Decomposition in orthogonal functions of data on an irregular mesh

Olaf Scholten

Kapteyn Institute & KVI, University of Groningen, The Netherlands

O.Scholten@rug.nl

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1 General Introduction

Orthonormal functions, like Legengre polynomials, show their orthonormality only when integrated over their full range. When decomposing data that has been measured ar random positions such orthonormality conditions have thus to be modified.

Assume we have a set of orthonormal functions (according to the usual mathematical definition) $f_\alpha(x)$ where $\alpha = 1, \cdots, M$ they obey

$$\delta_{\alpha,\beta} = \int dx f_\alpha(x)\, f_\beta(x) \; . \tag{1}$$

When this integral is limited to a sum over a finite set of values x_i with $i = 1, \cdots, N$ we have in general

$$\delta_{\alpha,\beta} \neq \sum_{i=1}^{N} dx f_\alpha(x_i)\, f_\beta(x_i) \; . \tag{2}$$

For decomposing data that is known on such an irregular mesh it will be nice to have such an orthonormality condition. To arrive at this we introduce weighting factors for each grid point, w_i with $i = 1, \cdots, N$, such that

$$\delta_{\alpha,\beta} = \sum_{i=1}^{N} dx\, w_i\, f_\alpha(x_i)\, f_\beta(x_i) \; . \tag{3}$$

The first (only?) problem we face is how to choose these wights.

To solve this problem it is simplest to introduce a vector notation

$$\overrightarrow{X} = \begin{pmatrix} x_1 & x_2 & \cdots & x_n \end{pmatrix} \; , \tag{4}$$

and similarly $\overrightarrow{W}$ for the wights at the grid points, $\overrightarrow{D}$ for the data, and $\overrightarrow{F_\alpha}$ for the function values at the grid points. We can define the function tensor (or matrix if you prefer) as $\overset{\Rightarrow}{F}$ where

$$\overset{\Rightarrow}{F}_{m,n} = \begin{pmatrix} f_1(x_1) & f_1(x_2) & \cdots & f_1(x_N) \\ f_2(x_1) & f_2(x_2) & \cdots & f_2(x_N) \\ \vdots & \vdots & \ddots & \vdots \\ f_M(x_1) & f_M(x_2) & \cdots & f_M(x_N) \end{pmatrix} \; .$$

The normality condition Eq. (3) can now be rewritten as

$$\mathbb{1} = \overrightarrow{\overrightarrow{F}}^T \, Diag(\overrightarrow{W}) \, \overrightarrow{\overrightarrow{F}}^T \tag{5}$$

where $\mathbb{1}$ is a unit matrix ($M \times M$ in this case) and $Diag(\overrightarrow{W})$ denotes a diagonal matrix with w_i on the diagonal. This leads to

$$\overrightarrow{\overrightarrow{F}}^{-1} \mathbb{1} \, {\overrightarrow{\overrightarrow{F}}^T}^{-1} = Diag(\overrightarrow{W}) \tag{6}$$

Assuming that $M = N$ the matrix can be decomposed as

$$\overrightarrow{\overrightarrow{F}} = \sum_j z_j^\dagger \lambda_j z_j \tag{7}$$

where z_j is a complex row vector, with

$$\overrightarrow{\overrightarrow{F}}^{-1} = \sum_j z_j^\dagger \lambda_j^{-1} z_j \tag{8}$$

since $z_j z_k^\dagger = \delta_{j,k}$ and $\sum_j z_j^\dagger z_j = \mathbb{1}$ and thus also

$$\overrightarrow{\overrightarrow{F}}^T = \sum_j z_j^T \lambda_j z_j^* = \sum_j z_j^\dagger \lambda_j^* z_j \tag{9}$$

where for the last step it is used that F is a real matrix and thus equal to its complex conjugate and

$${\overrightarrow{\overrightarrow{F}}^T}^{-1} = \sum_j z_j^\dagger \lambda_j^{*-1} z_j \; . \tag{10}$$

Theorem: if z is an eigenvector with a complex eigenvalue λ the z^* is also an eigenvector with eigenvalue λ^* for a real non-symmetric matrix. Now

$$\overrightarrow{\overrightarrow{F}}^{-1} \, {\overrightarrow{\overrightarrow{F}}^T}^{-1} = \sum_{j,k} z_j^\dagger \lambda_j^{-1} z_j z_k^\dagger \lambda_k^{*-1} z_k = \sum_j z_j^\dagger |\lambda_j|^{-2} z_j \neq Diag(|\lambda_j|^{-2}) \; . \tag{11}$$

The weights are thus not well defined.

In the literature this problem seems to be known as "empirical orthogonal functions irregular grid" and used in climatology. see EOF and in hydrology and in geomagnetism.