Space-time and spectral proper orthogonal decomposition

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Abstract: In this note we describe the theory and numerical implementation of proper orthogonal decomposition (POD). The original form – space-only or more suitably, space-time, as well as its spectral version (in frequency domain) will both be included. We note that POD along with its core mathematical foundation – singularvalue/eigenvalue decomposition, are well established. The only innovation left for us is to introduce and interpret them in a relatively newer way.

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)

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

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

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

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.

The goal of POD is to solve an optimization problem such that the space $\{\boldsymbol{\phi}_i\}_{i=1}^{\infty}$ 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

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

or, in terms minimization problem,

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

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

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1.2 Discrete estimate of the correlation tensor

The simulation data is arranged into

$$\boldsymbol{Q} = [\boldsymbol{q}_1, \boldsymbol{q}_2, \cdots, \boldsymbol{q}_{N_t}] \in \mathbb{R}^{N_d \times N_t} \tag{5}$$

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. The discrete estimate of the correlation tensor is then

$$\boldsymbol{R} = \langle \boldsymbol{q}\boldsymbol{q}^{\mathrm{T}} \rangle = \frac{1}{N_t - 1}\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}} = \frac{1}{N_t - 1}\sum_{i=1}^{N_t} \boldsymbol{q}_i \boldsymbol{q}_i^{\mathrm{T}} \tag{6}$$

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. 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 $\boldsymbol{R} = \boldsymbol{\Phi}\boldsymbol{\Lambda}\boldsymbol{\Phi}^{\mathrm{T}}$.

1.3 Method of snapshots

We note that $\boldsymbol{R} = \boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}}/(N_t - 1)$ is real symmetric, and the non-zero eigenvalues of $\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}}$ and $\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q}$ are the same. The spaces spanned by corresponding eigenvectors (eigenspaces) have the relation

$$\mathrm{eig}(\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}})\backslash\mathrm{null}(\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}}) = \mathrm{eig}(\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q})\backslash\mathrm{null}(\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q}), \tag{7}$$

where $\mathrm{null}(\cdot)$ denotes the null space spanned by eigenvectors associated with zero eigenvalues. 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. The dimension of the discrete EVPis $\min(N_d, N_t)$, which will commonly be N_t in numerical or experimental databases and hence the POD is typically performed in the temporal domain via the method of snapshot Sirovich (1987).

The discrete EVP reads

$$\boldsymbol{R}\boldsymbol{W}\boldsymbol{\Phi} = \boldsymbol{\Phi}\boldsymbol{\Lambda}, \tag{8}$$

or, equivalently, in the formulation of method of snapshots (Sirovich, 1987),

$$\frac{1}{N_t - 1}\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{W}\boldsymbol{Q}\boldsymbol{\Psi} = \boldsymbol{\Psi}\boldsymbol{\Lambda}, \tag{9}$$

where the POD eigenmodes are then recovered as

$$\tilde{\boldsymbol{\Phi}} = \boldsymbol{Q}\boldsymbol{\Psi}\boldsymbol{\Lambda}^{-1/2}, \tag{10}$$

which is just another way of saying the singular value decomposition of $\boldsymbol{Q}$:

$$\boldsymbol{Q} = \tilde{\boldsymbol{\Phi}}\boldsymbol{\Sigma}\boldsymbol{\Psi}^{\mathrm{T}}, \tag{11}$$

with the singular-value matrix being $\boldsymbol{\Sigma} = \boldsymbol{\Lambda}^{-1/2}$. 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 correspond to an eigen-expansion of $\boldsymbol{R}$ in spatial or temporal domain, respectively.

In the temporal 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 is then

$$\boldsymbol{q}(\boldsymbol{x}, t) = \sum_{i=1}^{N_t} a_i(t)\boldsymbol{\phi}_i(\boldsymbol{x}), \tag{12}$$

where the time-dependent amplitude $a_i(t) = \sqrt{\lambda_i}\psi_i(t)$ is the rescaled eigenfunctions in the temporal domain and (12) can be regarded as either an eigen-expansion in space or in time. We note the equivalence and separation of space and time in (12). 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

$$(\boldsymbol{\phi}_i, \boldsymbol{\phi}_j)_{\boldsymbol{W}} = \delta_{ij} \tag{13}$$

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

$$\langle a_i a_j \rangle = \delta_{ij}\lambda_i, \tag{14}$$

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 another Fourier expansion, but in 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

$$\boldsymbol{R}(\boldsymbol{x}, \boldsymbol{x}', t, t') = \langle \boldsymbol{q}(\boldsymbol{x}, t)\boldsymbol{q}^{\mathrm{H}}(\boldsymbol{x}', t') \rangle \tag{15}$$

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

$$\boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}', f) = \langle \hat{\boldsymbol{q}}(\boldsymbol{x}, f)\hat{\boldsymbol{q}}^{\mathrm{H}}(\boldsymbol{x}', f) \rangle. \tag{16}$$

