(\lambda+1)^4 - 2(\lambda+1)^2 + 1 = 0$$

$$((\lambda+1)^2 - 1)^2 = 0$$

$$\left(\lambda(\lambda+2)\right)^2 = 0$$

$$\lambda = 0 \ (multiple\ root), \lambda = -2 \ (mutiple\ root)$$

Calculation to obtain eigenvector belonging to eigenvalue $\lambda = 0$.

$$\begin{pmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = 0 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

$$-x_1 + x_3 = 0$$

$$x_2 - x_4 = 0$$

From this

$$x_1 = x_3, x_2 = x_4$$

We select following vector as simplest eigenvector.

$$\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

Calculation to obtain eigenvector belonging to eigenvalue $\lambda = -2$.

$$\begin{pmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = -2 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

$$x_1 + x_3 = 0$$

$$x_2 + x_4 = 0$$

From this

$$x_1 = -x_3, x_2 = -x_4$$

We select following vector as simplest eigenvector.

$$\begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}$$

Calculation of the other eigenvector belonging to eigenvalue $\lambda = 0$.

We use condition for orthogonality to upper two vectors. Following inner products should be 0.

$$(x_1 \quad x_2 \quad x_3 \quad x_4) \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = 0$$

$$(x_1 \quad x_2 \quad x_3 \quad x_4) \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix} = 0$$

$$x_1 + x_2 + x_3 + x_4 = 0$$
$$x_1 + x_2 - x_3 - x_4 = 0$$
$$x_1 = -x_2, x_3 = -x_4$$

We select following vector as simplest eigen vector.

$$\begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}$$

Calculation of the other eigenvalue belonging to eigen value $\lambda = -2$. We use condition for orthogonality to upper three vectors. Following inner products should be 0.

$$(x_1 \quad x_2 \quad x_3 \quad x_4) \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = 0$$

$$(x_1 \quad x_2 \quad x_3 \quad x_4) \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix} = 0$$

$$(x_1 \quad x_2 \quad x_3 \quad x_4) \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} = 0$$

$$x_1 + x_2 + x_3 + x_4 = 0$$
$$x_1 + x_2 - x_3 - x_4 = 0$$
$$x_1 - x_2 + x_3 - x_4 = 0$$
$$x_1 = -x_2, x_3 = -x_4, x_1 = x_4, x_2 = x_3$$

We select following vector as simplest eigenvector.

$$\begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}$$

We can obtain following matrix which diagonalize GnD^2Gn.

$$P = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & 1 & 1 & -1 \end{pmatrix}$$

$$GnD^2Gn = \begin{pmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}$$

For future convenience, we make orthogonalizing matrix to unit vector.

$$P = \begin{pmatrix} \dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2} \\ \dfrac{1}{2} & -\dfrac{1}{2} & \dfrac{1}{2} & -\dfrac{1}{2} \\ -\dfrac{1}{2} & -\dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2} \\ -\dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2} & -\dfrac{1}{2} \end{pmatrix}$$

$$P^{-1} = P^{\mathrm{T}}$$

$$\Lambda = \begin{pmatrix} -2 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Diagonalization

$$\begin{pmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} = P\Lambda P^{\mathrm{T}}$$

Using this

$$GnD^2Gn = \begin{pmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} \dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2} \\ \dfrac{1}{2} & -\dfrac{1}{2} & \dfrac{1}{2} & -\dfrac{1}{2} \\ -\dfrac{1}{2} & -\dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2} \\ -\dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2} & -\dfrac{1}{2} \end{pmatrix} \begin{pmatrix} -2 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \dfrac{1}{2} & \dfrac{1}{2} & -\dfrac{1}{2} & -\dfrac{1}{2} \\ \dfrac{1}{2} & -\dfrac{1}{2} & -\dfrac{1}{2} & \dfrac{1}{2} \\ \dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2} \\ \dfrac{1}{2} & -\dfrac{1}{2} & \dfrac{1}{2} & -\dfrac{1}{2} \end{pmatrix}$$

$$Z = \frac{Gn D^2 Gn}{-2}$$

$$= \frac{1}{-2}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}\begin{pmatrix} -2 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$$

