

Re: Distributing n points in space

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I have n points i don't have any coordinates, only thing i have is distance matrix por each pair of points distance from one to the other, i want to put them all in $k < n$ dimensional space, it is probably impossible to do it precisly what i want is to distripute points in space in in the way that minimize sum of diference between proper distance and the real one. Is there any solution of this, does the problem have any official name?

Consider the Gram matrix G:

$$G_{\{ij\}} = (x_i) \cdot (x_j)$$

G must be positive semidefinite. The $n \times n$ positive semidefinite matrix G is the Gram matrix for n points of R^k if and only if G has rank $\leq k$, and these points can be obtained using the diagonalization of G. If G has some negative eigenvalues or rank $> k$, the best approximation, in some sense, is obtained by using the (up to) k largest positive eigenvalues and eigenvectors.

Now given the distance matrix D:

$$D_{\{ij\}} = |x_i - x_j|$$

we can designate one of the points (say x_n) as the origin, and then

$$G_{\{ij\}} = (D_{\{in\}}^2 + D_{\{jn\}}^2 - D_{\{ij\}}^2) / 2$$

For example, suppose you have the 4 x 4 distance matrix

$$D = \begin{bmatrix} 0 & 2 & 2 & 3 \\ 2 & 0 & 3 & 2 \\ 2 & 3 & 0 & 1 \\ 3 & 2 & 1 & 0 \end{bmatrix}$$

and you want $k=2$. This leads to

$$G = \begin{bmatrix} 9 & 4.5 & 3 & 0 \\ 4.5 & 4 & -2 & 0 \\ 3 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

which has a negative eigenvalue. If λ_1 and λ_2 are the two

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positive eigenvalues and u_1 and u_2 the corresponding orthonormal eigenvectors, then we take the points of \mathbb{R}^2 corresponding to the rows of the matrix with columns $\sqrt{\lambda_1} u_1$ and $\sqrt{\lambda_2} u_2$, namely

[-3.01692215332068070, .520107363143339496],
[-1.58230163082378516, -1.45887821879530888],
[-.540150726393245684, 1.36862161370595770],
[0., 0.]

which would have the distance matrix

[0. 2.444283121 2.618085777 3.061426293]
[2.444283121 0. 3.013442187 2.152209123]
[2.618085777 3.013442187 0. 1.471355813]
[3.061426293 2.152209123 1.471355813 0.]

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