Quantitative Climate Science: Data Centric Methods, EOFs and EOF reconstructions

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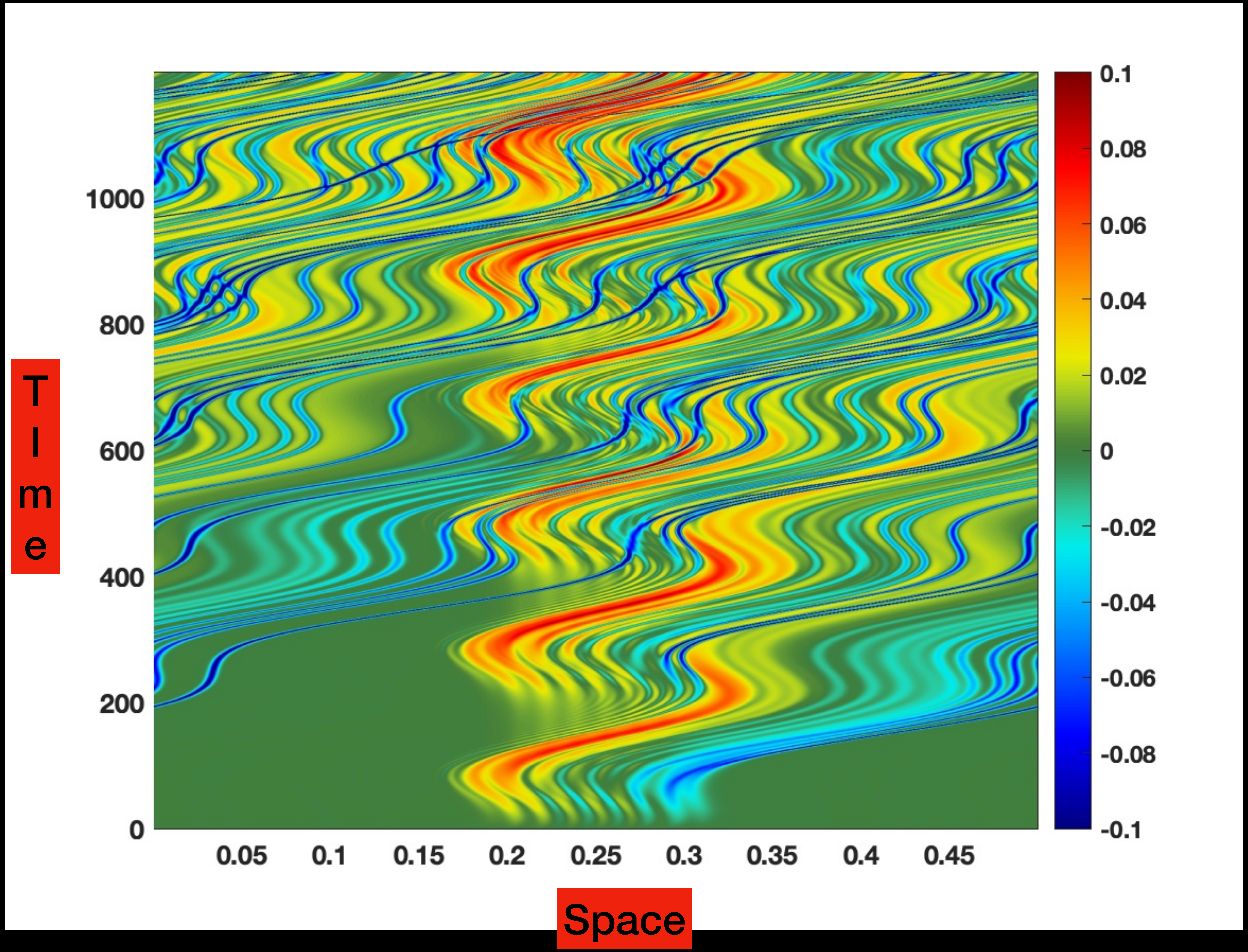
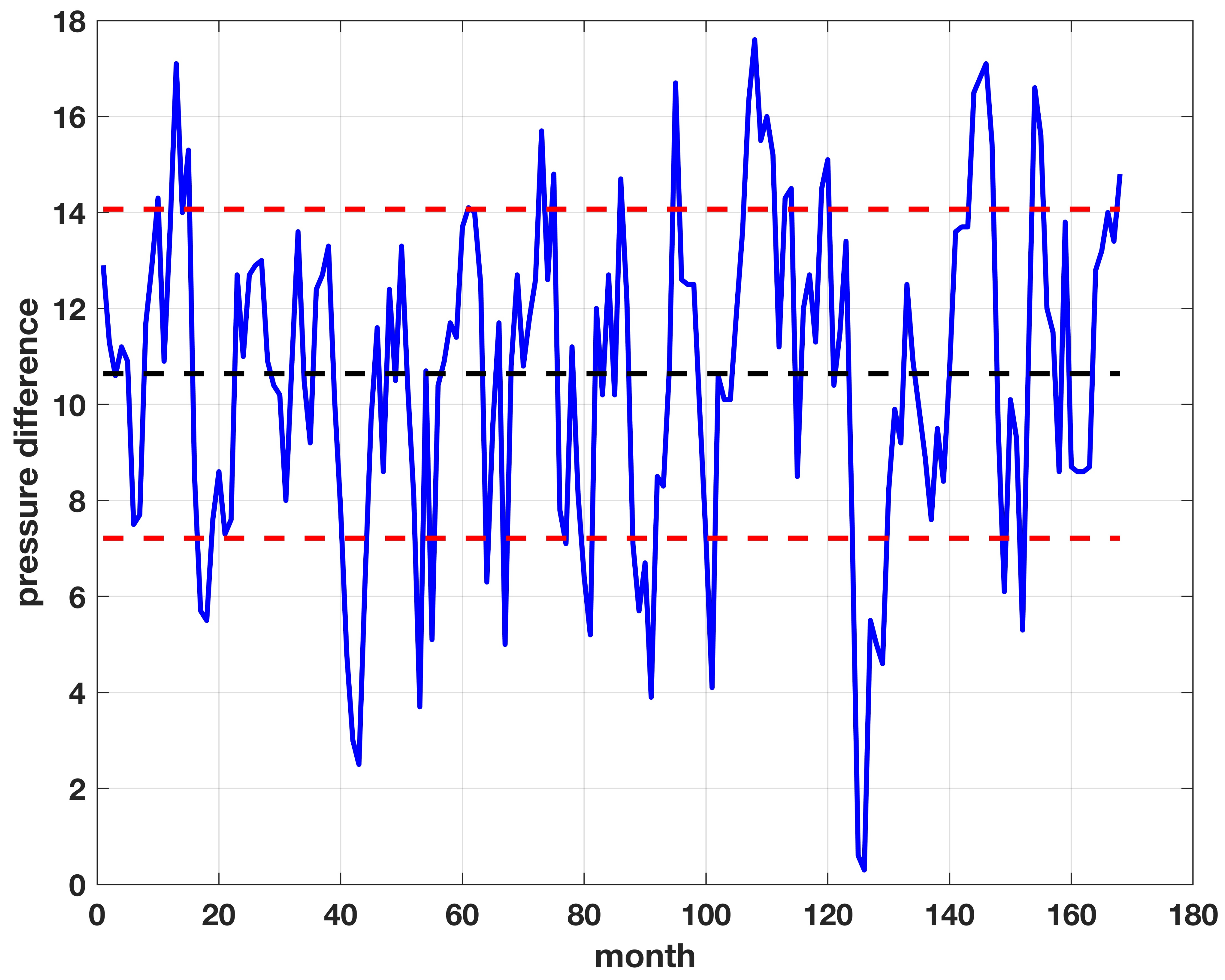
Review: the data

- Our focus will be on the data set is generated by the pseudo spectral integration of a nonlinear wave equation (the forced BBM equation).
- This time we will ask the question of whether we can come up with a better basis than sines and cosines.
- Of course we will have to define “better” first.
- To do so we start with more basic data.