Transform to the form of $P\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}}P^{\mathrm{T}}$.

$$P\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}}P^{\mathrm{T}} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$$

$$P\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}}P^{\mathrm{T}} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

What we need is $P\Lambda^{\frac{1}{2}}$.

$$P\Lambda^{\frac{1}{2}} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

$$\left(\frac{1}{2} \quad \frac{1}{2}\right), \left(\frac{1}{2} \quad -\frac{1}{2}\right), \left(-\frac{1}{2} \quad -\frac{1}{2}\right), \left(-\frac{1}{2} \quad \frac{1}{2}\right)$$
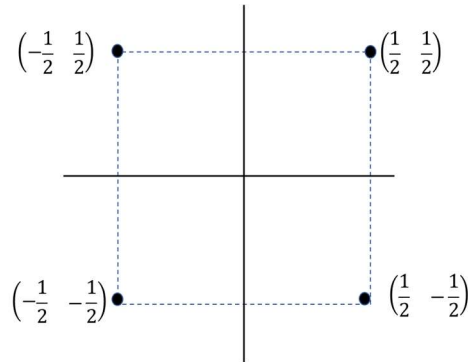
Fig.84. Two-dimensional plot of 4 vertexes

These vertexes form quadrate of which center is origin. We could understand that the es are distributing in 2-dimensinal space from the calculation of eigenvalues in which there are two vectors from four are $\lambda = 0$.

Example 3 (tetrahedron)

As an example of 3-dimensional data, we calculate tetrahedron of which lengths of sides are 1.

$$D = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

$$D^2 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Centralization.

$$GnD^2Gn = \begin{pmatrix} \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} \end{pmatrix}$$

$$= \begin{pmatrix} -\frac{3}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & -\frac{3}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & -\frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & -\frac{3}{4} \end{pmatrix} \begin{pmatrix} \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} \end{pmatrix}$$

$$= \begin{pmatrix} -\dfrac{3}{4} & \dfrac{1}{4} & \dfrac{1}{4} & \dfrac{1}{4} \\ \dfrac{1}{4} & -\dfrac{3}{4} & \dfrac{1}{4} & \dfrac{1}{4} \\ \dfrac{1}{4} & \dfrac{1}{4} & -\dfrac{3}{4} & \dfrac{1}{4} \\ \dfrac{1}{4} & \dfrac{1}{4} & \dfrac{1}{4} & -\dfrac{3}{4} \end{pmatrix} = \dfrac{1}{4}\begin{pmatrix} -3 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 \\ 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & -3 \end{pmatrix}$$

Concerning $\begin{pmatrix} -3 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 \\ 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & -3 \end{pmatrix}$, we calculate eigenvalue.

$$\begin{vmatrix} -3-\lambda & 0 & 1 & 0 \\ 0 & -3-\lambda & 0 & 1 \\ 1 & 0 & -3-\lambda & 0 \\ 0 & 1 & 0 & -3-\lambda \end{vmatrix} = 0$$

$$(\lambda+3)^4 - 2(\lambda+3)^2 + 1 = 0$$

$$((\lambda+3)^2 - 1)^2 = 0$$

$$(\lambda+3)^2 = 1$$

$$(\lambda+3) = \pm 1$$

$$\lambda = -4 \ (multiple\ root), \lambda = -2 \ (multiple\ root)$$

We calculate eigenvectors belonging to eigen value $\lambda = -4$.

$$\begin{pmatrix} -3 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 \\ 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & -3 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = -4\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

$$-3x_1 + x_2 + x_3 + x_4 = -4x_1$$

$$x_1 - 3x_2 + x_3 + x_4 = -4x_2$$

$$x_1 + x_2 - 3x_3 + x_4 = -4x_3$$

$$x_1 + x_2 + x_3 - 3x_4 = -4x_4$$

From all equations

$$x_1 + x_2 + x_3 + x_4 = 0$$

Simplest vector satisfying upper equation is as follow.

$$\begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}$$

Simplest orthogonal vector to upper vector satisfying the equation is as follow.

