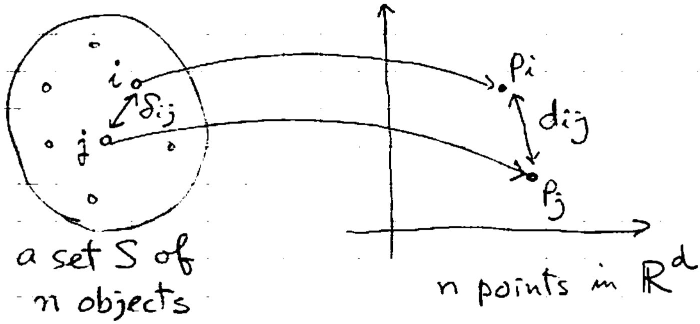
MDS : Multi-Dimensional Scaling



δ_{ij} : dissimilarity between objects i and j

$\wr\wr$

d_{ij} : Euclidean distance between two points p_i and p_j

> Given an integer $d>0$ and a matrix $\Delta=[\delta_{ij}]$ representing dissimilarity of every pair of objects, find a mapping of those objects to points in d-dimensional space $\mathbb{R}^d$ so that pointwise distance is approximately equal to the dissimilarity between corresponding objects.

approximation error : $e_{ij} = |\delta_{ij} - d_{ij}|$

objective function to be minimized :

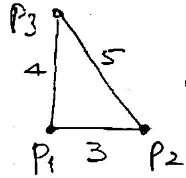
$f_1 : \sum_{i,j} e_{ij} \rightarrow \min$

$f_2 : \sum_{i,j} e_{ij}^2 \rightarrow \min$ ... etc.

(Example E1)

$$\Delta = \begin{array}{c|ccc} & 1 & 2 & 3 \\ \hline 1 & 0 & 3 & 4 \\ 2 & 3 & 0 & 5 \\ 3 & 4 & 5 & 0 \end{array}$$

$\delta_{12} = \delta_{21} = 3$
$\delta_{13} = \delta_{31} = 4$
$\delta_{23} = \delta_{32} = 5$.

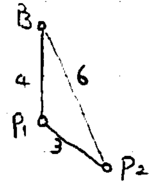


exact embedding in R^2

(Example E2)

$$\Delta' = \begin{array}{c|ccc} & 1 & 2 & 3 \\ \hline 1 & 0 & 3 & 4 \\ 2 & 3 & 0 & 6 \\ 3 & 4 & 6 & 0 \end{array}$$

Exact embedding is still possible



(Example E3)

$$\Delta' = \begin{array}{c|ccc} & 1 & 2 & 3 \\ \hline 1 & 0 & 3 & 4 \\ 2 & 3 & 0 & 8 \\ 3 & 4 & 8 & 0 \end{array}$$

violates triangular inequality
for $\forall i, j, k$
$d_{ij} + d_{jk} \geq d_{ik}$

$$\begin{cases} \text{Metric case : every triple satisfies triangular inequality} \\ \text{Non-metric case : otherwise} \end{cases}$$

> Given a set of n objects with associated dissimilarity matrix which is metric (ie., satisfying triangular inequality), those objects are mapped to points in the $(n-1)$ dimensional space so that $\delta_{ij} = d_{ij}$ for every pair (i, j).

$x_i = (x_{i1}, x_{i2}, \cdots, x_{id})^T$: point in $\mathbb{R}^d$

$\Rightarrow$ the Euclidian distance d_{ij}

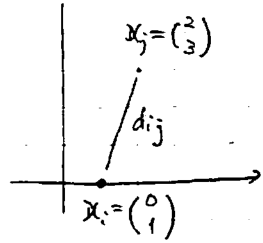
$$\boxed{d_{ij}^2 = (x_i - x_j)^T (x_i - x_j).} \qquad (1)$$

(Example E4)

$$x_i = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad x_j = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$$

$$\Rightarrow \quad x_i - x_j = \begin{pmatrix} 0-2 \\ 1-3 \end{pmatrix} = \begin{pmatrix} -2 \\ -2 \end{pmatrix}$$

$$d_{ij}^2 = (-2 \ \ -2) \begin{pmatrix} -2 \\ -2 \end{pmatrix} = (-2)^2 + (-2)^2 = 8$$



Let the inner product matrix be $\mathbb{B}$, where

$$[\mathbb{B}]_{ij} = b_{ij} = x_i^T x_j \qquad (2)$$

Want to find $\mathbb{B}$ using known squared distances $\{d_{ij}^2\}$

<u>To find $\mathbb{B}$</u>

Translation does not change pairwise distances

$\Downarrow$ as a natural assumption

$$\sum_{i=1}^{n} x_{ij} = 0 \quad \text{for } j = 1, \cdots, d. \qquad (3)$$

(means that the centroid of n points is placed at the origin)

$$d_{ij}^2 = (x_i - x_j)^T (x_i - x_j)$$
$$= x_i^T x_i + x_j^T x_j - 2 x_i^T x_j \qquad (4)$$

$$\frac{1}{n}\sum_{i=1}^{n} d_{ij}^2 = \frac{1}{n}\sum_{i=1}^{n}\left(x_i^T x_i + x_j^T x_j - 2x_i^T x_j\right)$$

Here $\sum_{i=1}^{n} x_i^T x_j = \left(\sum_{i=1}^{n} x_i^T\right) x_j = 0$ (due to (3))

$$\therefore \frac{1}{n}\sum_{i=1}^{n} d_{ij}^2 = \frac{1}{n}\sum_{i=1}^{n} x_i^T x_i + \frac{1}{n}\sum_{i=1}^{n} x_j^T x_j$$

$$= \frac{1}{n}\sum_{i=1}^{n} x_i^T x_i + x_j^T x_j \qquad (5)$$

$$\frac{1}{n}\sum_{j=1}^{n} d_{ij}^2 = \frac{1}{n}\sum_{j=1}^{n}\left(x_i^T x_i + x_j^T x_j - 2x_i^T x_j\right)$$

$$= x_i^T x_i + \frac{1}{n}\sum_{j=1}^{n} x_j^T x_j \qquad (6)$$

$$\therefore \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij}^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{1}{n}\sum_{j=1}^{n} d_{ij}^2\right) = \frac{1}{n}\sum_{i=1}^{n}\left(x_i^T x_i + \frac{1}{n}\sum_{j=1}^{n} x_j^T x_j\right)$$

$$= \frac{1}{n}\sum_{i=1}^{n} x_i^T x_i + \frac{1}{n^2}\sum_{j=1}^{n}\sum_{i=1}^{n} x_j^T x_j$$

$$= \frac{1}{n}\sum_{i=1}^{n} x_i^T x_i + \frac{1}{n}\sum_{j=1}^{n} x_j^T x_j$$

$$= \frac{2}{n}\sum_{i=1}^{n} x_i^T x_i \qquad (7)$$

From (5) and (7),

$$x_j^T x_j = \frac{1}{n}\sum_{i=1}^{n} d_{ij}^2 - \frac{1}{n}\sum_{i=1}^{n} x_i^T x_i = \frac{1}{n}\sum_{i=1}^{n} d_{ij}^2 - \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij}^2$$

Similarly

$$x_i^T x_i = \frac{1}{n}\sum_{j=1}^{n} d_{ij}^2 - \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij}^2$$

Now, combining (2) and (4), we have

$$b_{ij} = x_i^T x_j = \frac{1}{2}\left(x_i^T x_i + x_j^T x_j - d_{ij}^2\right)$$

$$= \frac{1}{2}\left(\frac{1}{n}\sum_{j=1}^{n} d_{ij}^2 - \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij}^2 + \frac{1}{n}\sum_{i=1}^{n} d_{ij}^2 - \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij}^2 - d_{ij}^2\right)$$

$$= \frac{1}{2}\left(\frac{1}{n}\sum_{i=1}^{n} d_{ij}^2 + \frac{1}{n}\sum_{j=1}^{n} d_{ij}^2 - \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij}^2 - d_{ij}^2\right)$$

$$\therefore b_{ij} = -\frac{1}{2}\left(d_{ij}^2 - \frac{1}{n}\sum_{i=1}^{n} d_{ij}^2 - \frac{1}{n}\sum_{j=1}^{n} d_{ij}^2 + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij}^2\right) \quad \text{---} \ (8)$$

