Multivariate Methods

Homework #2 (2020-2021), Answers

Here we work out a simple multidimensional scaling problem and see how negative eigenvalues can arise. Consider four points whose distances are the entries in the following matrix:

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

A. Calculate the doubly-centered distance matrix G, with entries

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

Note that all points have the same set of distances to its neighbors: two points at a distance of 1, and one point at a distance of b. So $\frac{1}{N}\sum_{i=1}^{N}d_{ij}^{\ 2}=\frac{1}{N}\sum_{j=1}^{N}d_{ij}^{\ 2}=\frac{1}{4}(1+1+b^2)=\frac{2+b^2}{4}$, and $\frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}d_{ij}^{\ 2}=\frac{2+b^2}{4}$ also. So,

$$G=-\frac{1}{2}\begin{pmatrix} 0 & 1 & b^2 & 1 \\ 1 & 0 & 1 & b^2 \\ b^2 & 1 & 0 & 1 \\ 1 & b^2 & 1 & 0 \end{pmatrix}+\frac{1}{2}\left(\frac{2+b^2}{4}\right)\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}=\frac{1}{8}\begin{pmatrix} +2+b^2 & -2+b^2 & +2-3b^2 & -2+b^2 \\ -2+b^2 & +2+b^2 & -2+b^2 & +2-3b^2 \\ +2-3b^2 & -2+b^2 & +2+b^2 & -2+b^2 \\ -2+b^2 & +2-3b^2 & -2+b^2 & +2+b^2 \end{pmatrix}.$$

B. We now find the eigenvectors of G. Observe that G, like D, is invariant under cyclic permutation of the labels (1234). Therefore, it commutes with $P=\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$, and consequently, has the same eigenvectors as P. What are the eigenvectors of P?

Since P corresponds to the rotations of a square, its eigenvectors are the Fourier basis: $\vec{\varphi}_1=\begin{pmatrix} +1 \\ +1 \\ +1 \\ +1 \end{pmatrix}$, $\vec{\varphi}_{-1}=\begin{pmatrix} +1 \\ -1 \\ +1 \\ -1 \end{pmatrix}$,

$\vec{\varphi}_i=\begin{pmatrix} +1 \\ +i \\ -1 \\ -i \end{pmatrix}$, and $\vec{\varphi}_{-i}=\begin{pmatrix} +1 \\ -i \\ -1 \\ +i \end{pmatrix}$.

C. Determine the eigenvalues of G corresponding to each of the eigenvectors above.

By direct multiplication, $G\vec{\varphi}_1 = 0$, $G\vec{\varphi}_{-1} = (1-\frac{b^2}{2})\vec{\varphi}_{-1}$, $G\vec{\varphi}_i = \frac{b^2}{2}\vec{\varphi}_i$, and $G\vec{\varphi}_{-i} = \frac{b^2}{2}\vec{\varphi}_{-i}$.

D. Find the embedding in 3-space that corresponds to the distance matrix in A.

The coordinates are given by $\vec{x}_k = \sqrt{\lambda_k}\vec{v}_k$, where $\vec{v}_i$ are the normalized eigenvectors. $\vec{\varphi}_1$ can be ignored since its eigenvalue is zero. For $\vec{\varphi}_{-1}$, we take $\vec{v}_{-1} = \frac{1}{2}\vec{\varphi}_{-1} = \frac{1}{2}\begin{pmatrix}+1\\-1\\+1\\-1\end{pmatrix}$. For the last two eigenvectors, we'd like to have real-valued coordinates. Since $\vec{\varphi}_i$, and $\vec{\varphi}_{-i}$ have the same eigenvalues, we replace them by

$\vec{v}_+ = \frac{\vec{\varphi}_i + \vec{\varphi}_{-i}}{2\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix}+1\\0\\-1\\0\end{pmatrix}$ and $\vec{v}_- = \frac{-i\vec{\varphi}_i + i\vec{\varphi}_{-i}}{2\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\+1\\0\\-1\end{pmatrix}$ (which have eigenvalue $\lambda_+ = \lambda_- = \frac{b^2}{2}$).

So, assuming all eigenvalues are positive, the coordinates are $\left[\sqrt{\lambda_{-1}}\vec{v}_{-1} \quad \sqrt{\lambda_+}\vec{v}_+ \quad \sqrt{\lambda_-}\vec{v}_-\right]$, i.e., the four rows of

$$\left[\frac{1}{2}\sqrt{1-\frac{b^2}{2}}\begin{pmatrix}+1\\-1\\+1\\-1\end{pmatrix} \quad \frac{b}{2}\begin{pmatrix}+1\\0\\-1\\0\end{pmatrix} \quad \frac{b}{2}\begin{pmatrix}0\\+1\\0\\-1\end{pmatrix}\right].$$

E. What values of b yield three equal eigenvalues?What does this indicate?

$\lambda_+ = \lambda_- = \frac{b^2}{2}$, and $\lambda_{-1} = 1-\frac{b^2}{2}$ becomes equal to the other eigenvalues at $b=1$. The points now lie at the vertices of a regular tetrahedron, and all three dimensions contribute equally. For $b<1$, the coordinate associated with $\vec{v}_{-1}$ dominates. For $b>1$, the coordinates associated with $\vec{v}_+$ and $\vec{v}_-$ dominate.

$\lambda_+ = \lambda_- = \frac{b^2}{2} \geq 0$ for all b, but $\lambda_{-1} = 1-\frac{b^2}{2}$ becomes negative when $b > \sqrt{2}$. The distances can no longer be achieved by four points in a Euclidean space.

F. What values of b yield negative eigenvalues?What does this indicate?

$\lambda_+ = \lambda_- = \frac{b^2}{2} \geq 0$ for all b, but $\lambda_{-1} = 1-\frac{b^2}{2}$ becomes negative when $b > \sqrt{2}$. The distances can no longer be achieved by four points in a Euclidean space.