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Sensitivity analysis of the strain criterion for multidimensional scaling

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Abstract

Multidimensional scaling (MDS) is a collection of data analytic techniques for constructing configurations of points from dissimilarity information about interpoint distances. Classsical MDS assumes a fixed matrix of dissimilarities. However, in some applications, e.g., the problem of inferring 3-dimensional molecular structure from bounds on interatomic distances, the dissimilarities are free to vary, resulting in optimization problems with a spectral objective function. A perturbation analysis is used to compute first- and second-order directional derivatives of this function. The gradient and Hessian are then inferred as representers of the derivatives. This coordinate-free approach reveals the matrix structure of the objective and facilitates writing customized optimization software. Also analyzed is the spectrum of the Hessian of the objective.

Keywords: Classical multidimensional scaling; Principal coordinate analysis; Distance matrices; Distance geometry; Spectral decomposition; Perturbation analysis

1. Introduction

Multidimensional scaling (MDS) is a collection of data analytic techniques for constructing configurations of points from dissimilarity information about interpoint distances. Developed primarily by psychometricians and statisticians, MDS is widely used in a variety of disciplines for visualization and dimension reduction. The extensive literature on MDS

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includes numerous books, e.g., Borg and Groenen (1997), Cox and Cox (1994), and Everitt and Rabe-Hesketh (1997); and book chapters, e.g., Everitt and Dunn (1991, Chapter 5), Krzanowski and Marriott (1994, Chapter 5), Mardia et al. (1979, Chapter 14), and Seber (1984, Section 5.5). Many specific formulations of MDS are possible; a useful organizing principle, adopted by de Leeuw and Heiser (1982) and by Trosset (1997b), is to formulate MDS as a collection of optimization problems. The method of Torgerson (1952) and Gower (1966), variously called classical MDS and principal coordinate analysis, can be formulated as an optimization problem with an objective function whose minimum value is sometimes called the strain criterion.

Formally, a matrix is a *dissimilarity matrix* if and only if it is symmetric and hollow (its diagonal entries vanish) with nonnegative entries. Given an $n \times n$ matrix $\Delta = (\delta_{ij})$ of *squared* dissimilarities and a target dimension p, a classical problem in distance geometry is to determine if Δ is a matrix of p-dimensional squared Euclidean distances, i.e., if there exist $x_1, \ldots, x_n \in \mathbb{R}^p$ such that $\|x_i - x_j\|^2 = \delta_{ij}$. It is well-known that the answer is affirmative if and only if the symmetric $n \times n$ matrix

$$A = \tau(\Delta) = -\tfrac{1}{2} P^{\mathrm{T}} \Delta P$$

is positive semidefinite with $\mathrm{rank}(A) \leqslant p$, where P is the $n \times n$ projection matrix $I - ee^{\mathrm{T}}/n$, I is the $n \times n$ identity matrix, and $e = (1, \ldots, 1)^{\mathrm{T}} \in \mathbb{R}^n$. This embedding theorem motivated classical MDS, which can be stated as the problem of finding the symmetric positive semidefinite $n \times n$ matrix of rank $\leqslant p$ that is nearest $\tau(\Delta)$ in squared Frobenius distance. The minimum value of the objective function, $\|B - \tau(\Delta)\|_F^2$, is the strain criterion. Detailed studies of the linear operator τ were made by Critchley (1988) and by Gower and Groenen (1991).

To evaluate the strain criterion for a fixed Δ, one computes the spectral decomposition $\tau(\Delta) = Q \Lambda Q^{\mathrm{T}}$ and sets $\bar{\Lambda} = \mathrm{diag}(\bar{\lambda})$, where

$$\bar{\lambda}_i = \left\{ \begin{array}{cl} \max(\lambda_i, 0) & i = 1, \ldots, p \\ 0 & i = p+1, \ldots, n \end{array} \right\}$$

and $\mathrm{diag}(\bar{\lambda})$ is the diagonal matrix whose diagonal entries are $(\bar{\lambda}_1, \ldots, \bar{\lambda}_n)$. Then $Q \bar{\Lambda} Q^{\mathrm{T}}$ is a global minimizer of $\|B - \tau(\Delta)\|_F^2$ and the global minimum is

$$\begin{aligned} F_p \circ \tau(\Delta) &= \|Q \bar{\Lambda} Q^{\mathrm{T}} - Q \Lambda Q^{\mathrm{T}}\|_F^2 = \sum_{i=1}^{n} (\bar{\lambda}_i - \lambda_i)^2 \\ &= \sum_{i=1}^{p} [\max(\lambda_i, 0) - \lambda_i]^2 + \sum_{i=p+1}^{n} \lambda_i^2 = \sum_{i=1}^{n} \lambda_i^2 - \sum_{i=1}^{p} [\max(\lambda_i, 0)]^2 \\ &= \|\tau(\Delta)\|_F^2 - \sum_{i=1}^{p} [\max(\lambda_i, 0)]^2. \end{aligned} \tag{1}$$

Notice that only the p largest eigenvalues are required to evaluate the strain criterion.

Classical MDS assumes that Δ is fixed. Recently, extensions of classical MDS have been developed for nonmetric MDS (Trosset, 1998b) and for various problems with bound constraints (Trosset, 1998a, 2000). The latter include the important problem of inferring