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}$$

We select these vectors as eigenvectors.

$$V_1 = \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \quad V_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}$$

Calculation for eigenvectors belonging to eigenvalue $\lambda = -2$.

$$\begin{pmatrix} -3 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 \\ 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = -2 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

$$-3x_1 + x_2 + x_3 + x_4 = -2x_1$$
$$x_1 - 3x_2 + x_3 + x_4 = -2x_2$$
$$x_1 + x_2 - 3x_3 + x_4 = -2x_3$$
$$x_1 + x_2 + x_3 - 3x_4 = -2x_4$$

$$x_1 = x_2 + x_3 + x_4 \quad \text{i}$$
$$x_2 = x_1 + x_3 + x_4 \quad \text{ii}$$
$$x_3 = x_1 + x_2 + x_4 \quad \text{iii}$$
$$x_4 = x_1 + x_2 + x_3 \quad \text{iv}$$

i − ii
$$x_1 - x_2 = x_2 - x_1$$
$$x_1 = x_2$$

Similarly from iii—iv,
$$x_3 = x_4$$

From ii+iii,

$$x_1 = -x_4$$

From i+iv,
$$x_2 = -x_3$$

We select following vectors as simplest vector satisfying the condition.

$$V_3 = \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}, V_3' = \begin{pmatrix} -1 \\ -1 \\ 1 \\ 1 \end{pmatrix}$$

Space $V_1, V_2 \cdot V_3$ and Space $V_1, V_2 \cdot V_3'$ are in the relation of mirror image, and V_3 and V_3' are oppositely oriented and is existing on the same line. We can combine V_3' to V_3.

$$V_1 = \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \quad V_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}, \quad V_3 = \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}$$

We transform them into unit vectors

$$
\begin{pmatrix} \dfrac{1}{\sqrt{2}} \\ -\dfrac{1}{\sqrt{2}} \\ 0 \\ 0 \end{pmatrix}, \quad
\begin{pmatrix} 0 \\ 0 \\ \dfrac{1}{\sqrt{2}} \\ -\dfrac{1}{\sqrt{2}} \end{pmatrix}, \quad
\begin{pmatrix} \dfrac{1}{2} \\ \dfrac{1}{2} \\ -\dfrac{1}{2} \\ -\dfrac{1}{2} \end{pmatrix}
$$

Conclusively, the diagonalizing matrix of $\begin{pmatrix} -3 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 \\ 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & -3 \end{pmatrix}$ is as follow.

$$
P = \begin{pmatrix}
\dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\
-\dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\
0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \\
0 & -\dfrac{1}{\sqrt{2}} & -\dfrac{1}{2}
\end{pmatrix}
$$

The eigenvalue of third eigenvector is $(-2) + (-2) = -4$.

$$
\Lambda = \begin{pmatrix} -4 & 0 & 0 \\ 0 & -4 & 0 \\ 0 & 0 & -4 \end{pmatrix}
$$

$$
\begin{pmatrix} -3 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 \\ 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & -3 \end{pmatrix} = P\Lambda P^T
$$

Using them.

$$
GnD^2Gn = \frac{1}{4} \begin{pmatrix} -3 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 \\ 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & -3 \end{pmatrix}
$$

$$
= \frac{1}{4} \begin{pmatrix}
\dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\
-\dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\
0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \\
0 & -\dfrac{1}{\sqrt{2}} & -\dfrac{1}{2}
\end{pmatrix}
\begin{pmatrix} -4 & 0 & 0 \\ 0 & -4 & 0 \\ 0 & 0 & -4 \end{pmatrix}
\begin{pmatrix}
\dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\
-\dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\
0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \\
0 & -\dfrac{1}{\sqrt{2}} & -\dfrac{1}{2}
\end{pmatrix}^T
$$

$$= \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\ -\dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\ 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \\ 0 & -\dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \\ \dfrac{1}{2} & \dfrac{1}{2} & -\dfrac{1}{2} & -\dfrac{1}{2} \end{pmatrix}$$

$$Z = \frac{GnD^2Gn}{-2}$$

$$= \frac{1}{-2} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\ -\dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\ 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \\ 0 & -\dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \\ \dfrac{1}{2} & \dfrac{1}{2} & -\dfrac{1}{2} & -\dfrac{1}{2} \end{pmatrix}$$

$$= \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\ -\dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\ 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \\ 0 & -\dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \end{pmatrix} \begin{pmatrix} \dfrac{1}{2} & 0 & 0 \\ 0 & \dfrac{1}{2} & 0 \\ 0 & 0 & \dfrac{1}{2} \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \\ \dfrac{1}{2} & \dfrac{1}{2} & -\dfrac{1}{2} & -\dfrac{1}{2} \end{pmatrix}$$