Now, define

$$a_{ij} = -\frac{1}{2} d_{ij}^2,$$

$$a_{i*} = \frac{1}{n}\sum_{j=1}^{n} a_{ij} = -\frac{1}{2n}\sum_{j=1}^{n} d_{ij}^2$$

$$a_{*j} = \frac{1}{n}\sum_{i=1}^{n} a_{ij} = -\frac{1}{2n}\sum_{i=1}^{n} d_{ij}^2$$

$$a_{**} = \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij} = -\frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij}^2 \qquad (9)$$

Then, we have

$$b_{ij} = a_{ij} - a_{i*} - a_{*j} + a_{**}. \qquad (10)$$

Define matrix $\mathbb{A}$ as $[\mathbb{A}]_{ij} = a_{ij}$, and hence the inner product matrix $\mathbb{B}$ is

$$\boxed{\mathbb{B} = \mathbb{H}\mathbb{A}\mathbb{H}} \qquad (11)$$

where $\mathbb{H}$ is the centering matrix

$$\mathbb{H} = \mathbb{I} - \frac{1}{n}\mathbb{1}\mathbb{1}^T, \quad \mathbb{1} = (\underbrace{1, 1, \ldots, 1}_{n})^T$$

e.g.

$$\mathbb{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbb{1} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad \mathbb{1}\mathbb{1}^T = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}(1\,1\,1) = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

$$\mathbb{I} - \frac{1}{3}\mathbb{1}\mathbb{1}^T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \end{pmatrix}$$

$$\mathbb{H}\mathbb{A}\mathbb{H} = \begin{pmatrix} 1-p & -p & -p \\ -p & 1-p & -p \\ -p & -p & 1-p \end{pmatrix}\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}\begin{pmatrix} 1-p & -p & -p \\ -p & 1-p & -p \\ -p & -p & 1-p \end{pmatrix} \quad p = \frac{1}{3}$$

$$= \begin{pmatrix} a_{11} - p\sum_{i=1}^{3} a_{i1}, & a_{12} - p\sum a_{i2}, & a_{13} - p\sum a_{i3} \\ \_\_\_ & \_\_\_ & \_\_\_ \\ \_\_\_ & \_\_\_ & \_\_\_ \end{pmatrix}\begin{pmatrix} 1-p & -p & -p \\ -p & 1-p & -p \\ -p & -p & 1-p \end{pmatrix}$$

(1,1) element

$$
\begin{aligned}
&= (1-p)\left[a_{11} - p\sum_{i=1}^{3} a_{i1}\right] - p\left[a_{12} - p\sum_{i=1}^{3} a_{i2}\right] - p\left[a_{13} - p\sum_{i=1}^{3} a_{i3}\right] \\
&= a_{11} - p\sum_{i=1}^{3} a_{i1} - p\left[a_{11} + a_{12} + a_{13} - p\sum a_{i1} - p\sum a_{i2} - p\sum a_{i3}\right] \\
&= a_{11} - p\sum a_{i1} - p\sum a_{1i} + p^2 \sum\sum a_{ij} \\
&= a_{11} - \frac{1}{n}\sum a_{i1} - \frac{1}{n}\sum a_{1i} + \frac{1}{n^2}\sum\sum a_{ij} \\
&= a_{11} - a_{*1} - a_{1*} + a_{**}.
\end{aligned}
$$

Now, we have

$$[\mathbb{B}]_{ij} = x_i^T x_j \qquad (2)$$

$$\mathbb{B} = \mathbb{HAH} \qquad (11)$$

Setting $\mathbb{X} = [x_1, x_2, \cdots, x_n]^T$

$$\Downarrow$$

$$\mathbb{B} = \mathbb{X}\mathbb{X}^T \qquad (12)$$

$$
\mathbb{X} = \begin{array}{c|ccc|c}
 & 1 & 2 & \cdots\ d & \\
\hline
1 & & & & x_1^T \\
2 & & & & x_2^T \\
\vdots & & & & \vdots \\
n & & & & x_n^T
\end{array}
$$

The rank of $\mathbb{B}$, $r(\mathbb{B})$, is then

$$r(\mathbb{B}) = r(\mathbb{X}\mathbb{X}^T) = r(\mathbb{X}) = d.$$

Now, $\mathbb{B}$ is symmetric, positive semi-definite and of rank d, and hence has d non-negative eigenvalues and $n-d$ zero eigen values.

$$\mathbb{B}v_i = \lambda_i v_i, \quad i = 1, 2, \cdots, n \qquad (13)$$

λ_i : eigenvalue

v_i : corresponding eigenvector

Define a matrix $\mathbb{V}$ by

$$\mathbb{V} = [v_1, v_2, \cdots, v_n]$$

Then, from (13) we have

$$\mathbb{B}\mathbb{V} = \mathbb{V}\Lambda, \qquad (14)$$

where

$$\Lambda = \begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_n \end{pmatrix}$$

with normalizations:

$$v_i^T v_i = 1. \qquad (15)$$

And for any $i \neq j$,

$$v_i^T v_j = 0. \qquad (16)$$

Therefore, we have

$$\mathbb{V}\mathbb{V}^T = \mathbb{I}.$$

Hence

$$\mathbb{B} = \mathbb{B}\mathbb{V}\mathbb{V}^T = \mathbb{V}\Lambda\mathbb{V}^T$$

i.e. $\boxed{\mathbb{B} = \mathbb{V}\Lambda\mathbb{V}^T}$ (17)

Because of the $n-d$ zero eigenvalues, $\mathbb{B}$ can be written as.

$$\mathbb{B} = \mathbb{V}_1 \Lambda_1 \mathbb{V}^T, \qquad (18)$$

$$\Lambda_1 = \mathrm{diag}(\lambda_1, \cdots, \lambda_d), \quad \mathbb{V}_1 = [v_1, \cdots, v_d].$$

Hence, as $\mathbb{B} = \mathbb{X}\mathbb{X}^T$, the coordinate matrix $\mathbb{X}$ is given by

$$\boxed{\mathbb{X} = \mathbb{V}_1 \Lambda_1^{1/2}} \qquad (19)$$

$$\Lambda_1^{1/2} = \mathrm{diag}(\sqrt{\lambda_1}, \sqrt{\lambda_2}, \cdots, \sqrt{\lambda_d})$$

$$\mathbb{X} = \begin{array}{c|c} & 1 \ 2 \ \cdots \ d \\ \begin{matrix} 1 \\ 2 \\ \vdots \\ n \end{matrix} & \begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix} \end{array} = [\mathbb{v}_1, \mathbb{v}_2, \cdots, \mathbb{v}_d] \begin{pmatrix} \sqrt{\lambda_1} & & & 0 \\ & \sqrt{\lambda_2} & & \\ & & \ddots & \\ 0 & & & \sqrt{\lambda_d} \end{pmatrix}$$

$$= (\sqrt{\lambda_1}\mathbb{v}_1, \sqrt{\lambda_2}\mathbb{v}_2, \cdots, \sqrt{\lambda_d}\mathbb{v}_d]$$

$\sqrt{\lambda_i}\mathbb{v}_i$ gives the i-th coordinate values of n points.