Example 1: The Tropical Pacific Atmosphere

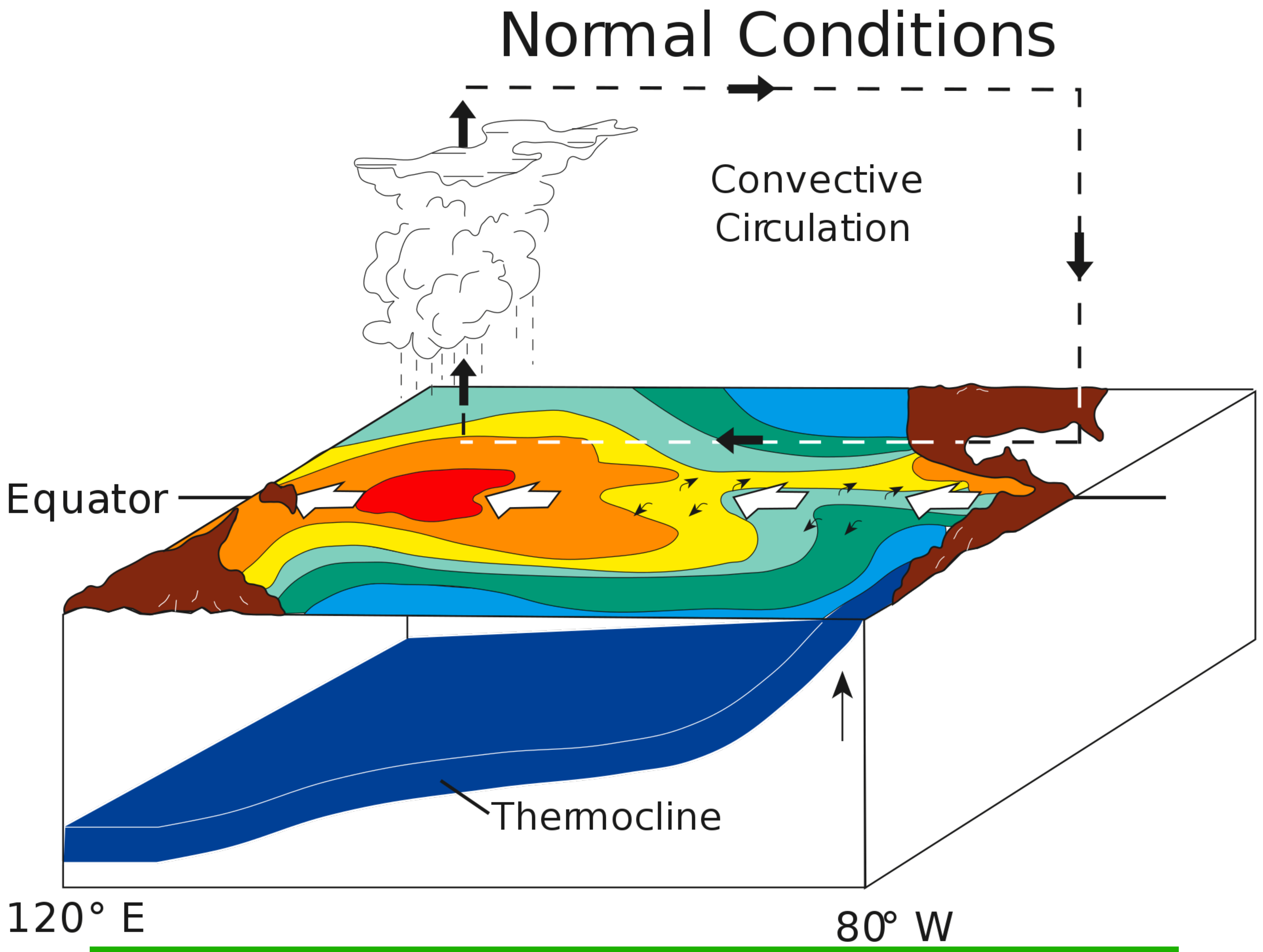
- The curve on the right shows the atmospheric pressure difference between Darwin, Australia and Easter Island.
- You can see that there are fairly, but not precisely, regular oscillations.
- Since the tropical Pacific is mostly ocean we could ask whether instead of the atmosphere we should be looking at the ocean.
- This YouTube movie shows the sea surface temperature (or SST) with the mean value subtracted off. This is called the SST anomaly.
- https://www.youtube.com/watch?v=d8KupSFlb9w



ENSO stands for the El Niño-Southern Oscillation. We will spend a week discussing this mode of climate variability later in the course.

Example 1: The Tropical Pacific Ocean Basic State

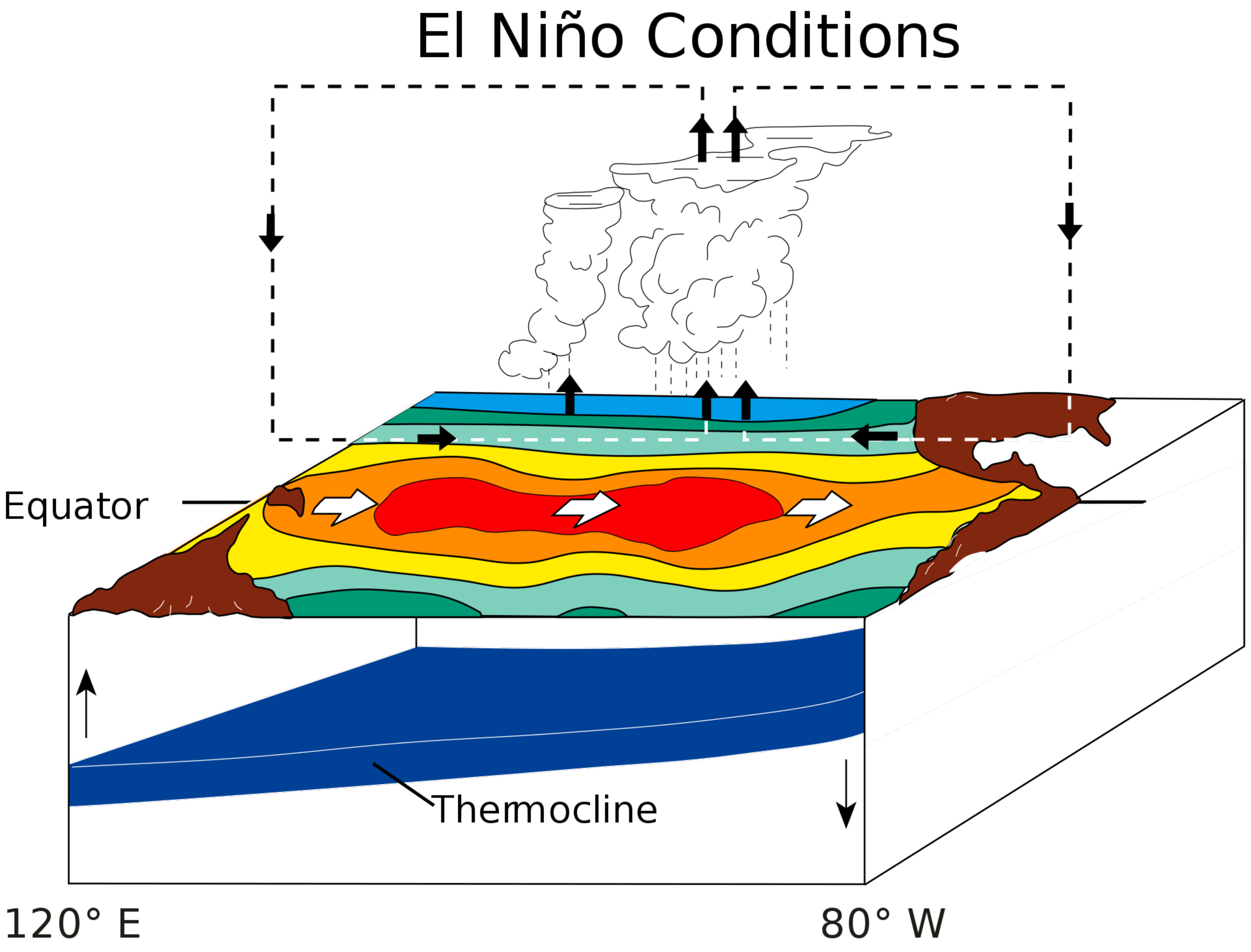
- On the right is a diagram of the state of the atmosphere-ocean system in the tropical Pacific.
- You should study ENSO in detail at some point, and can get a quick overview from https://en.wikipedia.org/wiki/El_Ni%C3%B1o
- For today, we focus on the Sea Surface Temperatures or SSTs.
- You can see a huge pool of warm water in the Western Pacific and white arrows indicating a net east to west flow.



Normal Pacific pattern: Warm pool in the west drives deep atmospheric convection. In the east local winds cause nutrient-rich cold water to upwell at the Equator and along the South American coast. (NOAA / PMEL / TAO)

Example 1: The Tropical Pacific El Niño

- On the right is a diagram of the state of the atmosphere-ocean system in the tropical Pacific during El Niño.
- You can see that the distribution of SST brings much more warm water into the Central and Eastern Pacific (i.e. closer to South America).
- Given that the Pacific is so wide that you could drop all of Canada into it and not even notice, this is a huge amount of moisture to move.
- The video we saw showed a lot of different things going on.
- A simple and useful mathematical question to ask is thus "what is the most important thing going on?" along with a mathematical definition of most important. Typically "captures the most vairance" is a good quantification of "most important".



