

Exponential Map of Symmetric Matrices

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Abstract. We show how to make symmetric nonnegative definite matrices into positive definite through the exponential map.

Problem statement

Consider $p \times p$ symmetric matrix X such as correlation and covariance matrices obtained from functional magnetic resonance imaging (fMRI). The matrix X is thermally assumed to be positive definite symmetric (PDS) but for various reasons, the observed matrix X may be nonnegative definite with multiple zero eigenvalues. The question is how to make them PDS. The approach here is based on the exponential mapping technique (Huang et al. 2020).

Method

Let Sym_p be the space of all $p \times p$ symmetric matrices with inner product $\langle A, B \rangle = \text{tr}(AB)$. Such space forms a vector space. The space of $p \times p$ symmetric positive-definite (SPD) matrices (Arsigny et al. 2007), denoted by Sym_p^+ , is a subspace of Sym_p but no longer forms a vector space. Given $X, Y \in Sym_p^+$, any positive sum $\alpha X + \beta Y \in Sym_p^+$ for $\alpha, \beta > 0$. Thus, Sym_p^+ is a convex set.

The matrix exponential of a symmetric matrix is SPD, and the logarithm of an SPD matrix is a symmetric matrix. Moreover, the exponential map is one-to-one between Sym_p and Sym_p^+ . Given $X \in Sym_p$, its exponential map $X \rightarrow e^X$ is defined through matrix exponential

$$e^X = \sum_{n=0}^{\infty} \frac{X^n}{n!}.$$

The exponential map may introduce too much error between X and e^X :

$$X - e^X = I + \frac{X^2}{2} + \frac{X^3}{6} + \cdots.$$

Thus, we use the basis expansion to increase the overall fit.

Let I_{ij} be the $p \times p$ matrix whose (i, j) -th and (j, i) -th entries are $1/\sqrt{2}$ if $i \neq j$ and all other entries are 0. Let I_{ii} be the $p \times p$ diagonal matrix whose (i, i) -th entry is 1 and all other entries are 0. For instance, for $p = 3$,

$$I_{31} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \text{ and } I_{22} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (1)$$

Then, we have

$$\langle I_{ij}, I_{kl} \rangle = \delta_{ik} \delta_{jl}.$$

and $\{I_{ij}, i \geq j\}$ forms an orthonormal basis in Sym_p (Huang et al. 2020). Then we expand any $X \in Sym_p^+$ as

$$X = \sum_{i \geq j} c_{ij} \exp(I_{ij}),$$

where $c_{ij} \geq 0$ can be estimated using the nonnegative least squares method (Esser et al. 2013).

Numerical implementation

The matrix exponential is computed more efficiently through singular value decomposition:

$$X = UDU^\top$$

where D is the diagonal matrix with diagonal entries d_i . Then, the matrix exponential is computed as

$$e^X = Ue^D U^\top,$$

where e^D is the diagonal matrix with diagonal entries given by e^{d_i} . For instance, the matrix exponentials of I_{31} and I_{22} in (1) are

$$e^{I_{31}} = \begin{pmatrix} 1.2606 & 0 & 0.7675 \\ 0 & 1 & 0 \\ 0.7675 & 0 & 1.2606 \end{pmatrix} \text{ and } e^{I_{22}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

In MATLAB, the nonnegative least squares estimation is performed using `lsqnonneg.m` by vectorizing the upper triangle matrix of symmetric matrices.

For instance, consider the following nonnegative definite matrix: $\begin{pmatrix} 1 & 2 & 3 \\ 2 & 2 & 2 \\ 3 & 2 & 1 \end{pmatrix}$ It has

eigenvalues $(0, 2, 6)$. This is estimated in Sym_3^+ as $\begin{pmatrix} 1.0205 & 1.8973 & 3.0000 \\ 1.8973 & 1.8973 & 2.0000 \\ 3.0000 & 2.0000 & 1.2865 \end{pmatrix}$. It

has eigenvalues $(0.0477, 1.8495, 6.0061)$ making it positive definite.

Bibliography

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