Space-time and spectral proper orthogonal decomposition

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Abstract: In this note we describe the theoretical background and the numerical implementation of proper orthogonal decomposition (POD). The original form – space-only or more suitably, space-time, as well as its spectral variant (in frequency domain) will both be included.

1 Proper orthogonal decomposition

1.1 The POD problem

The POD problem (Lumley, 1967, 1970; Holmes *et al.*, 2012) is to solve the following eigenvalue problem (EVP)

$$\mathcal{R}\phi_i(\boldsymbol{x}) = \int_{\mathcal{A}} \boldsymbol{R}(\boldsymbol{x}, \boldsymbol{x}')\boldsymbol{W}(\boldsymbol{x}')\phi_i(\boldsymbol{x}')\,\mathrm{d}\boldsymbol{x}' = \lambda_i\phi_i(\boldsymbol{x}), \tag{1}$$

with $\{\phi_i\}_{i=1}^{\infty}$ as the basis functions which are mutually orthogonal over the domain $\mathcal{A}$. Here

$$\boldsymbol{R}(\boldsymbol{x}, \boldsymbol{x}') = \langle \boldsymbol{q}(\boldsymbol{x}, t)\boldsymbol{q}^{\mathrm{T}}(\boldsymbol{x}', t)\rangle$$

is the two-point correlation tensor of a zero-mean time-homogeneous statistically stationary process $\boldsymbol{q}(\boldsymbol{x}, t)$ and $\boldsymbol{W}(\boldsymbol{x})$ is a symmetric weight matrix that makes the following inner product,

$$(\boldsymbol{q}_1, \boldsymbol{q}_2)_{\boldsymbol{W}} = \int_{\mathcal{A}} \boldsymbol{q}_2^{\mathrm{T}}(\boldsymbol{x})\boldsymbol{W}(\boldsymbol{x})\boldsymbol{q}_1(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \tag{2}$$

suitable for defining an energy norm ($\|\boldsymbol{q}\|_{\boldsymbol{W}} = (\boldsymbol{q}, \boldsymbol{q})^{1/2}$). Typically, $\boldsymbol{W}$ contains the constants of numerical quadrature in a discrete system and w.l.o.g. $\int_{\mathcal{A}} \boldsymbol{W}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = 1$.

The goal of POD is to solve an optimization problem such that the space $\{\phi_i\}_{i=1}^{\infty}$ can be represented by an optimal finite set of basis functions such that the energy of the signal is maximized when projected onto this basis as compared to any other basis with the same number of functions. In other words, the POD basis is the one that aligns best with the data in $\mathcal{L}_2$ (least-square) sense. The optimization problem is

$$\phi(\boldsymbol{x}) = \arg\max_{\|\phi\|_{\boldsymbol{W}}=1} \langle (\boldsymbol{q}, \phi)_{\boldsymbol{W}}\rangle, \tag{3}$$

or, in terms minimization problem,

$$\phi(\boldsymbol{x}) = \arg\min_{\|\phi\|_{\boldsymbol{W}}=1} \langle \|\boldsymbol{q} - (\boldsymbol{q}, \phi)_{\boldsymbol{W}}\phi\|_{\boldsymbol{W}}^2\rangle. \tag{4}$$

The optimization problem above is shown via a variational approach (Holmes *et al.*, 2012) to be equivalent to a Fredholm EVP as in (1).

Similarly, written in terms of the two-time correlation function

$$C(t, t') = (\boldsymbol{q}(\boldsymbol{x}, t), \boldsymbol{q}(\boldsymbol{x}, t'))_{\boldsymbol{W}}$$

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the EVP is

$$\mathcal{C}\psi_i(t) = \frac{1}{T}\int_0^T C(t,t')\psi_i(t')\,\mathrm{d}t' = \lambda_i\psi_i(t), \tag{5}$$

with exactly the same eigenvalues as in (1).

1.2   Matrix factorization; spatial and temporal modes

The discrete simulation data is arranged into

$$\boldsymbol{Q} = [\boldsymbol{q}_1, \boldsymbol{q}_2, \cdots, \boldsymbol{q}_{N_t}] \in \mathbb{R}^{N_d \times N_t} \tag{6}$$

where each $\boldsymbol{q}_i \in \mathbb{R}^{N_d}$ is one snapshot, N_d is the degree of freedom of the data (the dimension of the vector $\boldsymbol{q}_i$ multiplied by the number of discrete grid points), and N_t is the number of snapshots.

