Matrix Exponential

Moo K. Chung

University of Wisconsin-Madison, USA

mkchung@wisc.edu

Abstract. Correlation and covariance matrices arising in functional magnetic resonance imaging (fMRI) and EEG are theoretically assumed to be positive definite symmetric (PDS), but in practice are often only positive semidefinite with zero or near-zero eigenvalues due to finite sample size and noise. Such degeneracy violates the geometric assumptions underlying many statistical and manifold-based analyses. Motivated by this issue, we study the matrix exponential of symmetric matrices as the exponential map from the tangent space of symmetric matrices to the manifold of symmetric positive definite (SPD) matrices. We examine its basic properties and develop a tangent-space basis expansion framework that maps ill-conditioned symmetric matrices onto the SPD manifold via the exponential map, thereby enforcing positive definiteness in a geometrically principled and computationally stable manner.

Problem Statement

Consider $p \times p$ symmetric matrix A such as correlation and covariance matrices obtained from functional magnetic resonance imaging (fMRI). The matrix A is theoretically assumed to be positive definite symmetric (PDS) but for various reasons, the observed matrix A 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).

Dynamical Systems

Given a symmetric matrix A, the exponential of A (Moler & Van Loan 2003), denoted by e^A, is defined analogously to the scalar exponential function through its Taylor series expansion

$$e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!},$$

where A^k denotes the k-th matrix power of A. The matrix exponential arises naturally as the fundamental solution operator of dynamical systems or linear ordinary differential equations of the form

$$\frac{d\mathbf{x}(t)}{dt} = A\mathbf{x}(t),$$

for which the solution with initial condition $\mathbf{x}(0) = \mathbf{x}_0 \in \mathbb{R}^n$ is given by

$$\mathbf{x}(t) = e^{At}\mathbf{x}_0.$$

From a computational perspective, evaluating e^A directly from the infinite series is impractical for large matrices. While the series definition is conceptually useful, efficient computation for moderate to large matrices relies on alternative representations, such as spectral decomposition for symmetric matrices, which we describe next.

Matrix Exponential

A symmetric matrix A admits an eigenvalue decomposition of the form

$$A = PDP^{-1},$$

where $D = \text{diag}(\lambda_1, \ldots, \lambda_p)$ is a diagonal matrix containing the eigenvalues of A, and P is an orthogonal matrix whose columns are the corresponding eigenvectors, so that $P^{-1} = P^\top$. Using this decomposition, the matrix exponential can be computed as

$$e^A = Pe^D P^{-1}.$$

Since D is diagonal, its exponential is obtained by exponentiating each eigenvalue independently,

$$e^D = \text{diag}(e^{\lambda_1}, e^{\lambda_2}, \ldots, e^{\lambda_p}).$$

This spectral formulation is particularly efficient and numerically stable for symmetric matrices, as it reduces the computation of the matrix exponential to a standard eigenvalue decomposition followed by elementwise exponentiation.

We will illustrate how to compute the exponential map for a symmetric matrix of rank 2. Consider the symmetric matrix

```
X=[1 2 3
   2 2 2
   3 2 1]
```

Its singular value decomposition is obtained in MATLAB by

```
[U,S,V] = svd(X)
```

yielding

```
S = 6.0000         0            0
         0      2.0000          0
         0          0       0.0000
```

Thus, X is positive semidefinite with eigenvalues $(6, 2, 0)$ and is therefore not positive definite. However, the exponential map lifts all eigenvalues to strictly positive values, since $e^\lambda > 0$ even when $\lambda = 0$, implying that e^X is a symmetric positive definite matrix.

Space of Positive Definite Symmetric Matrices

We now introduce the matrix space in which the exponential map will be used. Let Sym_p denote the space of all $p \times p$ symmetric matrices equipped with the inner product

$$\langle A, B \rangle = \mathrm{tr}(AB).$$

This space forms a *vector space* under standard matrix addition and scalar multiplication. The space of $p \times p$ symmetric positive definite (SPD) matrices, denoted by Sym_p^+, is a subset of Sym_p. SPD matrices are of central importance because covariance and correlation matrices are often required to be positive definite in many applications.