(Example E5)

$$\text{dissimilarity matrix} = \begin{pmatrix} 0 & 3 & 4 \\ 3 & 0 & 5 \\ 4 & 5 & 0 \end{pmatrix} = (\delta_{ij})$$

$$a_{ij} = -\frac{1}{2}\delta_{ij}^2 = \begin{pmatrix} 0 & -9/2 & -8 \\ -9/2 & 0 & -25/2 \\ -8 & -25/2 & 0 \end{pmatrix}$$

$$a_{1*} = \frac{1}{3}\sum_{j=1}^{3} a_{1j} = \frac{1}{3}\left(0 - \frac{9}{2} - 8\right) = -\frac{25}{6} = a_{*1}.$$

$$a_{2*} = \frac{1}{3}\sum a_{2j} = \frac{1}{3}\left(-\frac{9}{2} + 0 - \frac{25}{2}\right) = -\frac{34}{6} = a_{*2}$$

$$a_{3*} = \frac{1}{3}\sum a_{3j} = \frac{1}{3}\left(-8 - \frac{25}{2} + 0\right) = -\frac{41}{6} = a_{*3}$$

$$a_{**} = \frac{1}{3}(a_{1*} + a_{2*} + a_{3*}) = \frac{1}{3}\left(-\frac{25}{6} - \frac{34}{6} - \frac{41}{6}\right) = -\frac{100}{18}$$

$$b_{11} = a_{11} - a_{1*} - a_{*1} + a_{**} = 0 + \frac{25}{6} + \frac{25}{6} - \frac{100}{18} = 50/18$$

$$b_{12} = a_{12} - a_{1*} - a_{*2} + a_{**} = -\frac{9}{2} + \frac{25}{6} + \frac{34}{6} - \frac{100}{18} = \frac{1}{18}(-81 + 75 + 102 - 100) = -\frac{4}{18}$$

$$b_{13} = a_{13} - a_{1*} - a_{*3} + a_{**} = -8 + \frac{25}{6} + \frac{41}{6} - \frac{100}{18} = \frac{1}{18}(-144 + 75 + 123 - 100) = -46/18$$

$$b_{22} = a_{22} - a_{2*} - a_{*2} + a_{**} = 0 + \frac{34}{6} + \frac{34}{6} - \frac{100}{18} = \frac{1}{18}(102 + 102 - 100) = \frac{104}{18}$$

$$b_{23} = a_{23} - a_{2*} - a_{*3} + a_{**} = -\frac{25}{2} + \frac{34}{6} + \frac{41}{6} - \frac{100}{18} = \frac{1}{18}(-225 + 102 + 123 - 100) = -\frac{100}{18}$$

$$b_{33} = a_{33} - a_{3*} - a_{*3} + a_{**} = 0 + \frac{41}{6} + \frac{41}{6} - \frac{100}{18} = \frac{1}{18}(123 + 123 - 100) = \frac{146}{18}$$

$$B = \frac{1}{18}\begin{pmatrix} 50 & -4 & -46 \\ -4 & 104 & -100 \\ -46 & -100 & 146 \end{pmatrix} = \begin{pmatrix} 2.78, & -0.22, & -2.56 \\ -0.22, & 5.78, & -5.56 \\ -2.55, & -5.56, & 8.11 \end{pmatrix}$$

$\lambda_1 = 12.96$, $\lambda_2 = 3.70$ $\sqrt{\lambda_1} = 3.6$, $\sqrt{\lambda_2} = 1.92$

$v_1^T = (-0.18, -0.59, 0.78)$

$v_2^T = (-0.79, 0.56, 0.24)$

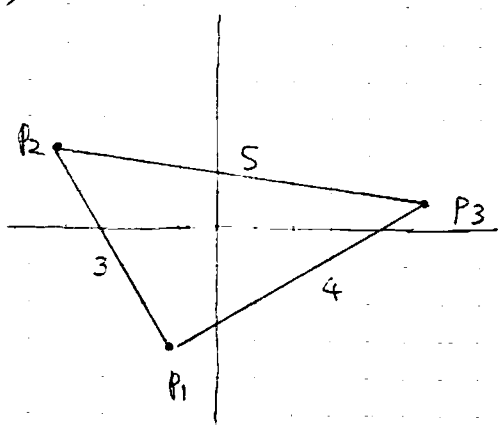
$\sqrt{\lambda_1}\, v_1^T = (-0.65, -2.12, 2.81)$

$\sqrt{\lambda_2}\, v_2^T = (-1.52, 1.08, 0.46)$

$\therefore$ $p_1 = (-0.65, -1.52)$

$p_2 = (-2.12, 1.08)$

$p_3 = (2.81, 0.46)$



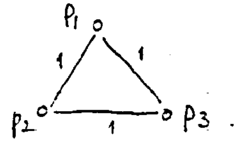
Given a dissimilarity matrix $\{\delta_{ij}\}$, can we always find an exact embedding if there is ?

Condition : $\mathbb{B}$ is positive semidefinite of rank d

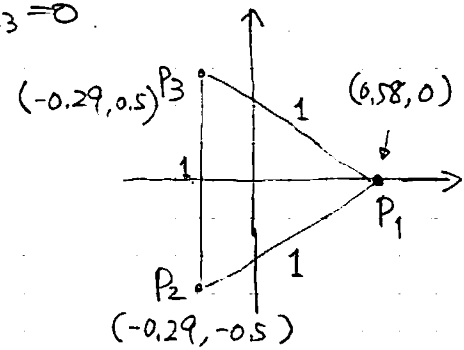
$\Rightarrow$ exact embedding in $\mathbb{R}^d$.

(Example E6)

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



$\lambda_1 = \lambda_2 = 0.5$, $\lambda_3 = 0$



> **Question.**
> How many dimensions are required ?

$\mathbb{B}$ has at least one 0 eigenvalue since

$$\mathbb{B}\mathbb{1} = \mathbb{H}\mathbb{A}\mathbb{H}\mathbb{1}$$

$$\mathbb{H} = \begin{pmatrix} 1-\frac{1}{n} & \cdots & -\frac{1}{n} \\ \vdots & 1-\frac{1}{n} \ddots & \vdots \\ -\frac{1}{n} & \cdots & 1-\frac{1}{n} \end{pmatrix} \quad \mathbb{1} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

$$\mathbb{H}\mathbb{1}_i = \left(1-\frac{1}{n}\right) + \underbrace{\left(-\frac{1}{n}\right) + \cdots + \left(-\frac{1}{n}\right)}_{n-1} = 0 \quad \therefore \mathbb{H}\mathbb{1} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\therefore \mathbb{B}\mathbb{1} = \mathbb{0} = 0\,\mathbb{1}$$

Suppose we are given a dissimilarity matrix $\{\delta_{ij}\}$ defined by pointwise distances. Then, can we find a configuration such that $d_{ij} = \delta_{ij}$ for every i, j?

YES by Mardia et al. in 1979.

if B is positive semi-definite of rank d.

$\Rightarrow B = V \Lambda V^T = X X^T$, where

$$\Lambda = \mathrm{diag}(\lambda_1, \cdots \lambda_d), \quad X = [x_1, \ldots, x_n]^T, \quad x_i = \lambda_i^{1/2} v_i.$$

$$d_{ij}^2 = (x_i - x_j)^T (x_i - x_j) = x_i^T x_i + x_j^T x_j - 2 x_i^T x_j$$

$$= b_{ii} + b_{jj} - 2 b_{ij}$$

$$= (a_{ii} - a_{i*} - a_{*i} + a_{**}) + (a_{jj} - a_{j*} - a_{*j} + a_{**}) - 2(a_{ij} - a_{i*} - a_{*j} + a_{**})$$

$$= a_{ii} + a_{jj} - 2a_{ij} \qquad (\because a_{i*} = a_{*i},\ a_{j*} = a_{*j}, \text{etc.})$$

$$= -2a_{ij} \qquad (\because a_{ii} = -\tfrac{1}{2}\delta_{ii}^2 = 0)$$

$$= \delta_{ij}^2$$

$$\therefore d_{ij}^2 = \delta_{ij}^2$$

Gower (1966) named this method "Principal Coordinates Analysis" (PCO).

in the embedding into $\mathbb{R}^{n-1}$,

$$d_{ij}^2 = \sum_{k=1}^{n-1} \lambda_k (x_{ik} - x_{jk})^2 \qquad (20)$$

So, if λ_i is small enough, then their contribution can be neglected.