An SVD can be applied to yield

$$\boldsymbol{Q} = \boldsymbol{\Phi}\boldsymbol{\Sigma}\boldsymbol{\Psi}^{\mathrm{T}} = \sum_{i=1}^{\mathrm{rank}(\boldsymbol{Q})} \phi_i\sigma_i\psi_i^{\mathrm{T}} \tag{7}$$

where the left and right singular-vectors, $\boldsymbol{\Phi} = \{\Phi_i\} \in \mathbb{R}^{N_d}$ and $\boldsymbol{\Psi} = \{\psi_i\} \in \mathbb{R}^{N_t}$, are the spatial and temporal bases, respectively. We note that the eigenvector of the original EVP, $\boldsymbol{\Phi}$, and the eigenvector in method of snapshots, $\boldsymbol{\Psi}$, are the left and right singular vectors of the data matrix $\boldsymbol{Q}$, and are the orthogonal bases of the columns (spatial structures) and rows (temporal evolution) of $\boldsymbol{Q}$. Correspondingly, they are form the eigen-expansion of $\boldsymbol{R} = \boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}}$ in the spatial domain or $\boldsymbol{C} = \boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q}$ in temporal domain, respectively. Since the spatial modes $\boldsymbol{\Phi}$ are linear combinations of the columns and the rows of $\boldsymbol{Q}$ and hence inherit any properties of the data columns invariant to linear operations, such as divergence-free of the velocity fields.

The energy content of the dataset, under certain matrix norms, for example, the Frobenius norm, is

$$\|\boldsymbol{Q}\|_F^2 = \mathrm{tr}(\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q}) = \mathrm{tr}(\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}}) = \sum_{i=1}^{\mathrm{rank}(\boldsymbol{Q})} \lambda_i, \tag{8}$$

where $\lambda_i = \sigma_i^2$ are the non-zero eigenvalues of $\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}}$ and $\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q}$. We note that the spaces spanned by their corresponding eigenvectors (eigenspaces) have the relation

$$\mathrm{eig}(\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}})\backslash\mathrm{null}(\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}}) = \mathrm{eig}(\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q})\backslash\mathrm{null}(\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q}), \tag{9}$$

where $\mathrm{null}(\cdot)$ denotes the null space spanned by eigenvectors associated with zero eigenvalues. Then we are left with two choices of EVPs to solve, either that of $\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}} = \boldsymbol{\Phi}\boldsymbol{\Sigma}\boldsymbol{\Phi}^{\mathrm{T}}$, which is proportional to the two-point correlation tensor $\boldsymbol{R}$, or $\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q} = \boldsymbol{\Psi}\boldsymbol{\Sigma}\boldsymbol{\Psi}^{\mathrm{T}}$, which is proportional to the two-time correlation matrix $\boldsymbol{C}$.

The discrete estimate of the spatial correlation tensor is then

$$\boldsymbol{R} = \langle \boldsymbol{q}\boldsymbol{q}^{\mathrm{T}}\rangle = \frac{1}{N_t - 1}\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}} = \frac{1}{N_t - 1}\sum_{i=1}^{N_t} \boldsymbol{q}_i\boldsymbol{q}_i^{\mathrm{T}} \tag{10}$$

where the factor $N_t - 1$ is the Bessel's correction such that the expectation of the sampled (co)variance converges to the (co)variance of the random signals. Here you can see that each time step (i) is one independent ensemble and the order of them can be permuted without affecting the final sum. Similarly, the temporal correlation matrix is

$$C(i,j) = \boldsymbol{q}_i^{\mathrm{T}}\boldsymbol{q}_j = (\boldsymbol{q}_j, \boldsymbol{q}_i), \ \boldsymbol{C} = \boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q}. \tag{11}$$

1.3 Method of snapshots

We note that the convergence problem of POD resides mostly in the convergence of the estimation of the correlation tensor $\boldsymbol{R}$, which will then be eigen-decomposed as $\boldsymbol{R} = \boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}}/(N_t - 1) = \boldsymbol{\Phi}\boldsymbol{\Lambda}\boldsymbol{\Phi}^{\mathrm{T}}/(N_t - 1)$. We note that $\boldsymbol{R}$ is real symmetric, and the non-zero eigenvalues of are the same as those of $\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q}/(N_t - 1)$. That being said, we can choose to solve the eigen-decomposition of one of $\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}}$ and $\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q}$, whichever has a smaller dimension. Typically, the dimension of the discrete EVP, $\min(N_d, N_t) = N_t$ in numerical or experimental databases and hence the POD will be performed in the temporal domain (solving for $\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q}$) via the method of snapshot Sirovich (1987).