Sym_p does not form a vector space (Arsigny et al. 2007). Any positive linear combination

$$\alpha X + \beta Y \in Sym_p^+, \qquad \alpha, \beta > 0,$$

remains positive definite for $X, Y \in Sym_p^+$, arbitrary linear combinations do not preserve positive definiteness. Consequently, Sym_p^+ is not a vector space and instead forms a smooth manifold with a non-flat (curved) geometric structure (Fig. 1). At each point $c \in Sym_p^+$, there is an associated tangent space, denoted by $T_c(Sym_p^+)$, which is a linear subspace of Sym_p. Unlike a vector space, these tangent spaces depend on the location c on Sym_p^+ and therefore vary from point to point, reflecting the curved geometric structure of Sym_p^+. Fig. 1 illustrates the relationship between the ambient space Sym_p and the embedded manifold Sym_p^+.

Approximating SPD Matrices Using Exponential Bases

The matrix exponential e^X guarantees positive definiteness for any symmetric matrix X. However, the resulting matrix may differ substantially from X, particularly when X contains large-magnitude entries. Consequently, relying on a single exponential mapping may lead to poor approximation accuracy. To address this issue while preserving positive definiteness, we represent a target matrix as a weighted combination of exponentials of simple symmetric basis matrices.

We begin by constructing an orthonormal basis for the space of symmetric matrices. Each basis element has either a single diagonal entry equal to one or a symmetric pair of off-diagonal entries equal to $1/\sqrt{2}$. For example, when $p = 3$, representative basis matrices are

$$I_{31} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \qquad I_{22} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

These basis matrices satisfy the orthonormality condition

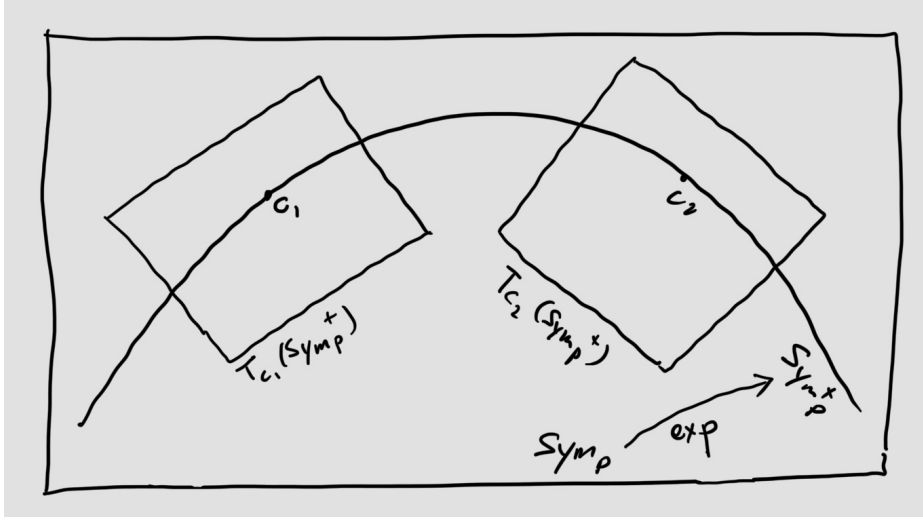$$\langle I_{ij}, I_{kl} \rangle = \delta_{ik} \delta_{jl},$$

Fig. 1: Sym_p^+ is a smooth manifold embedded in the ambient vector space of symmetric matrices Sym_p. For any point $c_i \in Sym_p^+$, the associated tangent space $T_{c_i}(Sym_p^+)$ is a linear subspace of Sym_p. The matrix exponential defines a smooth, one-to-one mapping $\exp : Sym_p \to Sym_p^+$, ensuring that the image of any symmetric matrix under this mapping lies in Sym_p^+.

and the collection $\{I_{ij},\ i \geq j\}$ forms an orthonormal basis of Sym_p (Huang et al. 2020).