We trans form this to the form of $P\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}}P^{\mathrm{T}}$.

$$= \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\ -\dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\ 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \\ 0 & -\dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \dfrac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \dfrac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \dfrac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \dfrac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \\ \dfrac{1}{2} & \dfrac{1}{2} & -\dfrac{1}{2} & -\dfrac{1}{2} \end{pmatrix}$$

From this we can obtain $P\Lambda^{\frac{1}{2}}$.

$$P\Lambda^{\frac{1}{2}} = \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\ -\dfrac{1}{\sqrt{2}} & 0 & \dfrac{1}{2} \\ 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \\ 0 & -\dfrac{1}{\sqrt{2}} & -\dfrac{1}{2} \end{pmatrix} \begin{pmatrix} \dfrac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \dfrac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \dfrac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \dfrac{1}{2} & 0 & \dfrac{1}{2\sqrt{2}} \\ -\dfrac{1}{2} & 0 & \dfrac{1}{2\sqrt{2}} \\ 0 & \dfrac{1}{2} & -\dfrac{1}{2\sqrt{2}} \\ 0 & -\dfrac{1}{2} & -\dfrac{1}{2\sqrt{2}} \end{pmatrix}$$

From this we can confirm vertexes of tetrahedron are existing in 3-dimensional space, and the coordinates of vertexes are as follow.

$$A: \left(\frac{1}{2} \quad 0 \quad \frac{1}{2\sqrt{2}} \right)$$

$$B: \left(-\frac{1}{2} \quad 0 \quad \frac{1}{2\sqrt{2}} \right)$$

$$C: \left(0 \quad \frac{1}{2} \quad -\frac{1}{2\sqrt{2}} \right)$$

$$D: \left(0 \quad -\frac{1}{2} \quad -\frac{1}{2\sqrt{2}} \right)$$

We confirm the distances among the points

$$|A - B| = \sqrt{\left(\left(\frac{1}{2}\right) - \left(-\frac{1}{2}\right)\right)^2 + \left((0) - (0)\right)^2 + \left(\left(\frac{1}{2\sqrt{2}}\right) - \left(\frac{1}{2\sqrt{2}}\right)\right)^2}$$

$$= \sqrt{\left((1)\right)^2 + 0 + 0} = 1$$

$$|A - C| = \sqrt{\left(\left(\frac{1}{2}\right) - (0)\right)^2 + \left((0) - \left(\frac{1}{2}\right)\right)^2 + \left(\left(\frac{1}{2\sqrt{2}}\right) - \left(-\frac{1}{2\sqrt{2}}\right)\right)^2}$$

$$= \sqrt{\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2} = \sqrt{\frac{1}{4} + \frac{1}{4} + \frac{1}{2}} = 1$$

$$|A - D| = \sqrt{\left(\left(\frac{1}{2}\right) - (0)\right)^2 + \left((0) - \left(-\frac{1}{2}\right)\right)^2 + \left(\left(\frac{1}{2\sqrt{2}}\right) - \left(-\frac{1}{2\sqrt{2}}\right)\right)^2}$$

$$= \sqrt{\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2} = \sqrt{\frac{1}{4} + \frac{1}{4} + \frac{1}{2}} = 1$$

$$|B - C| = \sqrt{\left(\left(-\frac{1}{2}\right) - (0)\right)^2 + \left((0) - \left(\frac{1}{2}\right)\right)^2 + \left(\left(-\frac{1}{2\sqrt{2}}\right) - \left(-\frac{1}{2\sqrt{2}}\right)\right)^2}$$