Here we introduce the weight matrix $\boldsymbol{W}$ which accounts for weights of non-uniform grid in numerical integration and the temporal correlation matrix becomes $\boldsymbol{C} = \boldsymbol{Q}^{\mathrm{T}}\boldsymbol{W}\boldsymbol{Q}$. The discrete POD EVP of (1) reads

$$\boldsymbol{R}\boldsymbol{W}\boldsymbol{\Phi} = \boldsymbol{\Phi}\boldsymbol{\Lambda}, \tag{12}$$

but, in the formulation of method of snapshots (Sirovich, 1987), the equivalent EVP (5),

$$\frac{1}{N_t - 1}\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{W}\boldsymbol{Q}\boldsymbol{\Psi} = \boldsymbol{\Psi}\boldsymbol{\Lambda}, \tag{13}$$

is solved first and then the spatial eigenmodes are then recovered as

$$\tilde{\boldsymbol{\Phi}} = \boldsymbol{Q}\boldsymbol{\Psi}\boldsymbol{\Lambda}^{-1/2}, \tag{14}$$

completing the singular value decomposition of $\boldsymbol{Q}$:

$$\boldsymbol{Q} = \tilde{\boldsymbol{\Phi}}\boldsymbol{\Sigma}\boldsymbol{\Psi}^{\mathrm{T}}, \tag{15}$$

where the singular-value matrix being $\boldsymbol{\Sigma} = \boldsymbol{\Lambda}^{-1/2}$. Here the tilded $\tilde{\boldsymbol{\Phi}}$ means the spatial modes are computed other than via solving its own EVP but via the projection of the data $\boldsymbol{Q}$ onto the temporal modes $\boldsymbol{\Psi}$, solved via an equivalent but typically less expensive EVP.

In the spatial domain, the eigen-expansion is now $\boldsymbol{R} = \tilde{\boldsymbol{\Phi}}\boldsymbol{\Lambda}\tilde{\boldsymbol{\Phi}}^{\mathrm{T}}$ with the orthonormality condition for the eigenmodes being $\tilde{\boldsymbol{\Phi}}^{\mathrm{T}}\boldsymbol{W}\tilde{\boldsymbol{\Phi}} = \boldsymbol{I}$. For convenience, the tilde will be dropped from now on. The POD expansion (of columns of $\boldsymbol{Q}$) is then

$$\boldsymbol{q}(\boldsymbol{x}, t) = \sum_{i=1}^{N_t} a_i(t)\boldsymbol{\phi}_i(\boldsymbol{x}), \tag{16}$$

where the time-dependent amplitude $a_i(t) = \sqrt{\lambda_i}\psi_i(t)$ is the rescaled eigenfunctions in the temporal domain and (16) can be regarded as either an eigen-expansion in space or in time. We note the equivalence and separation of space and time in (16). It can be interpreted as an expansion in spatial domain, with $\boldsymbol{\phi}_i(\boldsymbol{x})$ being the eigenfunctions and $a_i(t)$ being the temporal coefficients, or in temporal domain, with $a_i(t)$ being the eigenfunctions and $\boldsymbol{\phi}_i(\boldsymbol{x})$ being the spatial coefficients. That's also why we call it space-time POD instead of space-only.

We also note the orthonormality conditions of the spatial modes, $\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{W}\boldsymbol{\Phi} = \boldsymbol{I}$, or

$$(\boldsymbol{\phi}_i, \boldsymbol{\phi}_j)_{\boldsymbol{W}} = \delta_{ij} \tag{17}$$

and of the temporal modes (different coefficients are uncorrelated, like Fourier)

$$\langle a_i a_j \rangle = \delta_{ij}\lambda_i, \tag{18}$$

take the same form. For more discussions on the temporal domain and the equivalence, the readers are referred to Luchtenburg *et al.* (2009).