El Niño conditions: warm water and atmospheric convection move eastwards. In strong El Niños the deeper thermocline off S. America means upwelled water is warm and nutrient poor.

Some Mathematics Basics

- Consider two time series written like this: $f_i^{(1)}$ and $f_i^{(2)}$ where $i = 1 \ldots N$.
- We can denote the average with an overbar like this: $\bar{f}^{(1)} = \frac{1}{N} \sum_{i=1}^{N} f_i^{(1)}$
- The variance is defined in the standard way as var $\left[f_i^{(1)} \right] = \frac{1}{N-1} \sum_{i=1}^{N} \left(f_i^{(1)} - \bar{f}_i^{(1)} \right)^2$
- Because we have two time series we can also define the so-called covariance as cov $\left[f_i^{(1)} \right] = \frac{1}{N-1} \sum_{i=1}^{N} \left(f_i^{(1)} - \bar{f}_i^{(1)} \right) \left(f_i^{(2)} - \bar{f}_i^{(2)} \right)$
- The covariance tells us whether changes in one time series tend to follow the behaviour of the other time series.

The covariance matrix

- We can put all the information we can find about how the two time series vary into a matrix, which I will call $\mathbf{A}$, defined as

$$\mathbf{A} = \begin{pmatrix} \text{var}(f^{(1)}) & \text{cov}(f^{(1)}, f^{(2)}) \\ \text{cov}(f^{(1)}, f^{(2)}) & \text{var}(f^{(2)}) \end{pmatrix}$$

- The information **how variable each time series is can be found along the diagonal**, while the information of **how the two are related (the cross-correlation) is found along the off-diagonal**.

- The way we created $\mathbf{A}$ ensures that it is a symmetric, real valued matrix.

- From linear algebra we know the matrix has real eigenvalues, and orthonormal eigenvectors (their dot product is zero and their size is 1).

The eigenvectors of the covariance matrix

- Recall $\mathbf{A} = \begin{pmatrix} \text{var}(f^{(1)}) & \text{cov}(f^{(1)}, f^{(2)}) \\ \text{cov}(f^{(1)}, f^{(2)}) & \text{var}(f^{(2)}) \end{pmatrix}$ so that we can find eigenvalues (which we label $\sigma_1 \geq \sigma_2$) and eigenvectors (which we label $\overrightarrow{v_1}$ and $\overrightarrow{v_2}$)
- We learned in linear algebra that we can change bases so that our original time series can be written in terms of the eigenvectors (which are column vectors) like this:
- $(f_i^{(1)} f_i^{(2)})^T = \overrightarrow{v_1} a_i^{(1)} + \overrightarrow{v_2} a_i^{(2)}$.
- We can do even better if recall some more linear algebra, namely that for symmetric, real valued matrix $\mathbf{A}$ we can write $\mathbf{A} = \mathbf{S}^{-1}\mathbf{D}\mathbf{S}$ where $\mathbf{S}$ is a matrix made up of the eigenvectors.
- $\mathbf{S}$ is also called a “rotation” matrix, and we now know that we can get our new basis by “rotating” the data (this is one way geometry enters into modern data science).

The EOFs

- Let's unpack the meaning of the eigenvectors. With two measurements we can write the original data as: $(1,0)^T f_i^{(1)} + (0,1)^T f_i^{(2)}$ The transpose makes the basis vectors column vectors and $f_i^{(1)}$ and $f_i^{(2)}$ are row vectors (usually quite long ones).

- The rules of matrix multiplication make a matrix with two rows and N columns.

- We can also write $(f_i^{(1)} f_i^{(2)})^T = \overrightarrow{v_1} a_i^{(1)} + \overrightarrow{v_2} a_i^{(2)}$ where the eigenvectors are 2x1 column vectors, and $a_i^{(1)}$ and $a_i^{(2)}$ are 1xN row vectors.

- Thus we have rewritten our first data vector in terms of a new basis. On its own this is just a "I can do this" bit of pure math.

- But now imagine if $\sigma_1 \gg \sigma_2$. That means the first eigenvector is much more important than the second one and to a good approximation $(f_i^{(1)} f_i^{(2)})^T \approx \overrightarrow{v_1} a_i^{(1)}$ is just fine.

- With two data vectors it's a modest savings, but if we have lots of data vectors it would be a huge savings.

EOFs in general

- We now have N measurements which we organize as $\left[f_i^{(1)} \ldots f_i^{(M)}\right]$.

- We compute the covariance matrix which will be MxM (since we are averaging over the running time variable) and find its eigenvalues and eigenvectors. We assume the ordering is from the largest to the smallest eigenvalue.

- We can again write $(f_i^{(1)} \ldots f_i^{(M)})^T = \overrightarrow{v_1} a_i^{(1)} + \ldots + \overrightarrow{v_N} a_i^{(M)}$ where the eigenvectors are Mx1 column vectors, and $a_i^{(1)}$ … $a_i^{(M)}$ are 1xN row vectors.

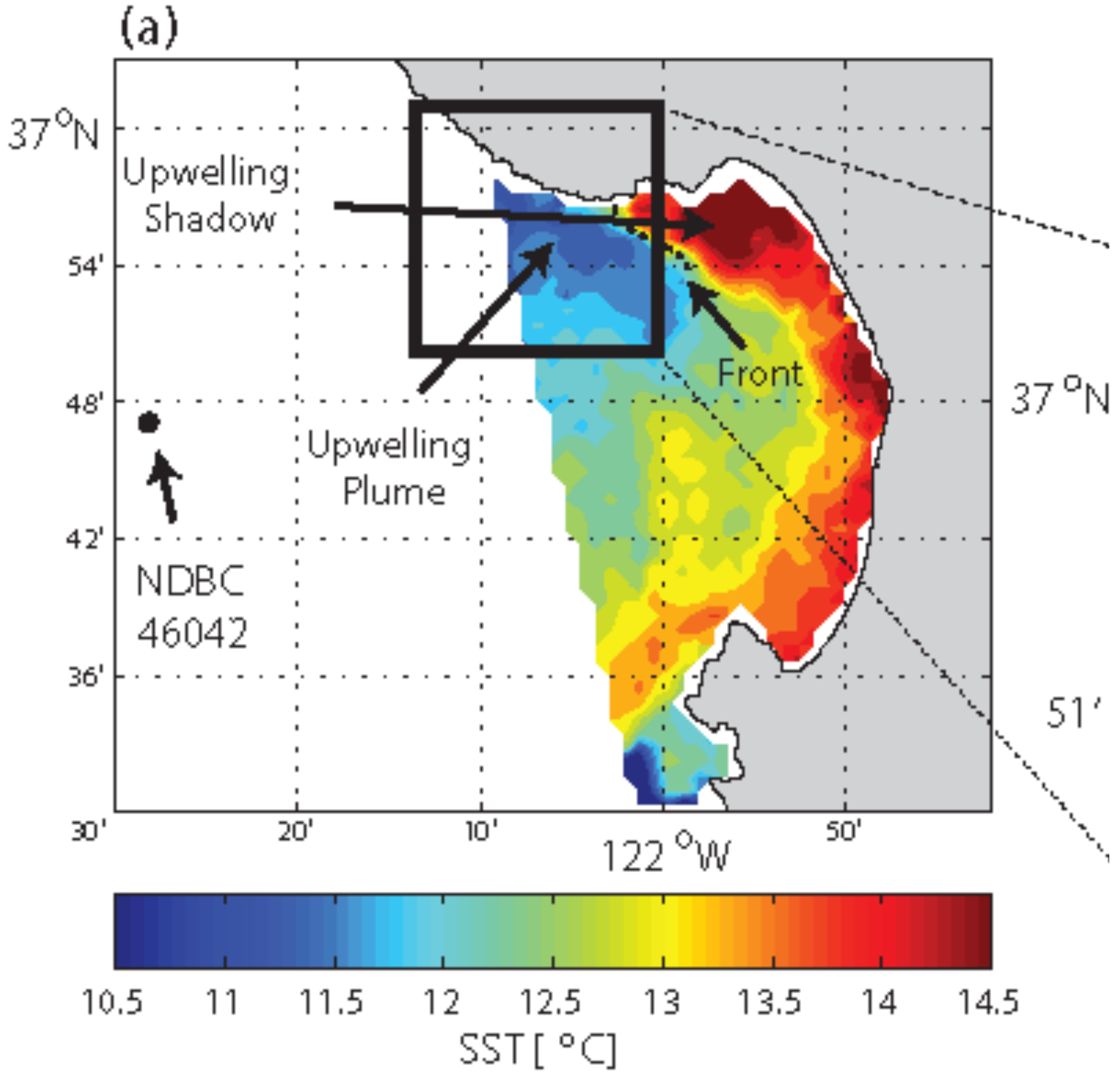
- Thus we have rewritten our data in terms of a new basis.