$$= \sqrt{\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2} = \sqrt{\frac{1}{4} + \frac{1}{4} + \frac{1}{2}} = 1$$

$$|B - D| = \sqrt{\left(\left(-\frac{1}{2}\right) - (0)\right)^2 + \left((0) - \left(-\frac{1}{2}\right)\right)^2 + \left(\left(\frac{1}{2\sqrt{2}}\right) - \left(\frac{1}{2\sqrt{2}}\right)\right)^2}$$

$$= \sqrt{\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2} = \sqrt{\frac{1}{4} + \frac{1}{4} + \frac{1}{2}} = 1$$

$$|C - D| = \sqrt{\left((0) - (0)\right)^2 + \left(\left(\frac{1}{2}\right) - \left(-\frac{1}{2}\right)\right)^2 + \left(\left(-\frac{1}{2\sqrt{2}}\right) - \left(-\frac{1}{2\sqrt{2}}\right)\right)^2}$$

$$= \sqrt{0^2 + (1)^2 + 0^2} = 1$$

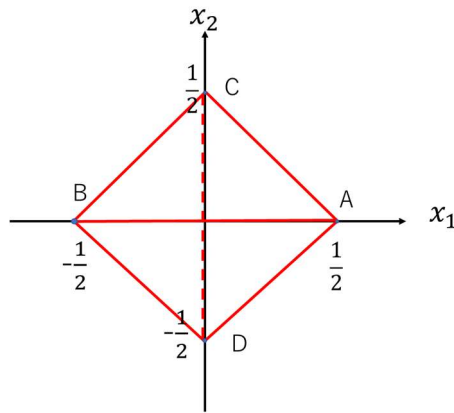Following is map of the pints on $x_1 - x_2$ flat.

Fig. 85. Two-dimensional plot of vertex of tetrahedron

No one can directly understand only from the two-dimensional plots that the figure is an image of tetrahedron.

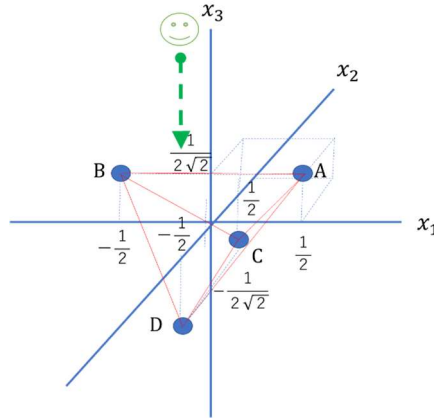Stereoscopic image of the points of vertexes is as follows.

Fig.86. Cubic diagram of tetrahedron and viewing direction projection view

The flat image is image looking from the direction of x_3 axis. We calculate cumulative contribution ratio by first and second axis from diagonal matrix of eigenvalues.

$$\Lambda = \begin{pmatrix} \dfrac{1}{2} & 0 & 0 \\ 0 & \dfrac{1}{2} & 0 \\ 0 & 0 & \dfrac{1}{2} \end{pmatrix}$$

Cumulative contribution ratio by first and second axis is

$$\frac{\dfrac{1}{2} + \dfrac{1}{2}}{\dfrac{1}{2} + \dfrac{1}{2} + \dfrac{1}{2}} = \frac{2}{3}$$

Flat image can explain only $\frac{2}{3}$ of the distribution of data. However, excepting diagonal lines in the flat image, distances between the vertexes are the same. Some may say that the flat image is explaining necessary information. Evaluation of adequacy and availability of the map changes depending on the purpose of analysis. What is most important is to make various flat images from different direction checking the cumulative contribution ratio. We cannot identify only from one map whether the flat image is representing quadrate or tetrahedron. Purpose of MDS is observation of multi-dimensional distribution of data. It is not drawing of a flat image.

VI-2-2-4. Additional discussion (relation between MDS and PCA)

We can draw a regular tetrahedron in example 3. The table of each vertex is as shown in table 48.