Using this basis, we approximate a symmetric matrix by a nonnegative linear combination of the exponentials of the basis elements,

$$X \approx \sum_{i \geq j} c_{ij}\, e^{I_{ij}},$$

where the coefficients c_{ij} are constrained to be nonnegative. This constraint ensures that the resulting approximation remains positive definite by construction. The coefficients $\{c_{ij}\}$ are estimated using nonnegative least squares (NNLS) (Boyd & Vandenberghe 2004).

Given a linear system $A\mathbf{x} = \mathbf{b}$, NNLS seeks a minimizer of

$$\min_{\mathbf{x} \geq 0} \|A\mathbf{x} - \mathbf{b}\|^2,$$

subject to the componentwise nonnegativity constraint. In contrast to ordinary least squares, the presence of inequality constraints generally precludes closed-form solutions. NNLS is particularly appropriate in settings where negative co-efficients are physically or conceptually meaningless, such as medical imaging applications involving intensities, concentrations, or energy contributions. Numerical solutions typically rely on iterative algorithms, including active-set and

projected gradient methods ([Boyd & Vandenberghe 2004]). In MATLAB, NNLS problems are conveniently solved using the built-in function `lsqnonneg.m`.

To illustrate the difference between ordinary least squares and NNLS, consider

```
A = [1  2;
     3  4;
     5  6];

b = [1;
     1;
     1];
```

Solving the overdetermined system $A\mathbf{x} = \mathbf{b}$ by ordinary least squares in MATLAB yields

```
A\b =
  -1.0000
   1.0000
```

which contains a negative component. Enforcing the nonnegativity constraint, we instead compute the NNLS solution

```
x = lsqnonneg(A,b)
x =
        0
   0.2143
```

This solution minimizes the residual norm subject to $\mathbf{x} \geq 0$, illustrating how NNLS provides a principled mechanism for estimating nonnegative coefficients in the exponential basis expansion.

Worked-out Example

Consider the following symmetric matrix of rank two:

```
X=[1 2 3
   2 2 2
   3 2 1]
```

Its eigenvalues are obtained via singular value decomposition:

```
[U,S,V] = svd(X)
```

yielding

```
S = 6.0000         0         0
         0    2.0000         0
         0         0    0.0000
```

Thus, X is positive semidefinite with eigenvalues $(0, 2, 6)$ and is therefore not positive definite. Applying the matrix exponential directly,

```
Y = exp(X);
[U,S,V] = svd(Y)
```

produces

```
S =
   28.0810          0          0
          0    17.3673          0
          0          0     2.1118
```

showing that the exponential map substantially inflates the original spectral scale.

We now apply the proposed exponential basis approximation method implemented in `PDS_find`.

```
X_estimate = PDS_find(X)
[U,S,V] = svd(X_estimate)
```

which yields

```
S =
    6.0061          0          0
          0     1.8495          0
          0          0     0.0477
```

The resulting estimate is

$$\widehat{X} = \begin{pmatrix} 1.0205 & 1.8973 & 3.0000 \\ 1.8973 & 1.8973 & 2.0000 \\ 3.0000 & 2.0000 & 1.2865 \end{pmatrix},$$

whose eigenvalues are $(0.0477, 1.8495, 6.0061)$, confirming that the matrix is positive definite and remains close to the original matrix X. The zero eigenvalue is lifted to a small positive value, while the nonzero eigenvalues remain close to their original magnitudes. The example demonstrate that the exponential basis approach yields SPD estimates that are significantly closer to the original matrix than the direct exponential map, both in spectral behavior and in the Frobenius norm sense.

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.

Boyd, S. & Vandenberghe, L. (2004), *Convex Optimization*, Cambridge University Press.

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.

Moler, C. & Van Loan, C. (2003), 'Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later', *SIAM review* **45**, 3–49.