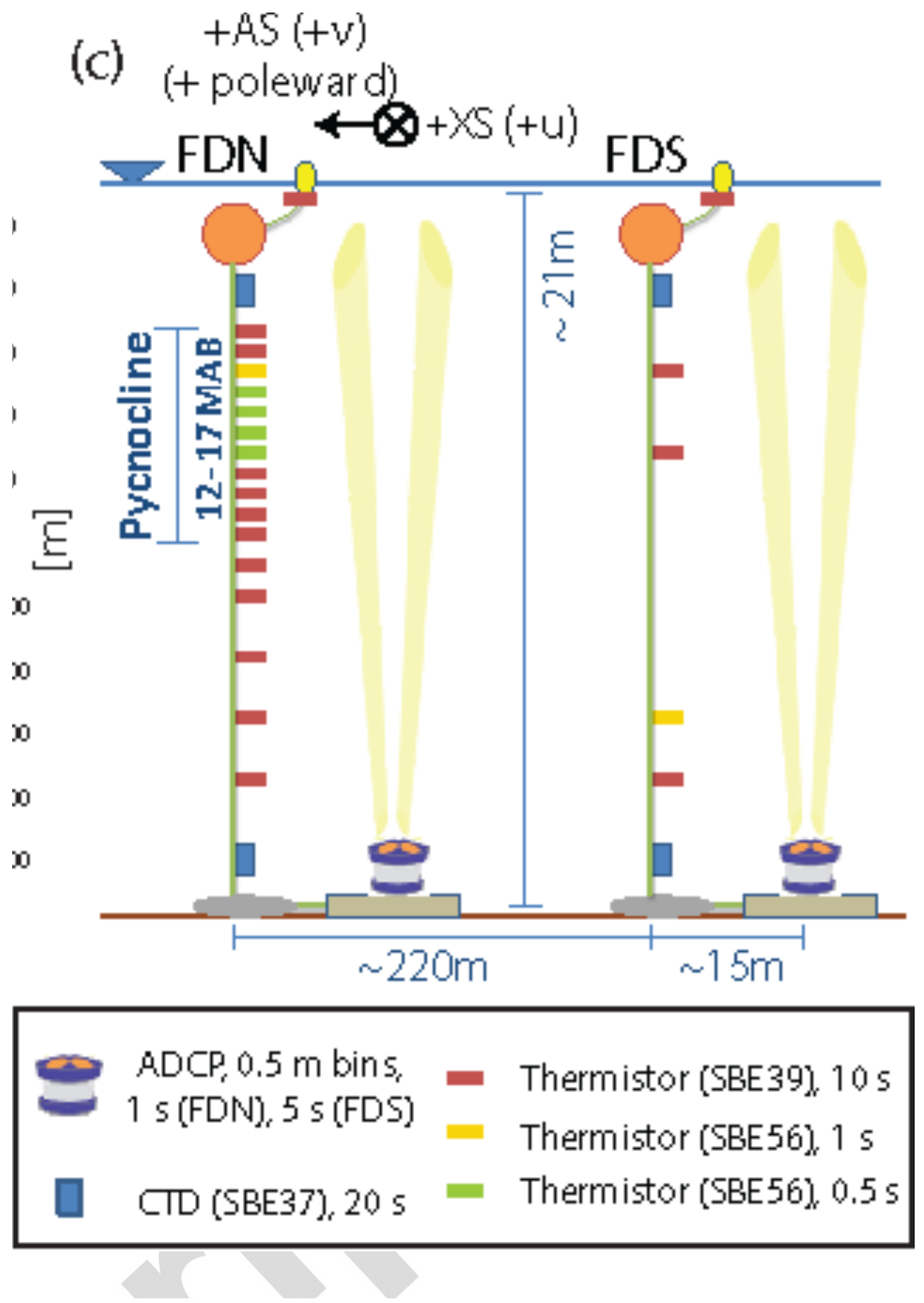
- We can now do successive approximations like with Fourier series, e.g. $(f_i^{(1)} \ldots f_i^{(M)})^T \approx \overrightarrow{v_1} a^{(1)} + \overrightarrow{v_2} a_i^{(2)} + \ldots + \overrightarrow{v_K} a_i^{(K)}$

- If we include all M eigenvectors we recover the original series, but in practice we may be able to get away with reconstructing with far fewer eigenvectors.

Example 2: Ocean Data

- A lot of information in the study of ENSO comes from satellite data, and satellite data along with its strengths and limitations merits a separate discussion.
- So for this example I am going to use "real" data, some times called *in situ w*hich is latin for "in it is original place".
- The data are from a mooring array in Monterey Bay as gathered and analyzed by my collaborator Ryan Walter (our paper is available on request).
- You don't need to be an oceanographer to get into analyzing the data set though.
- For our purposes we want to see how the EOF method makes sense of this data set.
- There are 35 measurements at different depths, and for each depth we measure 1992 times.

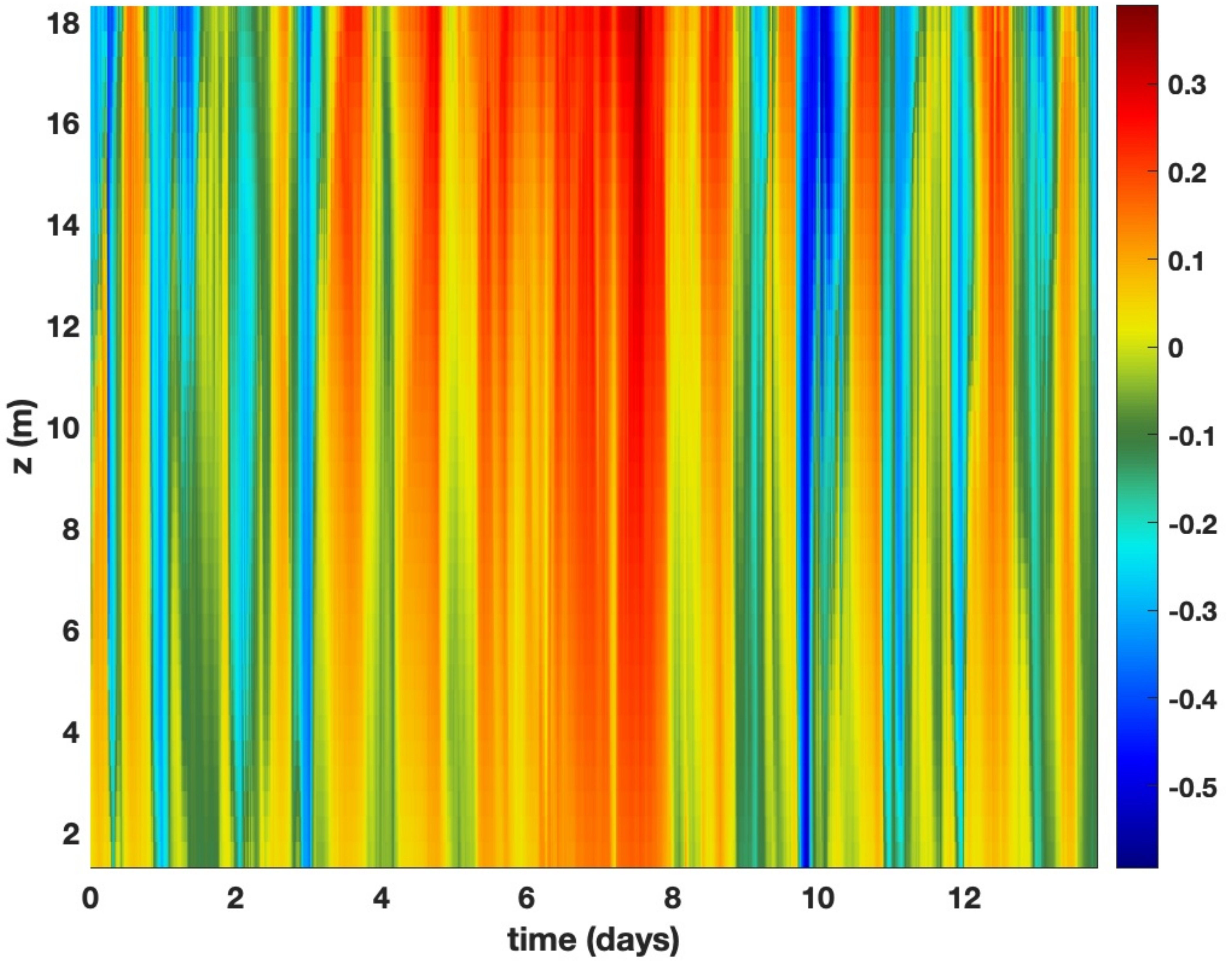




Monterey bay has a complex pattern of temperature variations that also vary in depth. The instrument array measures several quantities at different depths. We will concentrate on the scaled density.