Principal Coordinates Analysis

- $\{\delta_{ij}\}$: dissimilarity matrix
- Define a matrix B
- Find d largest eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d \geq 0$ and their corresponding eigenvectors $v_1, \cdots, v_d$.
- Compute a configuration by

$$X = [\sqrt{\lambda_1}\, v_1, \sqrt{\lambda_2}\, v_2, \cdots, \sqrt{\lambda_d}\, v_d]$$

Principal Coordinate Analysis (PCO) is expected to give a good embedding even if there is no exact embedding, but there is no theoretical bound on the performance (e.g. as an approximation ratio).

Metric Least Squares Scaling

loss function $\boxed{S = \sum_{i<j} \frac{1}{\delta_{ij}} (d_{ij} - \delta_{ij})^2 \Big/ \sum_{i<j} \delta_{ij}}$ (21)

$\downarrow$

to be minimized.

Now, $d_{ij}^2 = \sum_{k=1}^{d} (x_{ik} - x_{jk})^2$, and hence

$$\frac{\partial d_{ij}}{\partial x_{tk}} = \frac{\partial}{\partial x_{tk}} \sqrt{(x_{i1} - x_{j1})^2 + \cdots (x_{id} - x_{jd})^2}$$

$$= \frac{1}{2} \cdot \frac{1}{d_{ij}} \cdot \left[2 (x_{ik} - x_{jk}) \delta^{it} - 2 (x_{ik} - x_{jk}) \delta^{jt} \right]$$

$$= \frac{1}{d_{ij}} (x_{ik} - x_{jk}) (\delta^{it} - \delta^{jt}) \qquad (22)$$

where $\delta^{rs} = \begin{cases} 1 & \text{if } r = s \\ 0 & \text{if } r \neq s \end{cases}$

$$\frac{\partial S}{\partial x_{tk}} = \frac{\partial}{\partial x_{tk}} \left[\sum_{i<j} \frac{1}{\delta_{ij}} (d_{ij} - \delta_{ij})^2 \Big/ \sum_{i<j} \delta_{ij} \right]$$

$$= \left[\sum_{i<j} \frac{1}{\delta_{ij}} 2 (d_{ij} - \delta_{ij}) \frac{\partial d_{ij}}{\partial x_{tk}} \right] \Big/ \sum_{i<j} \delta_{ij}$$

$$= \left[\sum_{i<j} \frac{1}{\delta_{ij}} 2 (d_{ij} - \delta_{ij}) \frac{1}{d_{ij}} (x_{ik} - x_{jk}) (\delta^{it} - \delta^{jt}) \right] \Big/ \sum_{i<j} \delta_{ij}$$

$$= \left(\frac{1}{\sum_{i<j} \delta_{ij}} \right) \frac{\partial}{\partial x_{tk}} \left(\sum_{i=1}^{n} \frac{1}{\delta_{it}} (d_{it} - \delta_{it})^2 \right)$$

$$= \left(\frac{2}{\sum_{i<j} \delta_{ij}} \right) \sum_{i=1}^{n} \frac{d_{it} - \delta_{it}}{\delta_{it}} \cdot \frac{1}{d_{it}} (x_{ik} - x_{tk}) (\delta^{it} - \delta^{tt})$$

$$= \left(\frac{2}{\sum_{i<j} \delta_{ij}} \right) \sum_{i=1}^{n} \frac{d_{it} - \delta_{it}}{\delta_{it} d_{it}} (x_{tk} - x_{ik}).$$

The equations

$$\frac{\partial S}{\partial x_{tk}} = \left(\frac{2}{\sum_{i<j} \delta_{ij}} \right) \sum_{i=1}^{n} \frac{d_{it} - \delta_{it}}{d_{it}\,\delta_{it}} \left(x_{tk} - x_{ik} \right) = 0 \qquad (23)$$

$$t = 1, \cdots, n, \quad k = 1, \cdots, d$$

have to be solved numerically.

Sammon (1969) uses a steepest descent method, so that if $x_{tk}^{(m)}$ is the m-th iteration in minimizing S, then

$$x_{tk}^{(m+1)} = x_{tk}^{(m)} - MF \, \frac{\partial S}{\partial x_{tk}} \Big/ \left| \frac{\partial^2 S}{\partial x_{tk}^2} \right|, \qquad (24)$$

where MF is Sammon's magic factor to optimize convergence and was chosen as 0.3 or 0.4.

Least absolute residuals

$$LAR = \sum_{i<j} w_{ij} \left| d_{ij} - \delta_{ij} \right|. \qquad (25)$$

where w_{ij} are weights.

Unidimensional Scaling

in one dimension

$$d_{ij} = |x_i - x_j| \qquad (26)$$

and the loss function to be minimized is

$$S = \sum_{i<j} \left(\delta_{ij} - |x_i - x_j|\right)^2 \qquad (27)$$

$$\boxed{\begin{array}{l} x \text{ is a local minimum of } S \text{ if and only if} \\ \quad x_i = \frac{1}{n} \sum_{j=1}^{n} \delta_{ij}\, \mathrm{sign}(x_i - x_j), \quad i = 1, 2, \cdots, n. \end{array}} \qquad (28)$$

where $\quad \mathrm{sign}(a-b) = \begin{cases} 1 : a > b \\ 0 : a = b \\ -1 : a < b \end{cases} \qquad (29)$

Special case : ordering is fixd $\quad x_1 \geq x_2 \geq \cdots \geq x_n$

$$S = \sum_{i<j} \left(\delta_{ij} - (x_i - x_j)\right)^2 \qquad (30)$$

$$\frac{\partial S}{\partial x_k} = \sum_{k=i<j} \left(-2\delta_{kj} + 2(x_k - x_j)\right) + \sum_{i<k=j} \left(2\delta_{ik} + 2(x_k - x_i)\right)$$

$$= \sum_{j=k+1}^{n} \left(-2\delta_{kj} + 2(x_k - x_j)\right) + \sum_{i=1}^{k-1} \left(2\delta_{ik} + 2(x_k - x_i)\right)$$

$$= 2(n-1)x_k - \sum_{i \neq k} 2x_i + \sum_{i=1}^{k-1} 2\delta_{ik} - \sum_{i=k+1}^{n} 2\delta_{ik}$$

So, the equations to be satisfied are

$$(n-1)x_k - \sum_{i \neq k} x_i = -\sum_{i=1}^{k-1} \delta_{ik} + \sum_{i=k+1}^{n} \delta_{ik} \qquad (32)$$

Since we have at most (n-1) independent equations, the system of equations is expressed in the following matrix form:

$$\begin{pmatrix} n-1 & -1 & \cdots & -1 \\ -1 & n-1 & & \vdots \\ \vdots & -1 & \ddots & \vdots \\ -1 & -1 & & n-1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-1} \end{pmatrix} = \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_{n-1} \end{pmatrix},$$

where $C_i = -\sum_{j=1}^{i-1} \delta_{ij} + \sum_{j=i+1}^{n} \delta_{ij}$, $i=1,\cdots,n$.