Table 48. Components of the vertexes

Table 48. coordinate of each vertex

	x_1	x_2	x_3
A	$\dfrac{1}{2}$	0	$\dfrac{1}{2\sqrt{2}}$
B	$-\dfrac{1}{2}$	0	$\dfrac{1}{2\sqrt{2}}$
C	0	$\dfrac{1}{2}$	$-\dfrac{1}{2\sqrt{2}}$
D	0	$-\dfrac{1}{2}$	$-\dfrac{1}{2\sqrt{2}}$

When we are given this table as data at first, we consider implementation of PCA to observe multi-dimensional distribution of data. We can understand multi-dimensional distribution by drawing stereoscopic image from the data. It is meaningless performance to do PCA from this data practically. However, the author tries PCA for understanding of the relation between MDS and PCA.

At first, we calculate variance-covariance matrix.

Variance in x_1: $\left(\frac{1}{2}\right)^2 + \left(-\frac{1}{2}\right)^2 + (0)^2 + (0)^2 = \frac{1}{2}$

Variance in x_2: $(0)^2 + (0)^2 + \left(\frac{1}{2}\right)^2 + \left(-\frac{1}{2}\right)^2 = \frac{1}{2}$

Variance in x_3: $\left(\frac{1}{2\sqrt{2}}\right)^2 + \left(\frac{1}{2\sqrt{2}}\right)^2 + \left(-\frac{1}{2\sqrt{2}}\right)^2 + \left(-\frac{1}{2\sqrt{2}}\right)^2 = \frac{1}{2}$

Covariance between x_1 and x_2: $\left(\frac{1}{2}\right)(0) + \left(-\frac{1}{2}\right)(0) + (0)\left(\frac{1}{2}\right) + (0)\left(-\frac{1}{2}\right) = 0$

Covariance between x_1 and x_3: $\left(\frac{1}{2}\right)\left(-\frac{1}{2\sqrt{2}}\right) + \left(-\frac{1}{2}\right)\left(-\frac{1}{2\sqrt{2}}\right) + (0)\left(-\frac{1}{2\sqrt{2}}\right) + (0)\left(-\frac{1}{2\sqrt{2}}\right) = 0$

Covariance between x_2 and x_3: $(0)\left(\frac{1}{2\sqrt{2}}\right) + (0)\left(\frac{1}{2\sqrt{2}}\right) + \left(\frac{1}{2}\right)\left(-\frac{1}{2\sqrt{2}}\right) + \left(-\frac{1}{2}\right)\left(-\frac{1}{2\sqrt{2}}\right) = 0$

Variance-covariance matrix is

$$\begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix}$$

This is already diagonalized. We trans form this as follow.

$$\frac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The matrix is unit matrix. So, when we multiply this to the vector of each vertexs, we decrease original figure in size by $\frac{1}{2}$ keeping relative relation of original figure.

$$A': \left(\frac{1}{2} \quad 0 \quad \frac{1}{2\sqrt{2}} \right) \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{1}{2}\left(\frac{1}{2} \quad 0 \quad \frac{1}{2\sqrt{2}} \right)$$

$$B': \left(-\frac{1}{2} \quad 0 \quad \frac{1}{2\sqrt{2}} \right) \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{1}{2}\left(-\frac{1}{2} \quad 0 \quad \frac{1}{2\sqrt{2}} \right)$$

$$C': \left(0 \quad \frac{1}{2} \quad -\frac{1}{2\sqrt{2}} \right) \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{1}{2}\left(0 \quad \frac{1}{2} \quad -\frac{1}{2\sqrt{2}} \right)$$

$$D': \left(0 \quad -\frac{1}{2} \quad -\frac{1}{2\sqrt{2}} \right) \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{1}{2}\left(0 \quad -\frac{1}{2} \quad -\frac{1}{2\sqrt{2}} \right)$$

This procedure is only changing of the name of axes from x_1 component x_2 component and component x_3 to first principle component, second principle component and third principle component. We consider component which has small eigenvalue as error in PCA, and we assume that the eigenvalue of the component is 0. The eigenvalues are the same in this case. We can neglect any component. We can obtain the vertex of vertex on the flat between first and second component by following calculation.

$$A' = \left(\frac{1}{2} \quad 0 \quad \frac{1}{2\sqrt{2}} \right) \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} = \left(\frac{1}{2} \quad 0 \right)$$

This is natural consequence, though we can confirm the difference between MDS and PCA is difference in given data. The merit of MDS is construction of data structure only from distance data. Scientists who are thinking MDS as only a method for categorization of data using two or three-dimensional map sometimes waste important and useful information provided by MDS. It is important to consider multi-dimensional structure of data distribution checking maps from various direction with cumulative contribution ratio. Mapping is only a method to summarize the distribution.