Example 2: Ocean Data all the densities

- The density changes in Monterey bay are largely due to temperature changes.
- On the right I colour in the density (with a reference value subtracted off) as a function of time (horizontal axis) and z (vertical axis)
- You can see big fluctuations for about the first three days, and from day 9 on.
- In the middle is a long period where the whole record looks to be higher density than average.
- Some patterns are evident but it is hard to be unambiguous about what to say.

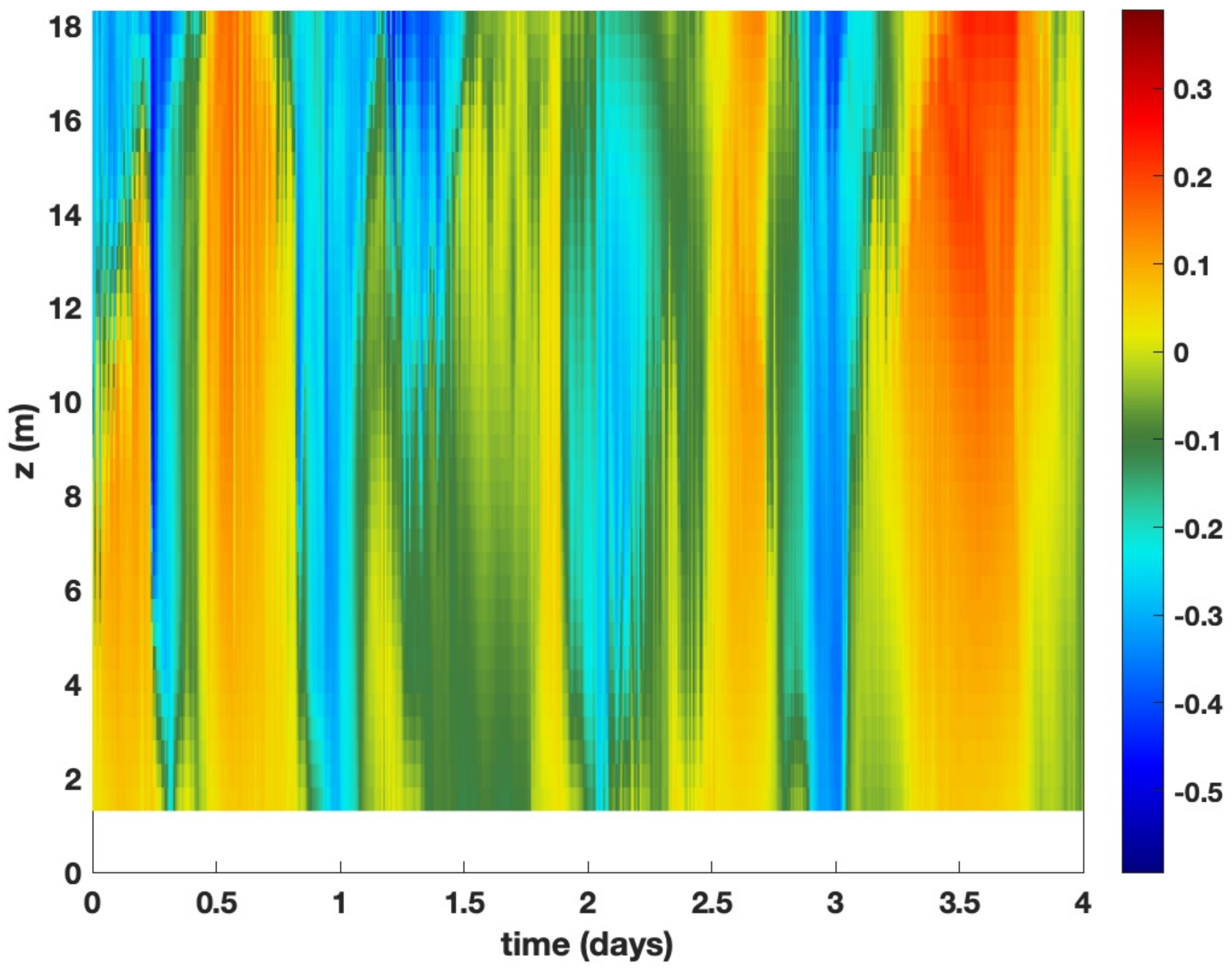


Example 2: Ocean Data early

- If we focus on the first four days we get a bit more clarity.

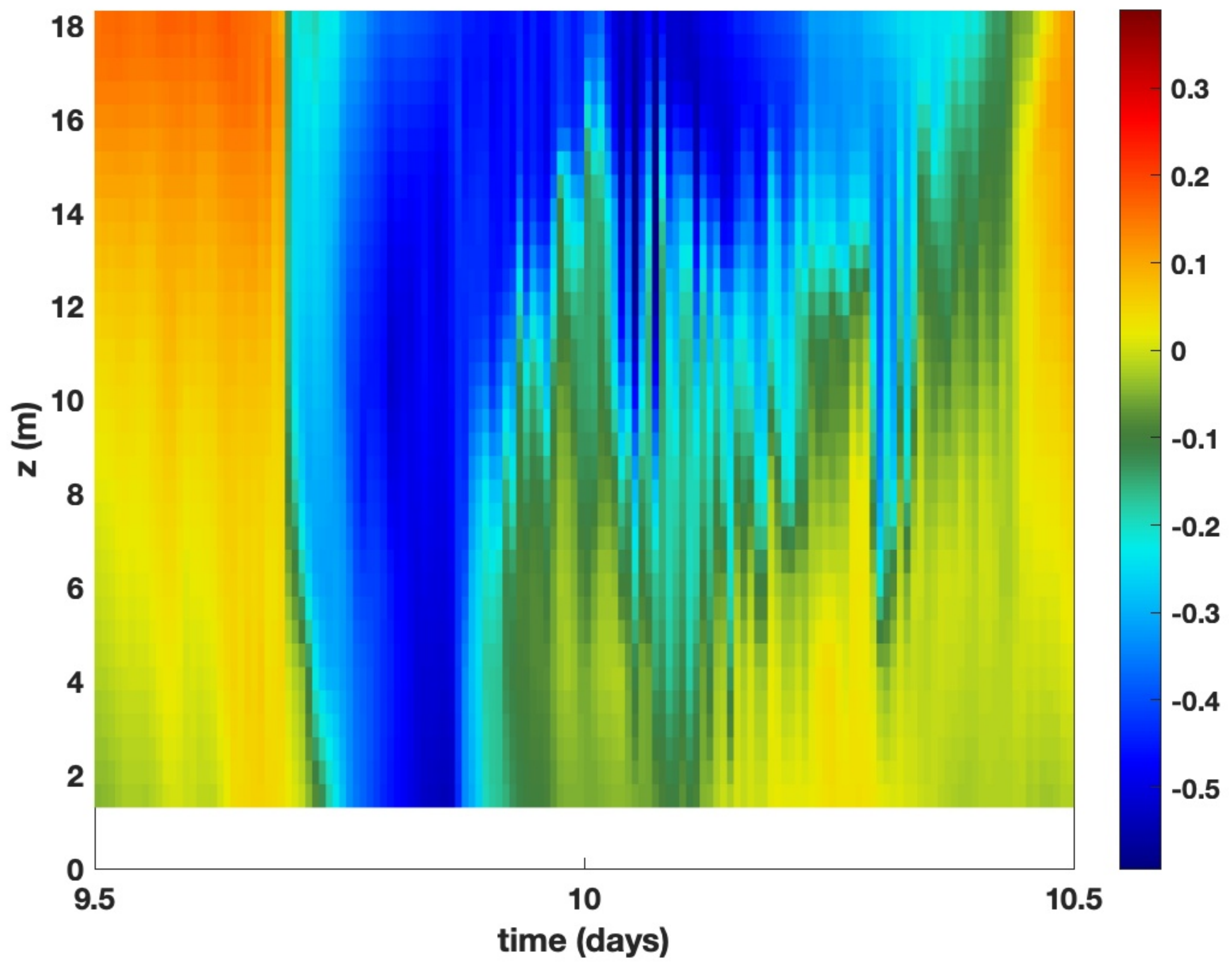
- Now one can see that sometimes the changed from more dense (warm) to less dense (cold) sometimes occurs all the way top the bottom and sometimes not so much.