We make a last comment that POD is just an analog to Fourier expansion, but it is empirical/data-based and for the inhomogeneous directions. If POD is done in homogeneous directions, Fourier modes will be recovered.

2 Spectral POD

Spectral POD (SPOD) could be established similarly.

2.1 The EVP

We denote the two-point, two-time correlation tensor as

$$\boldsymbol{R}(\boldsymbol{x}, \boldsymbol{x}', t, t') = \langle \boldsymbol{q}(\boldsymbol{x}, t)\boldsymbol{q}^{\mathrm{H}}(\boldsymbol{x}', t')\rangle \tag{19}$$

where $(\cdot)^{\mathrm{H}}$ denotes Hermitian transpose. With time-homogeneity, it reduces to $\boldsymbol{R}(\boldsymbol{x}, \boldsymbol{x}', \tau)$ as a function of $\tau = t - t'$, and is the Fourier transform pair of the spectral density tensor

$$\boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}', f) = \langle \hat{\boldsymbol{q}}(\boldsymbol{x}, f)\hat{\boldsymbol{q}}^{\mathrm{H}}(\boldsymbol{x}', f)\rangle. \tag{20}$$

Then the EVP similar to (1) is

$$\mathcal{R}\boldsymbol{\psi}^{(i)}(\boldsymbol{x}, t) = \int_{\mathcal{A}}\int_{-\infty}^{\infty} \boldsymbol{R}(\boldsymbol{x}, \boldsymbol{x}', t, t')\boldsymbol{W}(\boldsymbol{x}')\psi_i(\boldsymbol{x}', t')\,\mathrm{d}\boldsymbol{x}'\mathrm{d}t' = \lambda^{(i)}\boldsymbol{\psi}^{(i)}(\boldsymbol{x}, t). \tag{21}$$

Replacing $\boldsymbol{R}$ with its Fourier pair according to the relation

$$\boldsymbol{R}(\boldsymbol{x}, \boldsymbol{x}', \tau) = \int_{-\infty}^{\infty} \boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}', f)e^{i2\pi f\tau}\,\mathrm{d}f, \tag{22}$$

the EVP (21) becomes

$$\mathcal{S}\boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f) = \int_{\mathcal{A}} \boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}', f)\boldsymbol{W}(\boldsymbol{x}')\phi_i(\boldsymbol{x}', f)\,\mathrm{d}\boldsymbol{x}' = \lambda^{(i)}(f)\boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f), \tag{23}$$

with $\boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f) = \boldsymbol{\psi}^{(i)}(\boldsymbol{x}, t)e^{-i2\pi f\tau}$ being the corresponding eigenmodes. We note that the weighted inner-product is still the spatial integral,

$$(\boldsymbol{q}_1, \boldsymbol{q}_2)_{\boldsymbol{W}} = \int_{\mathcal{A}} \boldsymbol{q}_2^{\mathrm{H}}(\boldsymbol{x}, t)\boldsymbol{W}(\boldsymbol{x})\boldsymbol{q}_1(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x}, \tag{24}$$

over which the orthonormality and the variational/optimization problem are defined, since the time integration in (21) is absorbed in to the Fourier transform.

Here we use $\hat{\boldsymbol{q}}(\boldsymbol{x}, f)$ denotes the Fourier mode of $\boldsymbol{q}(\boldsymbol{x}, t)$ at a frequency f. Its can be represented by the eigenfunctions $\boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f)$ of $\boldsymbol{S}$ as

$$\hat{\boldsymbol{q}}(\boldsymbol{x}, f) = \sum_{i=1}^{\infty} \sqrt{\lambda^{(i)}(f)}\boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f). \tag{25}$$

We note that at the same frequency f, different eigenvectors $\boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f), \boldsymbol{\phi}^{(j)}(\boldsymbol{x}, f)$ are orthogonal under the spatial inner product (24) owing to the symmetric positive-definiteness of $\boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}', f)$. But eigenvectors $\boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f_1), \boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f_2)$ at the same rank (i) associated with different frequencies are not necessarily orthogonal.