Fortunately, the matrix has an inverse matrix. In fact,

$$\begin{pmatrix} 2/n & 1/n & \cdots & 1/n \\ 1/n & 2/n & & \vdots \\ \vdots & & \ddots & \vdots \\ 1/n & 1/n & & 2/n \end{pmatrix} \begin{pmatrix} n-1 & -1 & \cdots & -1 \\ -1 & n-1 & & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \cdots & n-1 \end{pmatrix} = \begin{pmatrix} 1 & & 0 \\ & 1 & \\ & & \ddots \\ 0 & & & 1 \end{pmatrix}$$

$\because$ diagonal $= \frac{2}{n} \times (n-1) + (n-2) \times \frac{1}{n} \times (-1) = \frac{1}{n}(2n-2-n+2) = \underline{1}$.

non-diagonal $= \frac{2}{n} \times (-1) + \frac{1}{n} \times (n-1) + (n-3) \times \frac{1}{n} \times (-1)$

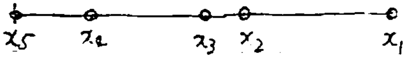
$= \frac{1}{n}(-2+n-1-n+3) = 0$

Thus, we have

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-1} \end{pmatrix} = \begin{pmatrix} \frac{2}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \\ \frac{1}{n} & \frac{2}{n} & \cdots & \frac{1}{n} \\ \vdots & \vdots & & \vdots \\ \frac{1}{n} & \frac{1}{n} & \cdots & \frac{2}{n} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_{n-1} \end{pmatrix}.$$

$$x_n = \frac{1}{n-1}\left[\sum_{i=1}^{n-1} x_i - \sum_{i=1}^{n-1} \delta_{in} \right]$$

(Example E7)



$$(\delta_{ij}) = \begin{array}{c|c} & \begin{matrix} 1 & 2 & 3 & 4 & 5 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{pmatrix} 0 & 4 & 5 & 8 & 10 \\ 4 & 0 & 1 & 4 & 6 \\ 5 & 1 & 0 & 3 & 5 \\ 8 & 4 & 3 & 0 & 2 \\ 10 & 6 & 5 & 2 & 0 \end{pmatrix} \end{array}$$

$$C_1 = -\sum_{j=1}^{0} \delta_{1j} + \sum_{j=2}^{5} \delta_{1j} = 27$$
$$C_2 = -\sum_{j=1}^{1} \delta_{2j} + \sum_{j=3}^{5} \delta_{2j} = -4 + 11 = 7$$
$$C_3 = -\sum_{j=1}^{2} \delta_{3j} + \sum_{j=4}^{5} \delta_{3j} = -6 + 8 = 2$$
$$C_4 = -\sum_{j=1}^{3} \delta_{4j} + \sum_{j=5}^{5} \delta_{4j} = -15 + 2 = -13$$
$$C_5 = -\sum_{j=1}^{4} \delta_{5j} = -23$$

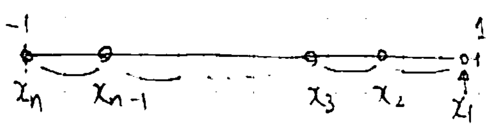
$$C_1 + C_2 + C_3 + C_4 + C_5 = 27 + 7 + 2 - 13 - 23 = 36 - 36 = 0$$
$$x_1 = \frac{1}{n} C_1 + \frac{1}{n} \sum C_i = \frac{27}{5}$$
$$x_2 = \frac{1}{n} C_2 + \frac{1}{n} \sum C_i = \frac{7}{5}$$
$$x_3 = \frac{1}{n} C_3 + \frac{1}{n} \sum C_i = \frac{2}{5}$$
$$x_4 = \frac{1}{n} C_4 + \frac{1}{n} \sum C_i = -\frac{13}{5}$$
$$x_5 = \frac{1}{4}\left[x_1 + x_2 + x_3 + x_4 + C_5\right] = \frac{1}{4}\left[\frac{1}{5}(27+7+2-13) - 23\right] = \frac{1}{4}\left(\frac{23}{5} - 23\right)$$
$$= -\frac{23}{5}$$

(Example E8)

$$\delta_{ij} = \begin{cases} 1 & \text{if } i \neq j \\ 0 & \text{if } i = j. \end{cases}$$

$$C_1 = n - 2$$
$$C_2 = n - 2 - 2 = n - 4$$
$$C_i = n - 2 - 2*(i-1) = n - 2i$$
$$C_n = n - 2 - 2(n-1) = -n$$

$$\sum_{i=1}^{n} C_i = \sum_{i=1}^{n} (n - 2i) = n(n-1) - 2 \cdot \frac{1}{2} n(n-1) = 0.$$
$$\therefore x_i = \frac{1}{n} C_i = \frac{1}{n}(n - 2i) = 1 - \frac{2i}{n}, \quad x_1 = 1 - \frac{2}{n}, \quad x_n = 1 - 2 = -1$$



Special Case $\delta_{ij} = \delta^{ij}$

$$(\delta_{ij}) = \begin{pmatrix} 0 & & 1 \\ & \ddots & \\ 1 & & 0 \end{pmatrix}$$

· In one dimension, there is an optimal embedding that minimizes $\sum_{i<j} (\delta_{ij} - d_{ij})^2$,
where $d_{ij} = |x_i - x_j|$ in $\mathbb{R}^1$.

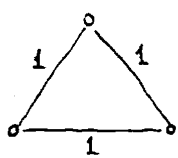
$$x_1 = 1 - \frac{2}{n},\ x_2 = 1 - \frac{4}{n},\ \cdots,\ x_{n-1} = 1 - \frac{2(n-1)}{n},\ x_n = -1.$$

• What is an optimal embedding in $\mathbb{R}^1$ if we add constraints $d_{ij} \geq \delta_{ij}$ for all i and j?

One solution is
$x_1 = 0,\ x_2 = 1,\ \cdots,\ x_n = n-1.$
The solution is optimal!

· In two dimensions

There is an exact embedding of three objects in $\mathbb{R}^2$.



← exact embedding for $\Delta_3 = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$

For n objects

$$a_{ij} = -\frac{1}{2}\delta_{ij}^2 \qquad \left(-\frac{1}{2} \text{ if } i \neq j,\ 0 \text{ if } i = j\right)$$

$$a_{i*} = a_{*i} = \frac{1}{n}\sum_{j=1}^{n} a_{ij} = -\frac{1}{2n}(n-1)$$

$$a_{**} = \frac{1}{n^2}\sum_i \sum_j a_{ij} = \frac{1}{n}\sum_{i=1}^{n} a_{i*} = \frac{1}{n}\cdot n \cdot \left(-\frac{n-1}{2n}\right) = -\frac{n-1}{2n}$$

$$\therefore\ b_{ij} = a_{ij} - a_{i*} - a_{*j} + a_{**}$$
$$= -\frac{1}{2} + \frac{1}{2n}(n-1) + \frac{1}{2n}(n-1) - \frac{1}{2n}(n-1) = -\frac{1}{2n} \quad \text{if } i \neq j$$
$$b_{ii} = a_{ii} - a_{i*} - a_{*i} + a_{**}$$
$$= 0 + \frac{1}{2n}(n-1) + \frac{1}{2n}(n-1) - \frac{1}{2n}(n-1) = \frac{1}{2} - \frac{1}{2n}$$

If we set $\varepsilon = -\frac{1}{2n}$, we have

$$B = \begin{pmatrix} \frac{1}{2}+\varepsilon & & & \\ & \frac{1}{2}+\varepsilon & & \varepsilon \\ & & \ddots & \\ \varepsilon & & & \frac{1}{2}+\varepsilon \end{pmatrix}$$

- The matrix B has an eigenvalue $1/2$:

  for any vector $v = (v_1, \cdots, v_n)^T$ such that $\sum_{i=1}^n v_i = 0$,
  $$Bv = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}, \quad x_i = \frac{1}{2}v_i + \varepsilon \sum_{j=1}^n v_j = \frac{1}{2}v_i$$
  $$\therefore\ Bv = \frac{1}{2}v \quad \Rightarrow \lambda = \frac{1}{2} \text{ is an eigenvalue}$$

- The matrix B has an eigenvalue 0:

  for the vector $\mathbb{1} = (1, \cdots, 1)^T$,
  $$B\mathbb{1} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}, \quad x_i = \frac{1}{2} + \varepsilon n = \frac{1}{2} + n \times \left(-\frac{1}{2n}\right) = 0.$$
  $$\therefore\ B\mathbb{1} = 0\,\mathbb{1} \quad \Rightarrow \lambda = 0 \text{ is an eigenvalue}$$

- B has no other eigenvalues.

  Let λ and $v = (v_1, \cdots, v_n)^T$ be a pair of eigenvalue and eigenvector of the matrix B.