- Also the change from more dense to less dense is sudden, while the change from more dense to less dense is more gradual.



Example 2: Ocean Data detail

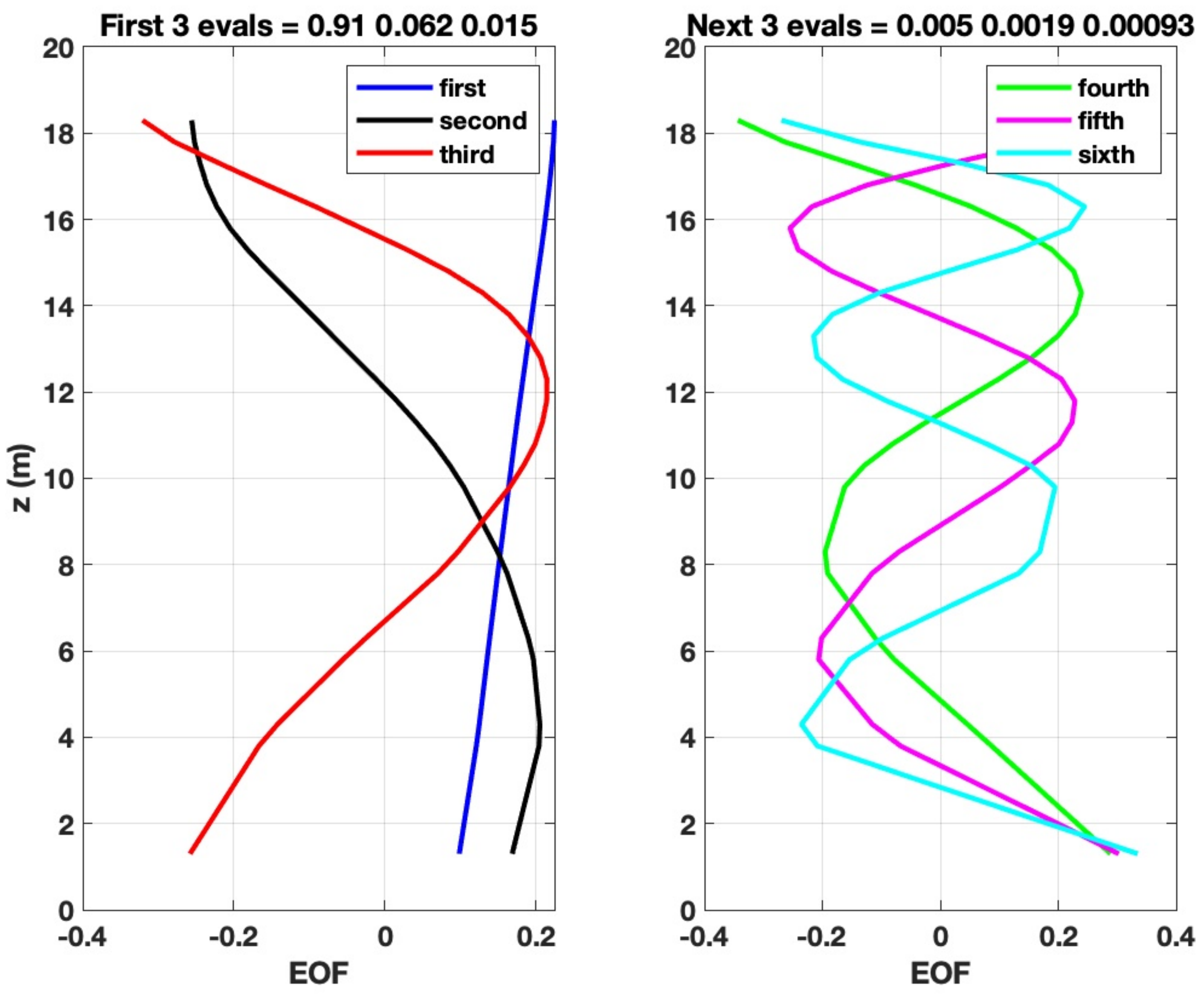
- If we focus on the “biggest event” in the record, we see more structure.
- This event occurs between day 9.5 and 10.5.
- It has a really neat structure with sharp transition around day 9.7, but a lot of fluctuations between day 9.9 and 10.2
- These turn out to be a special kind of wave found in the interior of oceans and lakes called internal waves.
- Those interested can see more in the paper we wrote on this that is posted under extra reading and as part of the lab.



Example 2: Ocean Data EOF results

EOFs are vectors with the same length as the number of rows in the covariance matrix (35 in this case)

- Computing EOFs is very easy in Matlab (you will get a chance to try it out on Wednesday).
- On the right I show the first six EOFs with the eigenvalues given in the titles.
- There is a huge jump from the first to the second to the third eigenvalue.
- The first EOF captures 91% of the variability, the second 6.2% and the third 1.2%. No other EOF is even near 1%.
- This means essentially everything about the data set can be learned from the first two EOFs, and that is an amazing example of how math allows us to understand the real world.

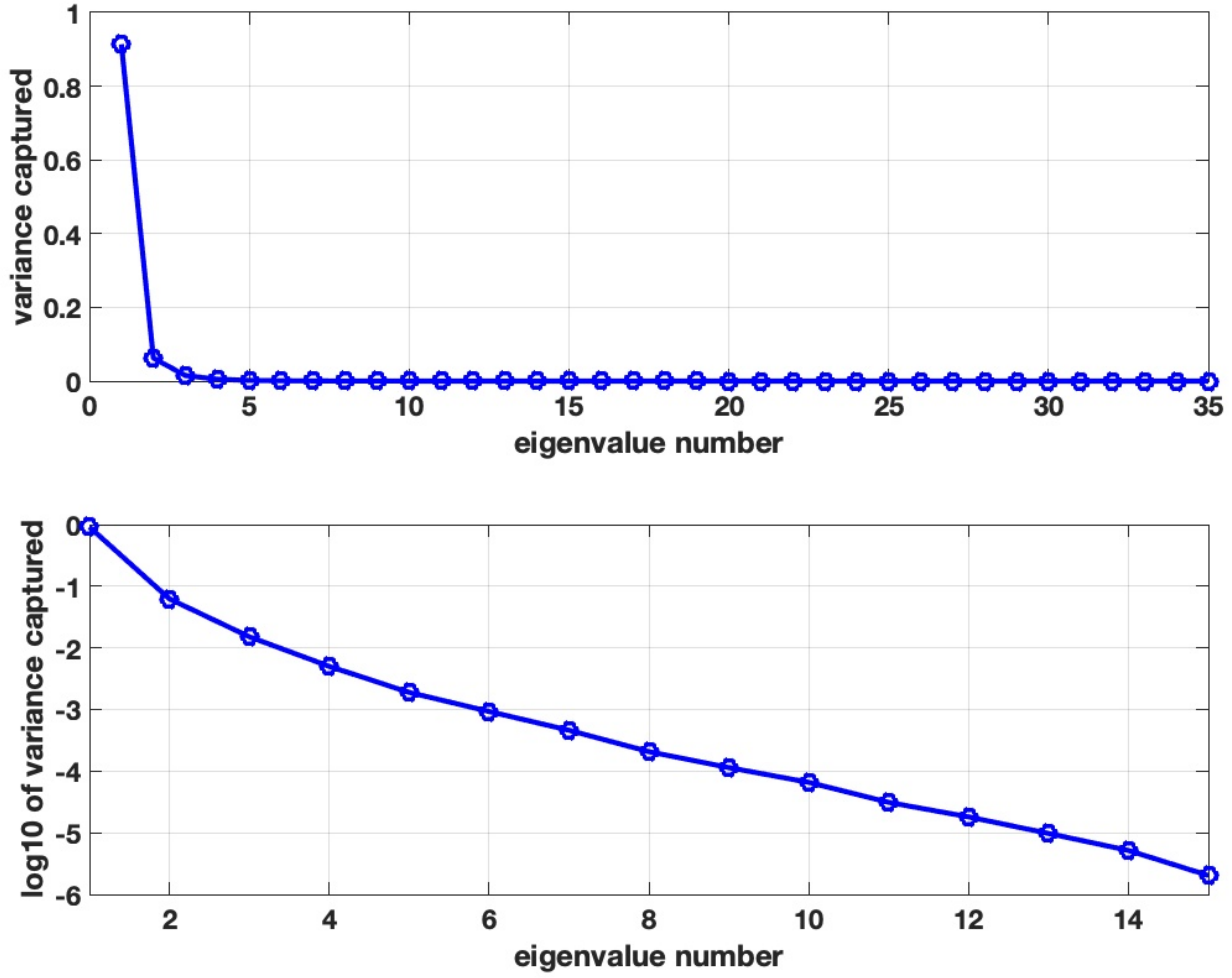


Remember that each EOF is a combination of the original measurements

Note that the first EOF (blue left panel) looks different from all others. Also note that it captures an incredible 91% of the variability.

