Exponential Map of Symmetric Matrices

Moo K. Chung

University of Wisconsin-Madison, USA

mkchung@wisc.edu

Abstract. Given a point in the manifold (space of positive definite symmetric matrices), we show how to estimate the point using basis in its tangent space (space of symmetric matrices) 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 theoretically 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 it PDS. The approach here is based on the exponential map technique that project the scatter points in the tangent space to scatter points to the underlying manifold (Huang et al. 2020).

Method

Let Sym_p be the space of all $p \times p$ symmetric matrices with inner product $\langle A, B \rangle = \mathrm{tr}(AB)$. Such space forms a vector space. The space of $p \times p$ symmetric positive-definite (SPD) matrices, denoted by Sym_p^+, is a subspace of Sym_p but no longer forms a vector space (Arsigny et al. 2007). 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 curved convex manifold. Sym_p is the tangent space of Sym_p^+.

The matrix exponential of a symmetric matrix is SPD, and the logarithm (inverse map) 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 $X \to e^X$ 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 $p = 3$,

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

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

$$e^X = Ue^DU^\top,$$

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

Arsigny, V., Fillard, P., Pennec, X. & Ayache, N. (2007), 'Geometric means in a novel vector space structure on symmetric positive-definite matrices', *SIAM journal on matrix analysis and applications* **29**, 328–347.

Esser, E., Lou, Y. & Xin, J. (2013), 'A method for finding structured sparse solutions to nonnegative least squares problems with applications', *SIAM Journal on Imaging Sciences* **6**, 2010–2046.

Huang, S.-G., Samdin, S.-T., Ting, C., Ombao, H. & Chung, M. (2020), 'Statistical model for dynamically-changing correlation matrices with application to brain connectivity', *Journal of Neuroscience Methods* **331**, 108480.