Then, we have

$$B v = \lambda v.$$

$$\Rightarrow \lambda v_i = \tfrac{1}{2} v_i + \varepsilon \textstyle\sum_{j=1}^{n} v_j \quad, i=1,2,\cdots,n, \quad \varepsilon = -\tfrac{1}{2n}.$$

Case 1: $\sum_{j=1}^{n} v_j = 0$

$$\lambda v_i = \tfrac{1}{2} v_i \quad , \quad \therefore \lambda = \tfrac{1}{2} \quad \text{(eigenvalue)}$$

Case 2: $\sum_{j=1}^{n} v_j \neq 0$

we must have

$$\lambda v_i = \frac{1}{2} v_i - \frac{1}{2n} \sum_{j=1}^{n} v_j .$$

For any $v_i \neq 0$, we must have

$$\lambda = \frac{1}{2} - \frac{1}{2n v_i} \textstyle\sum_{j=1}^{n} v_j ,$$

independently of i. Therefore, we must have $v_1 = v_2 = \cdots = v_n$. Then, we have

$$\lambda = \frac{1}{2} - \frac{1}{2n v_i} \cdot n v_i = \frac{1}{2} - \frac{1}{2} = 0. \quad \text{(eigenvalue)}$$

In this special case, eigenvector corresponding to the eigenvalue $\lambda_1 = 1/2$ is not uniquely determined. Any vector $v = (v_1, \cdots, v_n)^T$ with $\sum_{j=1}^{n} v_j = 0$ can be an eigenvector of $\lambda = 1/2$.

- <u>Special case : $n = 3$</u>

Let three points be $p_1(x_1, y_1)$, $p_2(x_2, y_2)$, and $p_3(x_3, y_3)$.

$\lambda_1 = \lambda_2 = 1/2$, $\quad v_1 = (x_1, x_2)^T$ and $v_2 = (y_1, y_2)^T$

condition : $x_1 + x_2 + x_3 = 0$ and $y_1 + y_2 + y_3 = 0$.

$$B = \begin{pmatrix} \frac{1}{2}+\varepsilon & \varepsilon \\ \varepsilon & \frac{1}{2}+\varepsilon \end{pmatrix} = \begin{pmatrix} \frac{1}{2}-\frac{1}{6} & -\frac{1}{6} \\ -\frac{1}{6} & \frac{1}{2}-\frac{1}{6} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} & -\frac{1}{6} \\ -\frac{1}{6} & \frac{1}{3} \end{pmatrix}$$

$$Bv_1 = \begin{pmatrix} \frac{1}{3}x_1 - \frac{1}{6}x_2 \\ -\frac{1}{6}x_1 + \frac{1}{3}x_2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$\therefore \ \frac{1}{3}x_1 - \frac{1}{6}x_2 = \frac{1}{2}x_1 \ \rightarrow \ x_1 = -x_2$$

$$-\frac{1}{6}x_1 + \frac{1}{3}x_2 = \frac{1}{2}x_2 \ \rightarrow \ x_1 = -x_2.$$

Similarly, from $Bv_2 = \frac{1}{2}v_2$, we have

$$y_1 = -y_2.$$

Thus, we have

① $x_1 + x_2 + x_3 = 0$
② $x_1 = -x_2$ $\Rightarrow$ $x_1 = -x_2$ and $x_3 = 0$
③ $y_1 + y_2 + y_3 = 0$ $\quad$ $y_1 = -y_2$ and $y_3 = 0$
④ $y_1 = -y_2$

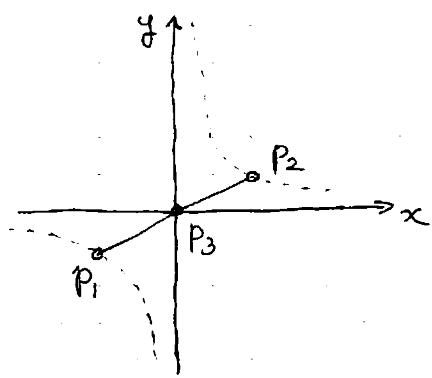
- Two vectors must be orthogonal

$$v_1^T v_2 = (x_1\ x_2\ x_3)\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = x_1y_1 + x_2y_2 + x_3y_3 = 1.$$

$$\Rightarrow x_1y_1 + (-x_1)(-y_1) + 0\cdot 0 = 2x_1y_1 = 1.$$

- Summarize the constraints, we have

① $x_1 = -x_2$, $x_3 = 0$
② $y_1 = -y_2$, $y_3 = 0$
③ $x_1y_1 = 1/2$.



Various Objective Functions

$$S_1 = \sum_{i<j} \left| d_{ij}^2 - \delta_{ij}^2 \right|$$

$$S_2 = \sum_{i<j} (d_{ij} - \delta_{ij})^2$$

$$S_3 = \sum_{i<j} \left| d_{ij} - \delta_{ij} \right|$$

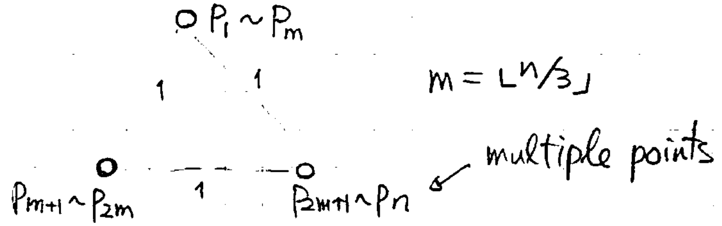
$$S_4 = \sum_{i<j} (d_{ij}^2 - \delta_{ij}^2)^2$$

many other variations, e.g.,

$$S_2' = \sum_{i<j} \frac{1}{\delta_{ij}} (d_{ij} - \delta_{ij})^2 \Big/ \sum_{i<j} \delta_{ij} .$$

$$S_1 = \sum_{i<j} \left| d_{ij}^2 - \delta_{ij}^2 \right|$$

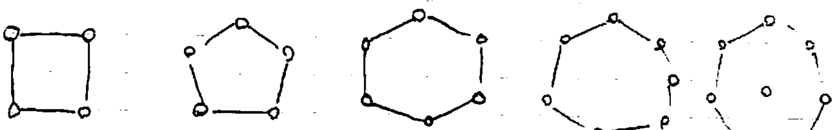
Special case : $\delta_{ij} = \begin{cases} 1 & \text{if } i \neq j \\ 0 & \text{if } i = j . \end{cases}$



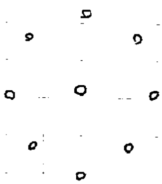
$m = \lfloor n/3 \rfloor$

$$S_2 = \sum_{i<j} (d_{ij} - \delta_{ij})^2$$

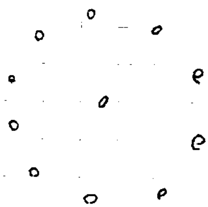
$$\delta_{ij} = \begin{cases} 1 & \text{if } i \neq j \\ 0 & \text{if } i = j. \end{cases}$$



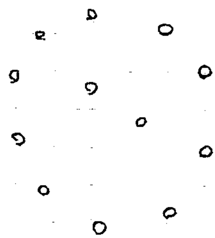
$n=4$ $n=5$ $n=6$ $n=7$ $n=8$.