Example 2: Ocean Data scree plot

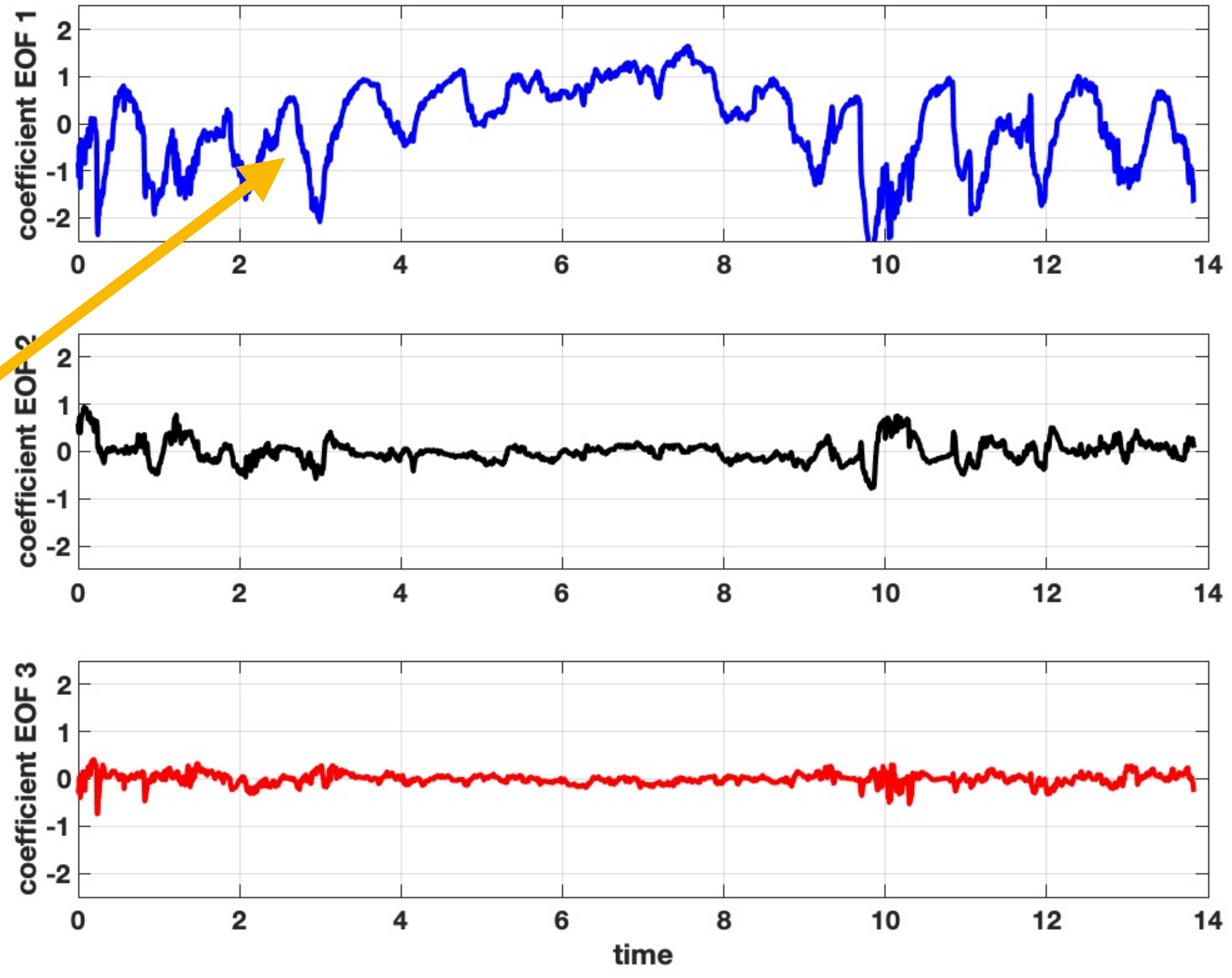
- In many data science applications the eigenvalues are plotted to show just how quickly they tend to zero.
- This is sometimes called a **scree plot** (the screen zone is usually a steep part near the top of a mountain where there are lots of broken up rocks).
- I sometimes like to plot things on a log scale because the variance captured typically falls off really fast.
- In practice all this means that the first few EOFs matter and the rest represent just minor details you may not care about.



Note how quickly the variance falls. The bottom panel is log scale so you can actually conclude something about eigenvalues beyond about 4.

Example 2: Ocean Data coefficients

- Each eigenvector has 1992 coefficients specifying its "weight" at any one time.
- Time is measured in days so the time values increase by 0.00694 days at each step.
- You can see from the picture on the right that the first eigenfunction has larger coefficients than the second and third eigenfunctions.
- This reflects the fact that the first eigenvalue is so much bigger than the others (the first EOF captures more variance).
- $(f_i^{(1)}, f_i^{(2)}, \ldots, f_i^{(35)})^T \approx \overrightarrow{v_1} a_i^{(1)}$ so that the whole data set is approximated by one 35x1 eigenvector and a (1x1992) vector of coefficients.

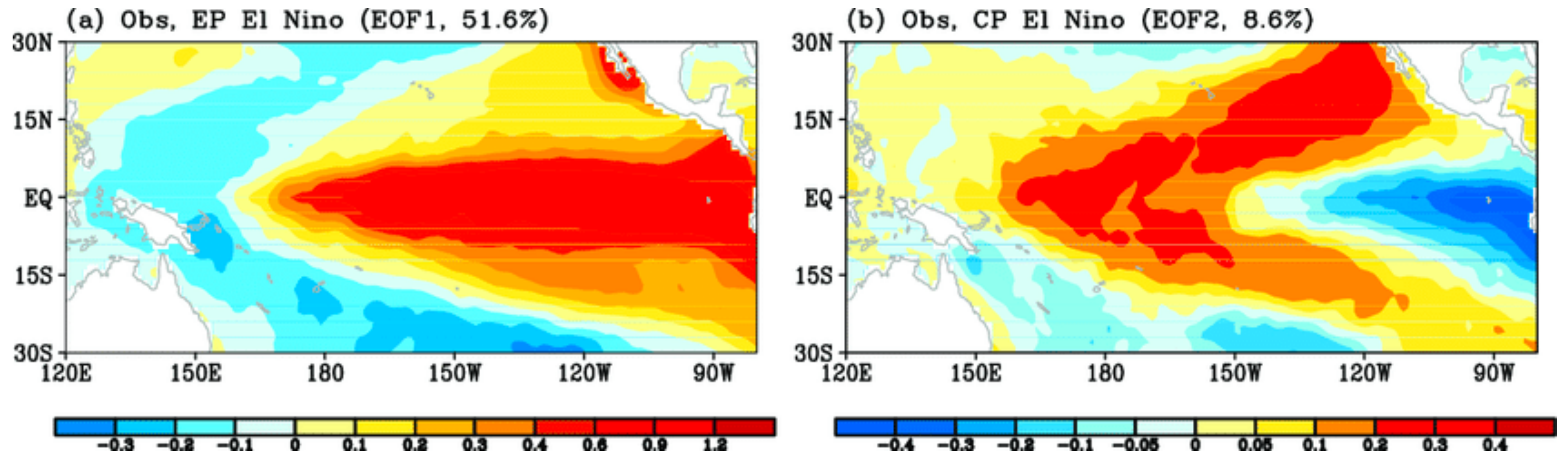


The idea would be that the first EOF matters more than any one measurement. So we want to know how its coefficient varies.

Example: EOFs of the tropical SST

- Many different studies have computed EOFs of the tropical Pacific SSTs.
- You can see that unlike our Monterey Bay data the leading EOF only captures just over 50% of the variability.
- It's shape is clearly over the central and western Pacific (i.e. near South America).
- The second EOF captures about 9% of the variability and is sort of wrapped around the first one.
- Given the complexity of the climate system it is amazing to me that something as simple as an EOF calculation corresponds so well to the overall understanding we have of El Niño.

EOFs are vectors with the same length as the number of rows in the covariance matrix.
Here the data would be the time series at all the points in the Pacific, may be something like 100x50=50,000 points.
That means the covariance matrix is quite large.



Xu et al, J. Climate, 2017.

