Multidimensional Scaling for Functional Data

Masahiro Mizuta
Center for Information and Multimedia Studies, Hokkaido University
N.11, W.5, Kita-ku,
Sapporo 060-0811, Japan
mizuta@cims.hokudai.ac.jp

1. Introduction

Nowadays, the area of data analysis is extended to the broad field. The types of data set that are dealt with data analysis are also extended. Ramsay and Silverman proposed the concept of Functional Data Analysis (FDA). FDA deals with functional data or deals with data as functional data. In the paper, we propose a method of FDA for functional dissimilarities data; the dissimilarities depending on a variable.

2. Multidimensional Scaling

Conventional MDS methods are developed for finding structures among n objects with configurations of n points on the p dimensional Euclidean space. The dissimilarities among n objects are denoted by $S = \{s_{ij}\}(i,j = 1,2,\cdots,n)$. We assume $s_{ij} \geq 0$, $s_{ij} = s_{ji}$ and $s_{ii} = 0$. The aim of MDS is to construct the configuration $X = \{\boldsymbol{x}_i\}(i = 1,2,\cdots,n)$ that represents the relations among n objects. The configuration is a set of n points on the p dimensional Euclidean space. The Euclidean distances between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ are denoted by d_{ij}; $d_{ij} := \|\boldsymbol{x}_i - \boldsymbol{x}_j\|$. Methods of MDS find a configuration X such as $d_{ij} \simeq s_{ij}$. The degree of the coincidence of d_{ij} and s_{ij} is defined for each MDS method, the values of them or the order of them.

3. Proposed Method

In the section, we propose a method of functional multidimensional scaling. Dissimilarities among n objects depending on a variable t are denoted by $S(t) = \{s_{ij}(t)\}(i,j = 1,2,\cdots,n), t \in [a,b]$. For the sake of explanation, we assume that the dimension of the space of the configuration is 2.

The proposed method needs a conventional MDS method for the first step, for example Torgerson's method. A conventional MDS method is applied to the dissimilarities data for each t. We can get 2 dimensional configurations of n objects for each t. They are denoted by $X(t) = \{\boldsymbol{x}_i(t)\}(i = 1,2,\cdots,n)$. There is no guarantee that $X(t)$ are continuous, but we assume that they are differentiable here. The key idea of the method is to find out orthogonal matrix function $Q(t)$ that adjusts $X(t)$ to $Q(t)X(t)$ because the distances between points are invariant under orthogonal transformations.

The length of the curve $\boldsymbol{x}_i(t)$ on the 2 dimensional space is

$$l = \int_a^b \sqrt{\left\| \frac{d\boldsymbol{x}(t)}{dt} \right\|^2} \, dt.$$

Then, we find the orthogonal matrix function $Q(t)$ that minimize

$$l(Q) = \int_a^b \sum_{i=1}^{n} \left\| \frac{dQ(t)\boldsymbol{x}_i(t)}{dt} \right\|^2 \, dt.$$

$Q(t)$ can be represented by $Q(t) = \begin{pmatrix} \sin\phi(t) & \cos\phi(t) \\ -\sin\phi(t) & \sin\phi(t) \end{pmatrix}$, where $\phi(t)$ is a function of t. Then

$$l(Q) = \int_a^b \left(\sum_{i=1}^{n} \left\| \frac{d\boldsymbol{x}_i(t)}{dt} \right\|^2 + 2 \left(\sum_{i=1}^{n} \frac{d\boldsymbol{x}_i(t)^T}{dt} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \boldsymbol{x}_i(t) \right) \phi'(t) + \left(\sum_{i=1}^{n} \|\boldsymbol{x}_i(t)\|^2 \right) \phi'(t)^2 \right) dt.$$

So when

$$\phi'(t) = \frac{-\sum_{i=1}^{n} \frac{d\boldsymbol{x}_i(t)^T}{dt} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \boldsymbol{x}_i(t)}{\sum_{i=1}^{n} \|\boldsymbol{x}_i(t)\|^2},$$

$l(Q)$ takes the minimum value.

The *functional* configuration $Q(t)X(t)$ is the result of the functional multidimensional scaling. The functional configuration can be shown with motions of n points by dynamic graphics. The n trajectories of $X(t)$ are also a good representation on a sheet.

REFERENCES

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RÉSUMÉ

Une méthode de Scaling Multidimensionnel pour les données de dissimilarities fonctionnelles est proposée. Quand les données de dissimilarities entre les objets sont données ont dépendu d'une variable, la méthode proposée peut dériver la configuration fonctionnelle qui représente les données de dissimilarities fonctionnelles.