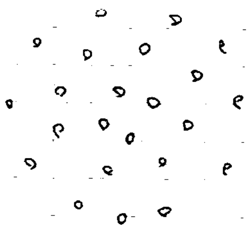
$n=9$



$n=11$



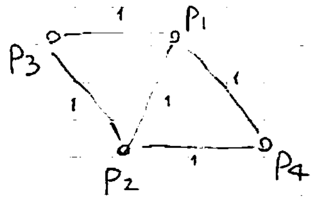
$n=12$

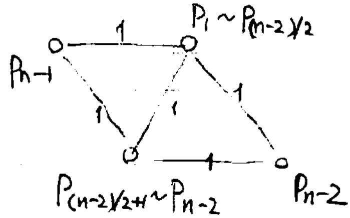


$n=?$

$$S_3 = \sum_{i<j} |d_{ij} - \delta_{ij}|$$

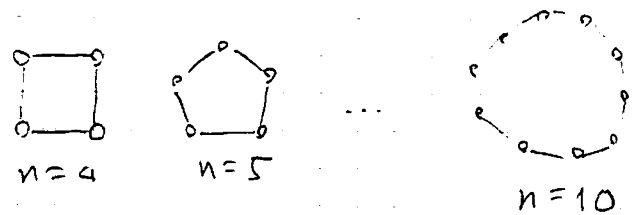
$$\delta_{ij} = \begin{cases} 1 & \text{if } i \neq j \\ 0 & \text{if } i = j. \end{cases}$$





$$S_4 = \sum_{i<j} \left(d_{ij}^2 - \delta_{ij}^2\right)^2$$

$$\delta_{ij} = \begin{cases} 1 & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}.$$



Inserting one point in the amidst of many points

Problem: Given n points $p_1, \cdots, p_n$ in the plane and n real values $\delta_1, \cdots, \delta_n$, find a point p that minimizes

$$\sum_{i=1}^{n} |d_i^2 - \delta_i^2|,$$

where d_i is the distance from p to p_i.

Note!

A similar problem with an objective function

$$\sum_{i=1}^{n} |d_i - \delta_i|$$

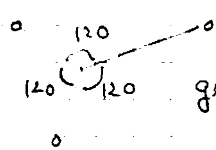
is hard.

$\because$ Consider a special case where $\delta_i = 0, i = 1, \cdots, n$.

This problem is to find a point that minimizes the sum of distances to the existing points.

→ It is called "Geometric Median"

For three points

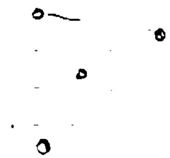


geometric median for three points

↳ known as "Fermat point"

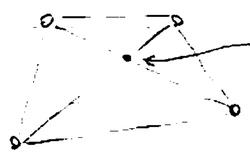
This problem is called the Fermat-Weber problem.

For four points



→ geometric center coincides with the internal point.

Case 1 : one point is inside the triangle formed by the remaing three points



intersection of two diagonals
→ geometric center

Case 2 : convex positions

For n points.

No formula is known to calculate the geometric median.

Good news : the sum of distances is a convex function
⇓
local optimum = global optimum.

Problem is hard even for 5 points.

Approximation algorithm (Bose - Maheshwari - Morin '03).

ε-approximation algorithms

$O(n \log n)$ time : deterministic

$O(n)$ time : randomized

FACT : The search space is convex.

Proof : the distance to each existing point p_i is convex.
($f_i = d(p, p_i)$)

- sum of convex functions is convex
- the sum of distances to the existing points is convex. $\sum d(p, p_i)$

Problem : Given n points $p_1, \cdots, p_n$ and n real values $\delta_1, \cdots, \delta_n$, find a point p that minimizes

$$\sum_{i=1}^{n} |d_i^2 - \delta_i^2|,$$

where d_i is the distance from p to p_i.

◦ Special case $\delta_i = 0$, $i = 1, \cdots, n$

Find a point p : $\sum_{i=1}^{n} d_i^2 \to \min$

Again, the search space is convex.

$$S = \sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} (x - x_i)^2 + (y - y_i)^2$$

At a global optimum, we must have

$$\frac{\partial S}{\partial x} = \frac{\partial S}{\partial y} = 0.$$

Thus, we have

$$\frac{\partial S}{\partial x} = 2\sum_{i=1}^{n} (x - x_i) = 0 \quad \therefore x = \frac{1}{n}\sum x_i$$

$$\frac{\partial S}{\partial y} = 2\sum_{i=1}^{n} (y - y_i) = 0 \quad \therefore y = \frac{1}{n}\sum y_i$$

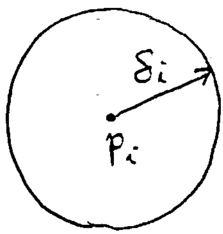
So, the centroid is the global optimum. //

Original problem: $S = \sum_{i=1}^{n} |d_i^2 - \delta_i^2| \to \min$

unfortunately, the function $|d_i^2 - \delta_i^2|$ is not convex.
So, the search space is not convex.

How to calculate $|d_i^2 - \delta_i^2|$

Draw a circle C_i of radius δ_i and center at p_i



In the interior of C_i
$|d_i^2 - \delta_i^2| = \delta_i^2 - d_i^2$
In the exterior of C_i
$|d_i^2 - \delta_i^2| = d_i^2 - \delta_i^2$

For n points

Draw n circles $C_1, \cdots, C_n$
→ arrangement of those circles
$O(n^2)$ cells.

At each cell R_i we have a quadratic polynomial
$a_i(x^2+y^2) + b_i x + c_i y + d_i$

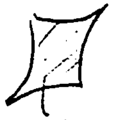
$$\frac{\partial S}{\partial x} = 2a_i x + b_i = 0 \qquad x = -\frac{b_i}{2a_i}$$

$$\frac{\partial S}{\partial y} = 2a_i y + c_i = 0 \qquad y = -\frac{c_i}{2a_i}$$

$\left(-\frac{b_i}{2a_i}, -\frac{c_i}{2a_i}\right)$: apex point.

If the apex point is within the cell, the apex point is a candidate of an optimal point.

If the apex point is outside the cell



Case 1: $a_i > 0$

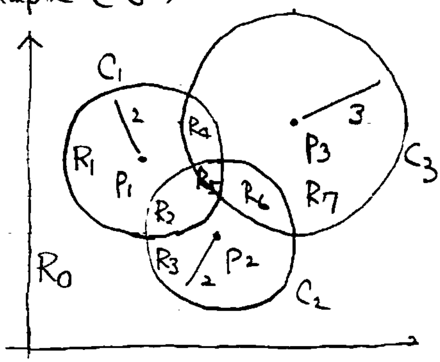
find a point on the boundary of R_i that is nearest to the apex point.

→ candidate for the cell.

Case 2: $a_i < 0$

find a point on the boundary of R_i that is farthest to the apex point.

(Example E8)



$p_1(3,5)$ $\delta_1 = 2$

$p_2(5,3)$ $\delta_2 = 2$

$p_3(7,6)$ $\delta_3 = 3$.

Cells are coded by three signs $(\sigma_1, \sigma_2, \sigma_3)$

$$\sigma_i = \begin{cases} 1 & \text{if the cell is outside the circle } C_i \\ -1 & \text{otherwise} \end{cases}$$

Then, the objective function

$$S = \sigma_1\left[(x-3)^2+(y-5)^2-2^2\right]+\sigma_2\left[(x-5)^2+(y-3)^2-2^2\right]+\sigma_3\left[(x-7)^2+(y-6)^2-3^2\right]$$

$$= (\sigma_1+\sigma_2+\sigma_3)(x^2+y^2)-2(3\sigma_1+5\sigma_2+7\sigma_3)x-2(5\sigma_1+3\sigma_2+6\sigma_3)y$$

