Lecture 14: Part 1: More on EOFs and Part 2: Generalized inverse with SVD

Recap

We've been discussing matrix inversion, eigenvalues, and the singular value decomposition. Last lecture was a refresher on linear algebra and we're not going to return to EOFs and SVDs.

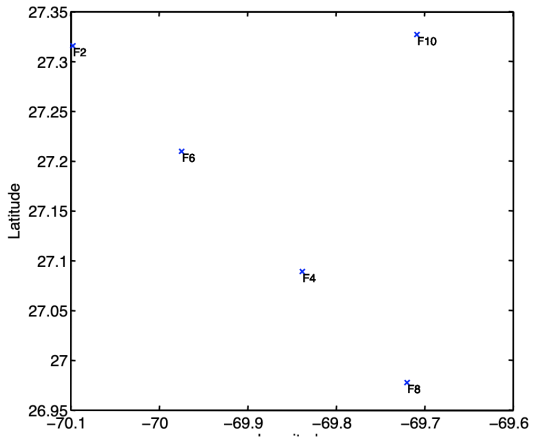

Figure 1: Mooring locations in the Frontal Air-Sea Interaction Experiment (FASINEX).

Moored temperature data, an example

As an example, consider moored temperature data from the North Atlantic, taken in the vicinity of the subtropical front. An array of five moorings was deployed to observe air-sea interaction in the region of the front (Figure 1). The array was in the form of a right triangle, with the hypotenuse oriented roughly parallel to the anticipated acrossfront direction. A total of 38 temperature sensors were divided roughly evenly among the 5 moorings, with each time series 2448 hours in length.

The temperature time series from one of the moorings reveals some of the processes occurring in the region (Figure 2). The upper 40 m are mostly uniform in temperature, as the curves for these time series nearly always overlap. The main exception to this patter is that temperature at 1 m is warmer on a daily cycle, especially near the end of the record as spring warming sets in. From 80-160 m, the ocean is stratified, although the stratification weakens during the last month of the record. The largest variability is at a period of nearly one month, and is present at all depths, although it is strongest at 160 m. This variability is caused by the passage of mesoscale fronts and eddies, which were a focus of the experiment.

EOFs and amplitudes of the temperature data are found by doing a singular value decomposition. The first step in the analysis is to examine the fraction of variance accounted for by each EOF (Figure 3). The first EOF accounts for 57% of the variance, the second 18%, and so on. The first 5 EOFs together account for 90% of the variance, so we get a reasonably complete description of the variance with only 5 spatial functions (EOFs) and time series (amplitudes). If the goal is a description of the largest variance, this is certainly a simpler than having to look at all 38 temperature time series.

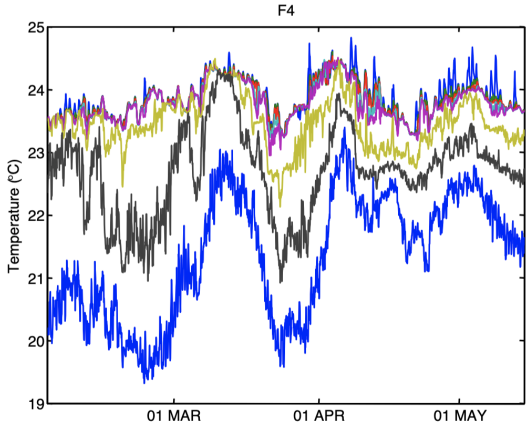

Figure 2: Temperature records from FASINEX mooring F4 at depths 1, 10, 20, 30, 40, 80, 120, and 160 m.

The first EOF of temperature describes most of the variance observed in all 38 time series (Figure 4). Temperature at all depths and moorings is in phase, with the largest signal at depth. The EOF is nearly uniform in the upper 40 m, consistent with the presence of a mixed layer. The structure of the amplitude is similar to the large fluctuations in Figure 2. A first mode like this one, with all locations in phase is common in EOF analysis.

The second EOF describes variability that is of opposite phase on either side of the array (Figure 4). The combination of the first two EOFs are able to describe the passage of mesoscale features past the array. The second EOF is generally larger at depth, consistent with Figure 2. Playing this game of describing EOFs is fun, but not necessarily useful as there is no guarantee that the EOFS have a one-to-one correspondence to physical modes. However, no other functions can describe more variance than the EOFs, even if the physical modes were known perfectly.