2.2 Numerical implementation

The numerical implementation can be referred to Towne *et al.* (2018); Schmidt & Colonius (2020). Data are sampled into blocks of sequenced snapshots (shown below is the l-th block)

$$\boldsymbol{Q}^{(l)} = [\boldsymbol{q}_1^{(l)}, \boldsymbol{q}_2^{(l)}, ..., \boldsymbol{q}_{N_{\mathrm{FFT}}}^{(l)}] \in \mathbb{R}^{N_d \times N_{\mathrm{FFT}}}, \tag{26}$$

where each column $\boldsymbol{q}_i^{(l)}$ is one snapshot. The total number of snapshots in one block (ensemble) is N_{FFT}. The degree of freedom of one snapshot is $N_d = N_x \times N_y \times N_z \times N_{\mathrm{var}}$, where N_{var} is the dimension of the vector $\boldsymbol{q}(\boldsymbol{x}, t)$.

A discrete Fourier transform (DFT) is performed on $\boldsymbol{Q}$ to yield

$$\hat{\boldsymbol{Q}}^{(l)} = [\hat{\boldsymbol{q}}_1^{(l)}, \hat{\boldsymbol{q}}_2^{(l)}, ..., \hat{\boldsymbol{q}}_{N_{\mathrm{FFT}}}^{(l)}] \in \mathbb{C}^{N_d \times N_{\mathrm{FFT}}}. \tag{27}$$

Then the Fourier modes are sampled in overlapping blocks following the standard Welch's method (Welch, 1967) to construct

$$\hat{\boldsymbol{Q}}_k = [\hat{\boldsymbol{q}}_k^{(1)}, \hat{\boldsymbol{q}}_k^{(2)}, ..., \hat{\boldsymbol{q}}_k^{(N_{\mathrm{blk}})}] \in \mathbb{C}^{N_d \times N_{\mathrm{blk}}}, \tag{28}$$

where k denotes the k-th discrete frequency and N_{blk} the number of blocks. The sampled spectral density at the k-th frequency is then $\boldsymbol{S}_k = \hat{\boldsymbol{Q}}_k \hat{\boldsymbol{Q}}_k^{\mathrm{H}}/(N_{\mathrm{blk}} - 1)$, where each block is treated as an ensemble (analogy to individual times in (6) for the estimation of $\boldsymbol{R}$). The discrete version of the eigenvalue problem (23) is

$$\boldsymbol{S}_k \boldsymbol{W} \boldsymbol{\Phi}_k = \boldsymbol{\Phi}_k \boldsymbol{\Lambda}_k. \tag{29}$$

Using the method of snapshots, (29) will instead be solved with

$$\frac{1}{N_{\mathrm{blk}} - 1} \hat{\boldsymbol{Q}}_k^{\mathrm{H}} \boldsymbol{W} \hat{\boldsymbol{Q}}_k \boldsymbol{\Psi}_k = \boldsymbol{\Psi}_k \boldsymbol{\Lambda}_k, \tag{30}$$

which provides the eigenmodes of $\boldsymbol{S}_k$ as $\tilde{\boldsymbol{\Phi}}_k = \hat{\boldsymbol{Q}}_k \boldsymbol{\Psi}_k \boldsymbol{\Lambda}_k^{-1/2}$ such that the eigenvalue decomposition is

$$\boldsymbol{S}_k = \tilde{\boldsymbol{\Phi}}_k \boldsymbol{\Lambda}_k \tilde{\boldsymbol{\Phi}}_k^{\mathrm{H}} = \sum_{i=1}^{N_{\mathrm{blk}}} \lambda_k^{(i)} \tilde{\boldsymbol{\phi}}_k^{(i)} (\tilde{\boldsymbol{\phi}}_k^{(i)})^{\mathrm{H}}. \tag{31}$$

The physical meaning of the spatial modes $\tilde{\boldsymbol{\Phi}}_k(\boldsymbol{x})$ can be interpreted as either the eigenvectors of the spectral density tensor $\boldsymbol{S}_k$ or the left singular vectors (spatial bases) of the Fourier mode $\hat{\boldsymbol{q}}_k$, at the discrete frequency f_k.

We note that unlike the separation of space and time in (16), the coefficients of the spatial modes in (25) are already sorted to the selected frequency at which the EVP is solved. And the SPOD modes are spatio-temporally coherent (as they come from eigen-decomposing the two-point, two-time correlation tensor) as opposed to only spatially OR temporally coherent in a POD problem (as the modes are EITHER eigenvectors of the spatial OR temporal correlation tensors).

Acknowledgement

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