$+ \text{const}.$

$$\frac{\partial S}{\partial x} = 2(\sigma_1+\sigma_2+\sigma_3)x - 2(3\sigma_1+5\sigma_2+7\sigma_3) = 0$$

$$\frac{\partial S}{\partial y} = 2(\sigma_1+\sigma_2+\sigma_3)y - 2(5\sigma_1+3\sigma_2+6\sigma_3) = 0$$

$$\therefore (x,y) = \left(\frac{3\sigma_1+5\sigma_2+7\sigma_3}{\sigma_1+\sigma_2+\sigma_3}, \frac{5\sigma_1+3\sigma_2+6\sigma_3}{\sigma_1+\sigma_2+\sigma_3}\right)$$

cell R_0 (1,1,1) $x=15/3=5$ $y=14/3$ $(x,y)=(5,14/3)$

cell R_1 (-1,1,1) $x=9/1=9$ $y=4/1=4$ $(x,y)=(9,4)$

cell R_2 (-1,-1,1) $x=-1/(-1)=1$ $y=-2/(-1)=2$ $(x,y)=(1,2)$

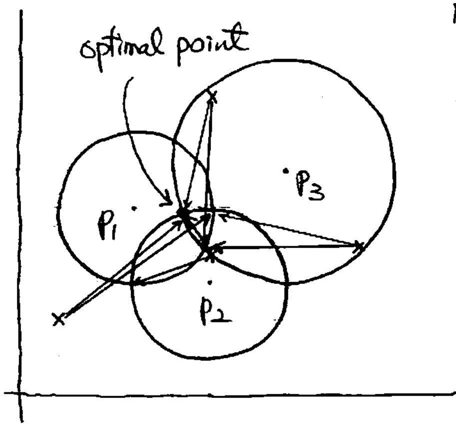
cell R_3 (1,-1,1) $x=5/1=5$, $y=8/1=8$ $(x,y)=(5,8)$

cell R_4 (-1,1,-1) $x=(-5)/(-1)=5$, $y=(-8)/(-1)=8$ $(x,y)=(5,8)$

cell R_5 (-1,-1,-1) $x=(-15)/(-3)=5$, $y=(-14)/(-3)=14/3$ $(x,y)=(5,14/3)$

cell R_6 (1,-1,-1) $x=-9/(-1)=9$, $y=-4/(-1)=4$ $(x,y)=(9,4)$

cell R_7 (1,1,-1) $x=1/1=1$, $y=2/1=2$. $(x,y)=(1,2)$



No apex point lies in the interior of the corresponding cell.

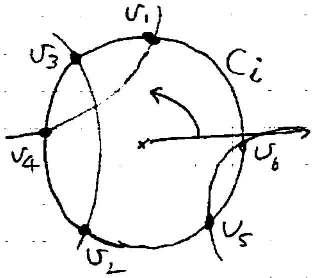
for each cell, find a nearest/farthest point from the apex point

Construct an arrangement of circles.

① Compute all intersections of circles
→ $O(n^2)$ intersections

we compute a list of all intersections for each circle

circle C_i $\boxed{v_1 \mid v_2 \mid \cdots \mid}$ ← list of intersections on C_i

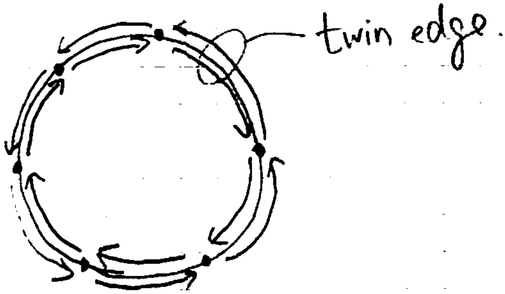


Sort all the intersections by angles from the horizontal ray to the right from the center of C_i.

$(v_{i_0}, v_{i_1}, \cdots, v_{i_{k-1}})$: sorted list

→ make edges $e_{i_0} = (v_{i_0}, v_{i_1}), \cdots, e_{i_{k-1}} = (v_{i_{k-2}}, v_{i_{k-1}}),$
$e_{i_k} = (v_{i_{k-1}}, v_{i_0})$

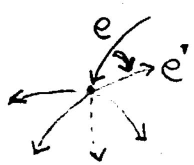
→ for each edge, we create its twin edge of the opposite direction



Now we have all vertices (intersections) and edges connecting vertices.

Next, we enumerate all the cells

while(there is an unvisited edges){
  Choose one unvisited edge e arbitrarily;
  Make a new cell Ri lying to the left of e;
  Put the edge into a list L(Ri) associated with Ri.
  do{
    Among those edges outgoing from the target point of the edge e, choose the one that is next to e in the clockwise order.



let it be e'.

    Put e' into the list L(Ri) and label it as "visited".
    e = e';
  }while (the list L(Ri) is not a cycle);
}.

<u>Algorithm</u>

(1) Draw n circles $C_1, \cdots, C_n$;

(2) Construct an arrangement of those circles.

(3) Compute a dual graph G;

(4) Compute a spanning tree T of G;

(5) Compute a walk along T; $\rightarrow$ sequence of cells.

(6) R = initial cell in the sequence
Compute the objective function S
(compute coefficients A, B, C, and D
$A(x^2+y^2)+Bx+Cy+D$)
Solve a system of equation $\partial S/\partial x = \partial S/\partial y = 0$;
let $p(R)$ be a point satisfying the system;
Check whether $p(R)$ lies inside R or not
by traversing the boundary of R;
if $p(R)$ lies inside R then $p^*(R) = p(R)$;
else if $A > 0$ then
find a point on the boundary of R that
is closest to $p(R)$
else $A < 0$ then
find a point on the boundary of R that
is farthest from $p(R)$
else $A = 0$ then
find a point on the boundary of R that
minimizes $Bx + Cy + D$;
all by traversing the boundary of R;

Now, we have a dual graph $G = (V, \bar{E})$.

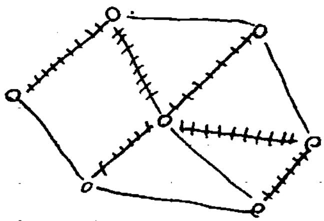
$\#$ of vertices $= \#$ of cells $= O(n^2)$

$\#$ of edges $\leq \#$ of twin edges $= O(n^2)$

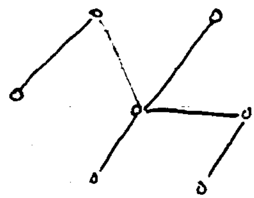
time to compute the dual graph $= O(n^2)$.

$\Downarrow$

Then, compute a spanning tree T of G



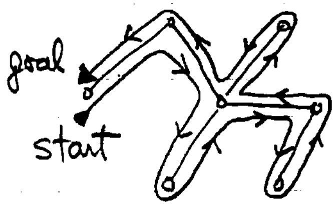
dual graph



tree edge.

$\Downarrow$

Define a walk along T



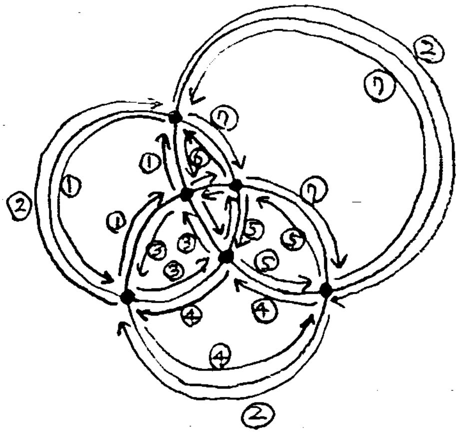
Walk

= a sequence of vertices visiting each edge exactly twice.

two vertices are adjacent in a walk

$\Rightarrow$ their corresponding cells are adjacent

(Example E9)



Now, we can traverse the boundary of any cell.

Constructing a dual graph

Dual graph $G = (V, E)$

vertex ← cell.

edge ← between two cells adjacent to each other.

For each cell R_i

traverse the boundary of R_i

for each edge e

find its twin edg e'

let R_j be the cell associated with e'

define an edge (R_i, R_j) if it is not found.

while (R is not the last cell in the sequence){

let R' be the next cell in the sequence;

modify the objective function using the information of the edge between R and R';

(this modification can be done in $O(1)$ time).

let R = R';

repeat the same calculation as above;

→ find an optimal point $p^*(R)$ for R;

}.

Note that the boundary of a cell is traversed only twice. Thus, the total time for Traverse is $O(n^2)$.

Therefore, the total running time is

$O(n^2 \log n)$ for sorting intersections

$O(n^2)$ for remaining computation

in total $O(n^2 \log n)$ time and

$O(n^2)$ space

⇓

can improve the running time into $O(n^2)$?

space can be improved $O(n)$

while keeping the running time in $O(n^2 \log n)$

⇐ Plane Sweep Algorithm.