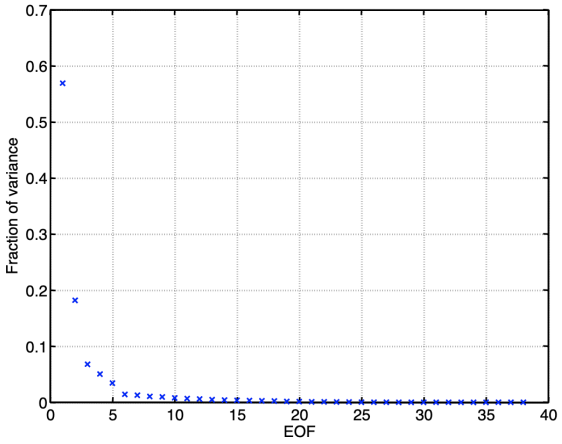

Figure 3: The fraction of variance accounted for by the EOFs of temperature on the FASINEX moorings.

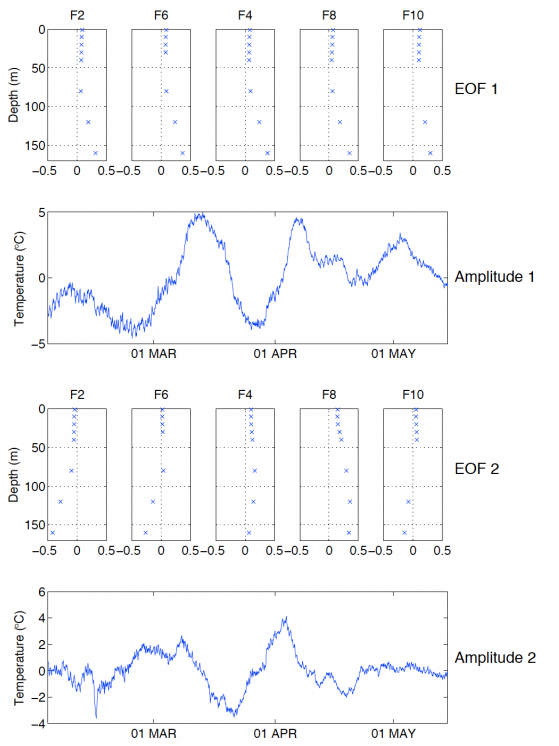

Figure 4: First two EOFs and amplitudes of temperature. The EOFs are shown by crosses as a function of depth on each mooring, and the amplitudes are shown as time series. In this case, the EOFs are dimensionless and the amplitudes carry the units of °C.

EOFs and physical modes, weighting

A common misconception about EOFs is to associate them with physical modes. An easy way to see the folly in this is to consider the orthogonality relations:

$$(e_i, e_j) = \delta_{ij} \text{ for physical modes} \tag{1}$$

$$\mathbf{b}_i^T \mathbf{b}_j = \delta_{ij} \text{ for EOFs} \tag{2}$$

These are not the same. The inner product for normal modes in the ocean, for instance, is a vertical integral weighted by the buoyancy frequency squared, while that for EOFs is a simple dot product. The normalization for a physical mode is generally an expression of some conserved quantity such as energy. The normalization for EOFs is somewhat arbitrary, depending on the locations of the data. While a dominant physical process ought to be represented in the first few EOFs, there is no one-to-one correspondence between physical modes and EOFs.

We can attempt to approximate the integral in (1), thus changing our estimate of energy, by weighting and using the orthogonality relation:

$$\mathbf{b}_i^T \mathbf{W} \mathbf{b}_j = \delta_{ij}. \tag{3}$$

Similarly we might use some sort of weighting in the definition of our ensemble average. In any case the problem is easily solved by transforming to new coordinates

$$\mathbf{b}' = \mathbf{W}^{1/2} \mathbf{b}, \tag{4}$$

and solving the eigensystem

$$\mathbf{W}^{-1/2}\langle \mathbf{y}\mathbf{y}^T \rangle \mathbf{W}^{-1/2}\mathbf{b}' = \lambda \mathbf{b}' \tag{5}$$

All of the results above immediately follow.