The difference between MDS and PCA is difference in form of given dataset, and we can get similar result. This means that we can evaluate similarity among individual data from given values of various measurement item calculating distance in multi-dimensional space after PCA. In this meaning, MDS is completely inverse procedure of PCA. However, PCA has several advantages to MDS. Firstly, we can categorize the data using result of PCA. As an example, we sample all benthic organisms in a quadrate and record the number of each species in each sampling site as measurement item. We can apply PCA to the dataset. And we can categorize species or sampling site using distance

among each data on multidimensional space as anti-similarity. Secondary, we can discuss the relation between distribution of each species or sampling site with other factors such as environment factors or seasonality or social background. This is so called correspondence analysis if we measure such background data simultaneously. There are several historically different correspondence analyses. All correspondence analysis is considered an application of PCA now a days. We already learned a kind of correspondence analysis in VI-2-1-4. However, there is a unique function in MDS which cannot be achieve by PCA. Sometimes MDS provide least expected findings. MDS does not need prier information and makes structure only by difference. For correspondence analysis by PCA we have to include measurement item relating to the phenomena using prior information. MDS can make draw structure of data distribution without clear cause and result relationship. This sometime provides new information.

In the case of coastal ecological survey, we can implement PCA directly from variance-covariance matrix or correlation matrix, when individual number of each species in each sampling site is a measurement item. Another idea is to make round robin distance table from anti-similarities of species composition. And then we implement MDS. There various similarity coefficients, namely Jaccard coefficient, Simpson coefficient, Dice coefficient and so on in ecological studies. Commonly we use $1 - similarity\ coefficent$ as distance. After making distant data among sampling site or among species from similarity coefficient, we can perform MDS. In such case, we need to select MDS or PCA. The author cannot make any recommendation mathematically for solution of this question. We consider that each species has same weight at the starting point in PCA, and we obtain the distance from correlation angle of vector） as the result. On the contrary, we start the analysis from the distances among points and we obtain the relative position of each point in MDS. We have to discuss the adequacy of treating each species in the same weight. Each species has each characteristic in distribution. Some species are rare species and existence of an individual of such species has important meaning. Some species are distribute making patch in a small area. Number of individuals in a patch is huge. Appearance ratio of other species became negligible small, when we express the appearance of species in actual count of individuals. This decrease of adequacy and reliability of analysis. There are several mitigation methods of this issue such as making similarity coefficient using binary data or using of logarithm of individual number and so on. However, there is no complete adaptive measure to all cases. This issue can sometimes be solved by PCA after standardization of data by standard deviation or PCA by correlation matrix, however it is not useful in all cases. In the impression of the author, most of the researcher in ecology prefer to use MDS than PCA.

We should think these issues adaptively depending on the experience and case studies. The author has not rich experiences to use MDS and PCA. The author is expecting readers to refer previous works in each research field.

VI-2-2-4. Non-metric multidimensional scaling.

Upper explanations are for classic MDS of metric DMS. MDS is developing recently using computer machine power. There are various MDS particularly in application of MDS to non-linear data. Interest of MDS is exist in allocation of data which we do not know the elements of data in multi-dimensional space from the difference. The author thinks that there are large possibilities of MDS in the analytical method to qualitative data and nominal scale data. The author expect application of MDS to analysis of all difference data. The point for the application is that the differences should be expressed as distance. This means that we cannot apply this method to data in which distance from A to B is different to distance from B to A (time distance of ship in stream between A and B is a typical example) or sum of distance A to B and B to C is not shorter than A to C. We need devices to express the distance. It reaches limit of capacity of the author to explain all of them. Readers who need method of non-metric MDS, please refer other text books and relating papers.