Multiscale Analysis of Complex Time Series: Integration of Chaos and Random Fractal Theory, and Beyond
by Jianbo Gao, Yinhe Cao, Wen-wen Tung and Jing Hu

APPENDIX B

PRINCIPAL COMPONENT ANALYSIS (PCA), SINGULAR VALUE DECOMPOSITION (SVD), AND KARHUNEN-LOÈVE (KL) EXPANSION

PCA is the eigenanalysis of the autocorrelation (or autocovariance) matrix R:

$$R = \begin{pmatrix} R_{11} & R_{12} & \cdots & R_{1n} \\ R_{21} & R_{22} & \cdots & R_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ R_{n1} & R_{n2} & \cdots & R_{nn} \end{pmatrix}.$$

Let λ_i and ϕ_i be the ith eigenvalue and corresponding eigenvector; then we have

$$R\phi_i = \lambda_i \phi_i, \quad i = 1, 2, \cdots, n.$$

Since the matrix R is symmetric and positive-definite, the eigenvalues are all positive, and the eigenvectors corresponding to different eigenvalues are orthogonal.

The SVD of a matrix $A_{n\times m}$ is

$$A = U\Sigma V^T,$$

where $U_{n\times n}$ and $V_{m\times m}$ are orthogonal matrices, $\Sigma_{n\times m}$ is a specific matrix that will be specified shortly, and T denotes the transpose of a matrix. The computation can be carried out by first forming AA^T or A^TA, and then doing eigenanalysis by finding all the positive eigenvalues and eigenvectors. The elements of Σ are all zero except that $\Sigma_{ii} = \sigma_i$ for $i = 1, 2, \cdots, r$, where r is the number of positive eigenvalues from either AA^T or A^TA and σ_i^2 is the ith eigenvalue of AA^T (or A^TA). The relation between PCA and SVD is clear if one forms the matrix A by taking delayed coordinates as its row vectors.

Under the KL expansion, a signal $x(t)$ is expanded as

$$x(t) = \sum_{n=1}^{\infty} c_n \psi_n(t) \quad 0 < t < T,$$

where $\psi(t)$ is a set of orthonormal functions in the interval $(0, T)$

$$\int_0^T \psi_n(t)\psi_m^*(t)dt = \delta[n-m]$$

and the coefficients c_n are random variables given by

$$c_n = \int_0^T x(t)\psi_n^*(t)dt,$$

where $*$ denotes a complex conjugate. The basis functions $\psi(t)$ are the solutions to the following integral equation:

$$\int_0^T R(t_1, t_2)\psi(t_2)dt_2 = \lambda\psi(t_1) \quad 0 < t_1 < T,$$

where $R(t_1, t_2)$ is the autocorrelation function of the process $x(t)$. Note that the KL expansion does not require the process $x(t)$ to be stationary.