Then the EVP (1) is cast as

$$\mathcal{R}\boldsymbol{\psi}^{(i)}(\boldsymbol{x}, t) = \int_{\mathcal{A}} \int_{-\infty}^{\infty} \boldsymbol{R}(\boldsymbol{x}, \boldsymbol{x}', t, t')\boldsymbol{W}(\boldsymbol{x}')\boldsymbol{\psi}_i(\boldsymbol{x}', t')\, \mathrm{d}\boldsymbol{x}'\mathrm{d}t' = \lambda^{(i)}\boldsymbol{\psi}^{(i)}(\boldsymbol{x}, t), \tag{17}$$

with the weighted inner-product being a space-time integral

$$(\boldsymbol{q}_1, \boldsymbol{q}_2)_{\boldsymbol{W}} = \int_{\mathcal{A}} \int_{-\infty}^{\infty} \boldsymbol{q}_2^{\mathrm{H}}(\boldsymbol{x}, t)\boldsymbol{W}(\boldsymbol{x})\boldsymbol{q}_1(\boldsymbol{x}, t)\, \mathrm{d}\boldsymbol{x}\mathrm{d}t, \tag{18}$$

over which is also the orthonormality defined. Replacing with

$$\boldsymbol{R}(\boldsymbol{x}, \boldsymbol{x}', \tau) = \int_{-\infty}^{\infty} \boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}', f)e^{i2\pi f\tau}\, \mathrm{d}f, \tag{19}$$

the EVP (17) becomes

$$\mathcal{S}\boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f) = \int_{\mathcal{A}} \boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}', f)\boldsymbol{W}(\boldsymbol{x}')\boldsymbol{\phi}_i(\boldsymbol{x}', f)\, \mathrm{d}\boldsymbol{x}' = \lambda^{(i)}(f)\boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f), \tag{20}$$

with $\boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f) = \boldsymbol{\psi}^{(i)}(\boldsymbol{x}, t)e^{-i2\pi f\tau}$ being the corresponding eigenmodes.

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

$$\hat{\boldsymbol{q}}(\boldsymbol{x}, f) = \sum_{i=1}^{\infty} \sqrt{\lambda^{(i)}(f)} \boldsymbol{\phi}^{(i)}(\boldsymbol{x}, f). \tag{21}$$

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 (2) due 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 under space-only inner product.

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)

$$\boldsymbol{Q}^{(l)} = [\boldsymbol{q}_1^{(l)}, \boldsymbol{q}_2^{(l)}, ..., \boldsymbol{q}_{N_{\mathrm{FFT}}}^{(l)}] \in \mathbb{R}^{N_d \times N_{\mathrm{FFT}}}, \tag{22}$$

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

$$\hat{\boldsymbol{Q}}^{(l)} = [\hat{\boldsymbol{q}}_1^{(l)}, \hat{\boldsymbol{q}}_2^{(l)}, ..., \hat{\boldsymbol{q}}_{N_{\mathrm{FFT}}}^{(l)}] \in \mathbb{C}^{N_d \times N_{\mathrm{FFT}}}. \tag{23}$$

Then the Fourier modes are sorted according to frequency (labeled as the k-th discrete frequency) to form

$$\hat{\boldsymbol{Q}}_k = [\hat{\boldsymbol{q}}_k^{(1)}, \hat{\boldsymbol{q}}_k^{(2)}, ..., \hat{\boldsymbol{q}}_k^{(N_{\mathrm{blk}})}] \in \mathbb{C}^{N_d \times N_{\mathrm{blk}}}, \tag{24}$$

where N_{blk} the number of blocks used in Welch's method (Welch, 1967).

The sampled spectral density at the k-th frequency is then $\boldsymbol{S}_k = \hat{\boldsymbol{Q}}_k \hat{\boldsymbol{Q}}_k^{\mathrm{H}} / (N_{\mathrm{blk}} - 1)$. The eigenvalue problem (20) takes the form of

$$\boldsymbol{S}_k \boldsymbol{W} \boldsymbol{\Phi}_k = \boldsymbol{\Phi}_k \boldsymbol{\Lambda}_k. \tag{25}$$

In the method of snapshots (Sirovich, 1987), (25) becomes

$$\frac{1}{N_{\mathrm{blk}} - 1} \hat{\boldsymbol{Q}}_k^{\mathrm{H}} \boldsymbol{W} \hat{\boldsymbol{Q}}_k \boldsymbol{\Psi}_k = \boldsymbol{\Psi}_k \boldsymbol{\Lambda}_k. \tag{26}$$

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

$$\boldsymbol{S}_k = \tilde{\boldsymbol{\Phi}}_k \boldsymbol{\Lambda}_k \tilde{\boldsymbol{\Phi}}_k^{\mathrm{H}} = \sum_{i=1}^{N_{\mathrm{blk}}} \lambda_k^{(i)} \tilde{\boldsymbol{\phi}}_k^{(i)} (\tilde{\boldsymbol{\phi}}_k^{(i)})^{\mathrm{H}}. \tag{27}$$

The physical meaning of the spatial modes $\tilde{\boldsymbol{\Phi}}_k(\boldsymbol{x})$ can be interpreted as either the eigenvector of the spectral density tensor $\boldsymbol{S}_k$ or the left singular vector 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 (12), the coefficients of the spatial modes in (21) are alreayd sorted to the selected frequency at which the EVP is solved.

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