Generalized inverse

We can define the generalized inverse (or pseudoinverse, or Moore-Penrose inverse). The unique minimum length solution to the inverse problem of minimizing $||\mathbf{Gm} - \mathbf{d}||$ is

$$\mathbf{m} = \mathbf{G}^+\mathbf{d}, \tag{6}$$

where

$$\mathbf{G}^+ = \mathbf{V}\mathbf{S}^+\mathbf{U}^T \tag{7}$$

$$\mathbf{S}^+ = \begin{bmatrix} \mathbf{S}_K^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \tag{8}$$

Note that $\mathbf{S}_K$ is easy to invert as it is a diagonal matrix. This is a suitable inverse for you if your idea of the best model is the one with minimum length as measured by the L_2 norm of $\mathbf{m}$.

Practical use of the singular value decomposition

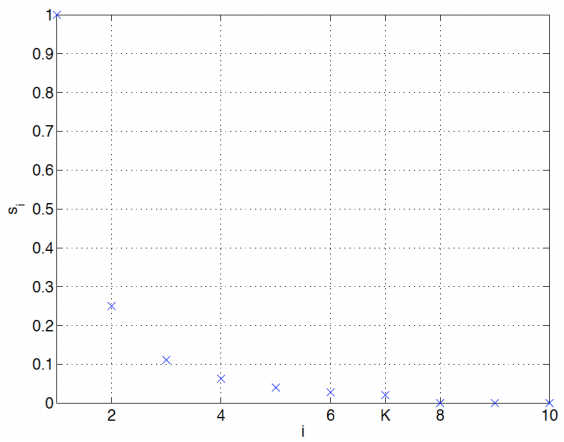

Figure 5: Singular values of a matrix of rank K.

Singular value decompositions have some powerful uses for data analysis, both for carrying out matrix inversion and also for assessing variability in general. Here are some things to consider.

1. *Rank.* The singular value decomposition is used primarily because it tells us immediately about the rank of the problem. Typically, one plots the singular values against their index numbers (Figure 5). This is often called the "spectrum" of the data kernel. The first K singular values are nonzero, but some of the nonzero singular values are very small. In practice, some of these small singular values are set to zero, increasing misfit, but reducing model size. This sounds similar to the procedure we used in simultaneously minimizing misfit and model size, because it is essentially the same thing.

2. *Minimizing the model size.* Consider the generalized inverse (6), for which the model size is

$$||\tilde{\mathbf{m}}_K||^2 = ||\mathbf{S}_K^{-1}\tilde{d}_K||^2 = \sum_{i=1}^{K}\left(s_i^{-1}\tilde{d}_i\right)^{-2} \tag{9}$$

3. *Characterizing misfit.* The misfit is contained within the null space of the matrix and is

$$||\tilde{\mathbf{d}}_0||^2 = \sum_{i=K+1}^{N} d_i^2 \tag{10}$$

   As small singular values are set to zero, the model size will decrease, while the misfit increases.

4. *Assessing the solution covariance.* Recall the model covariance matrix, which for the generalized inverse is

$$\langle \mathbf{m}'\mathbf{m}'^T\rangle = \mathbf{G}^+\langle \mathbf{d}'\mathbf{d}'^T\rangle\mathbf{G}^{+T}. \tag{11}$$

   Substituting the identity matrix for the data covariance matrix yields the **unit covariance matrix**:

$$\langle \mathbf{m}'\mathbf{m}'^T\rangle_u = \mathbf{G}^+\mathbf{G}^{+T}. \tag{12}$$

   Using (7-8) the unit covariance matrix can be written

$$\begin{aligned}
\langle \mathbf{m}'\mathbf{m}'^T\rangle_u &= \mathbf{V}\mathbf{S}^+\mathbf{U}^T\mathbf{U}\mathbf{S}^{+T}\mathbf{V}^T && (13)\\
&= \mathbf{V}\begin{bmatrix}\mathbf{S}_K^{-1} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\mathbf{S}_K^{-1} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{bmatrix}\mathbf{V}^T && (14)\\
&= \mathbf{V}\begin{bmatrix}\mathbf{S}_K^{-2} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{bmatrix}\mathbf{V}^T && (15)\\
&= \mathbf{V}_K\mathbf{S}_K^{-2}\mathbf{V}_K^T, && (16)
\end{aligned}$$

   where $\mathbf{V}_K$ is the matrix made of the first K columns of $\mathbf{V}$. The model variance is dominated by the smallest singular values. The fact that the small singular values dominate the covariance of $\mathbf{m}$ tells us that small, erroneous singular values could corrupt our estimates of model paramters. This is one more reason to zero out the small singular values, and move those components of the solution to the null space.