Computing EOFs in Matlab

- Matlab was designed as a way to do various bits of linear algebra on the computers of the 1970s.
- It thus has at least a couple ways of carrying out EOFs.
- The biggest practical issue is making sure the data is ordered the right way (I take care of this for you by preparing the data).

```
load Monterey_Bay

mymn=mean(myden,2);
myden = bsxfun(@minus, myden, mean(myden,2));
mytime=mytime-mytime(1);

%% The EOF calculation
cov_mat=cov(myden');
[vv, dd]=eig(cov_mat);
[evals, evalsi]=sort(diag(dd),'descend');

evals=evals/sum(evals);
evecs=vv(:,evalsi);
```

Loads in the data.
“myden” is the array of measurements with rows being depths and columns being times
Computes the mean in the second entry of the array
Removes the mean using a pretty fancy Matlab function (great for big data)
Shift the time so it starts at zero

Get Matlab to make the covariance matrix
Get the eigenvalues and eigenvectors
Sort the eigenvalues from biggest to smallest, and record the order in evils

Scale the eigenvalues (this is technically unnecessary, but I do it for safety)
Reorder the eigenvectors. Matlab makes sure these are already orthonormal

EOF theory summarized 1

- We first make a matrix, often called $\mathbf{X}$, of our time series. Each row is a different time series and we assume they all have a length **N**.
- The covariance matrix would thus be $\mathbf{C} = \dfrac{1}{N-1}\mathbf{X}\mathbf{X}^{\mathbf{T}}$. It is positive, real-valued, and symmetric by construction.
- In practice before we make $\mathbf{X}$, we subtract the mean from each time series.
- We can use the fact that $\mathbf{C}$ is symmetric, real valued and positive to write $\mathbf{C} = \dfrac{1}{N-1}\mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{\mathbf{T}}$ where $\mathbf{U}$ is a rotation (or change of basis) matrix made up of the orthonormal eigenvectors of $\mathbf{C}$ as columns and $\boldsymbol{\Lambda}$ is a diagonal matrix of eigenvalues. Note that $\mathbf{U}^{-\mathbf{1}} = \mathbf{U}^{\mathbf{T}}$
- We can order the eigenvalues and corresponding eigenvectors so the first row in $\boldsymbol{\Lambda}$ is the biggest value, and the first column in $\mathbf{U}$ is the corresponding eigenvector. The second row in $\boldsymbol{\Lambda}$ is the second biggest eigenvalue and the second column in $\mathbf{U}$ is the corresponding eigenvector, and so on.

EOF theory summarized 2

- We can change the basis in which the data is written by letting $\mathbf{Y} = \mathbf{U}^{\mathbf{T}}\mathbf{X}$ and we can also define a covariance matrix in this new basis.

- $\mathbf{C}_Y = \dfrac{1}{N-1}\mathbf{Y}\mathbf{Y}^{\mathbf{T}} = \mathbf{U}^{\mathbf{T}}\mathbf{X}\mathbf{X}^{\mathbf{T}}\mathbf{U} = \dfrac{1}{N-1}\boldsymbol{\Lambda}$, which means by changing the basis to the eigenvectors we have eliminated the off-diagonal (or cross correlation terms). That is quite amazing!

- Thus the eigenvectors are the “optimal” basis to make the covariance matrix as easy to understand as possible.

- The eigenvectors thus form an **empirical basis**, one built completely from the data set.

- In practice this basis also ends up being super efficient at representing the key components of the data (basically you need 1-3 of the eigenvectors in many cases).

EOF approximation

- Many presentations of EOFs stop at this point.
- The idea is that EOFs are good, and the first EOF may well tell you something rather smart about your data. But the connection to the original physical system is unclear.
- The observation that EOFs are unphysical became fodder for many studies, and EOFs have been extended in a variety of ways (we will see a couple).
- In his PhD thesis Justin Shaw made the observation that while individual EOFs are unphysical, the reconstruction of the original data set using EOFs is by construction physical.
- In other words instead of the loose: $(f_i^{(1)}..f_i^{(M)})^T \approx \overrightarrow{v_1}a^{(1)} + \overrightarrow{v_2}a_i^{(2)} + \ldots + \overrightarrow{v_K}a_i^{(K)}$let $X_K = \overrightarrow{v_1}a^{(1)} + \overrightarrow{v_2}a_i^{(2)} + \ldots + \overrightarrow{v_K}a_i^{(K)}$be the kth approximation and now you can ask how well this approximation does at representing the underlying data.
- The recorded presentation by Justin Shaw explains the philosophy and details of the error map method, with the published paper (in extra readings) providing additional info.

Fourier Series: Generalized

$$F_n(x) = \sum_{k=1}^{n} c_k \phi_k(x) \qquad c_k = \langle f(x), \phi_k(x) \rangle$$

- The Fourier idea for a general basis; this is exactly what we have "rediscovered" for EOFs!
- Only instead of choosing a convenient basis we get one from the eigenvalue problem!

EOF challenges

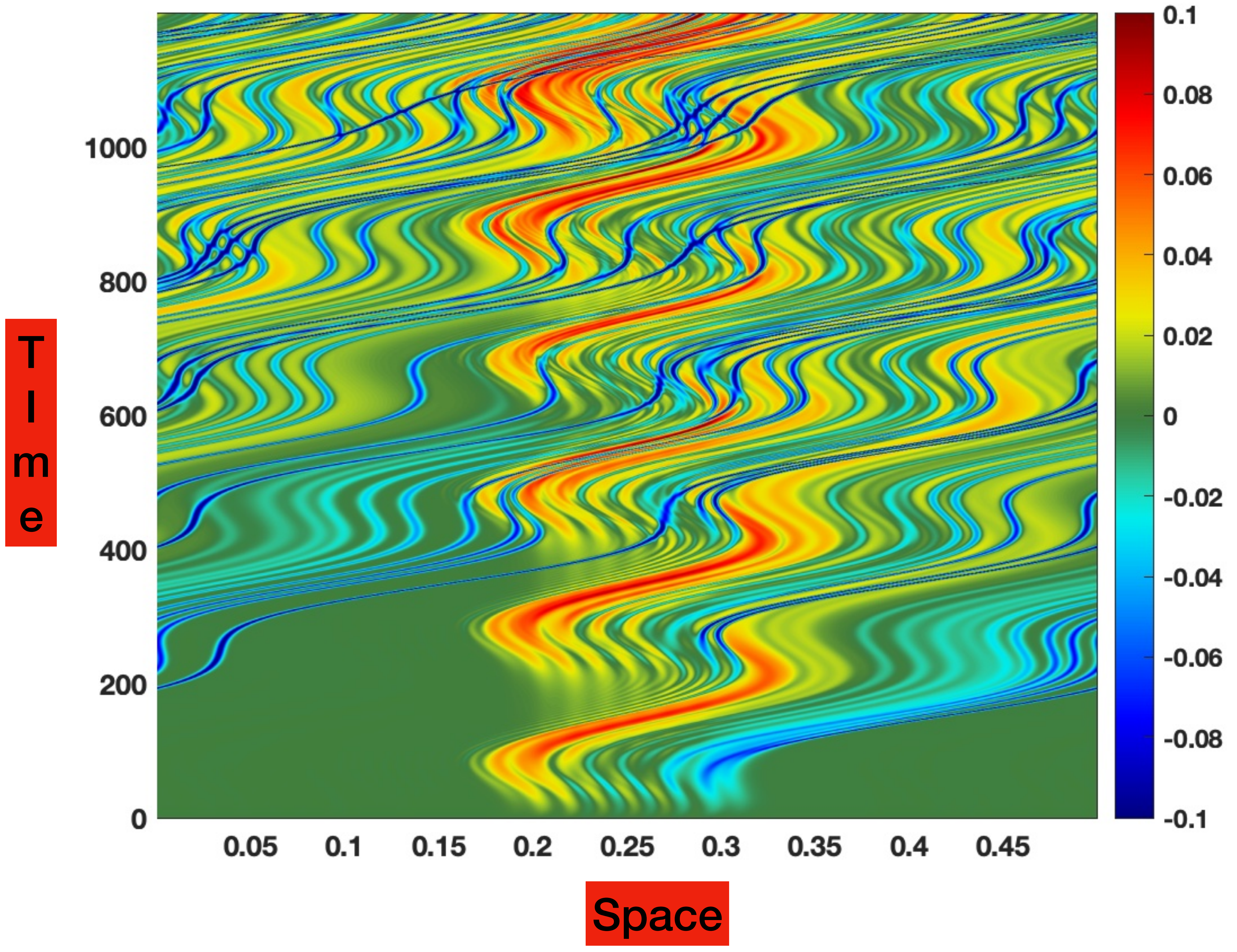
- If we want to apply EOFs and (eventually) the Error map method to our data set we have some numerical challenges to consider.

- Recall that the data set is 2048 points in space by 1200 points in time. So the resulting covariance matrix is 2048x2048 and is full.

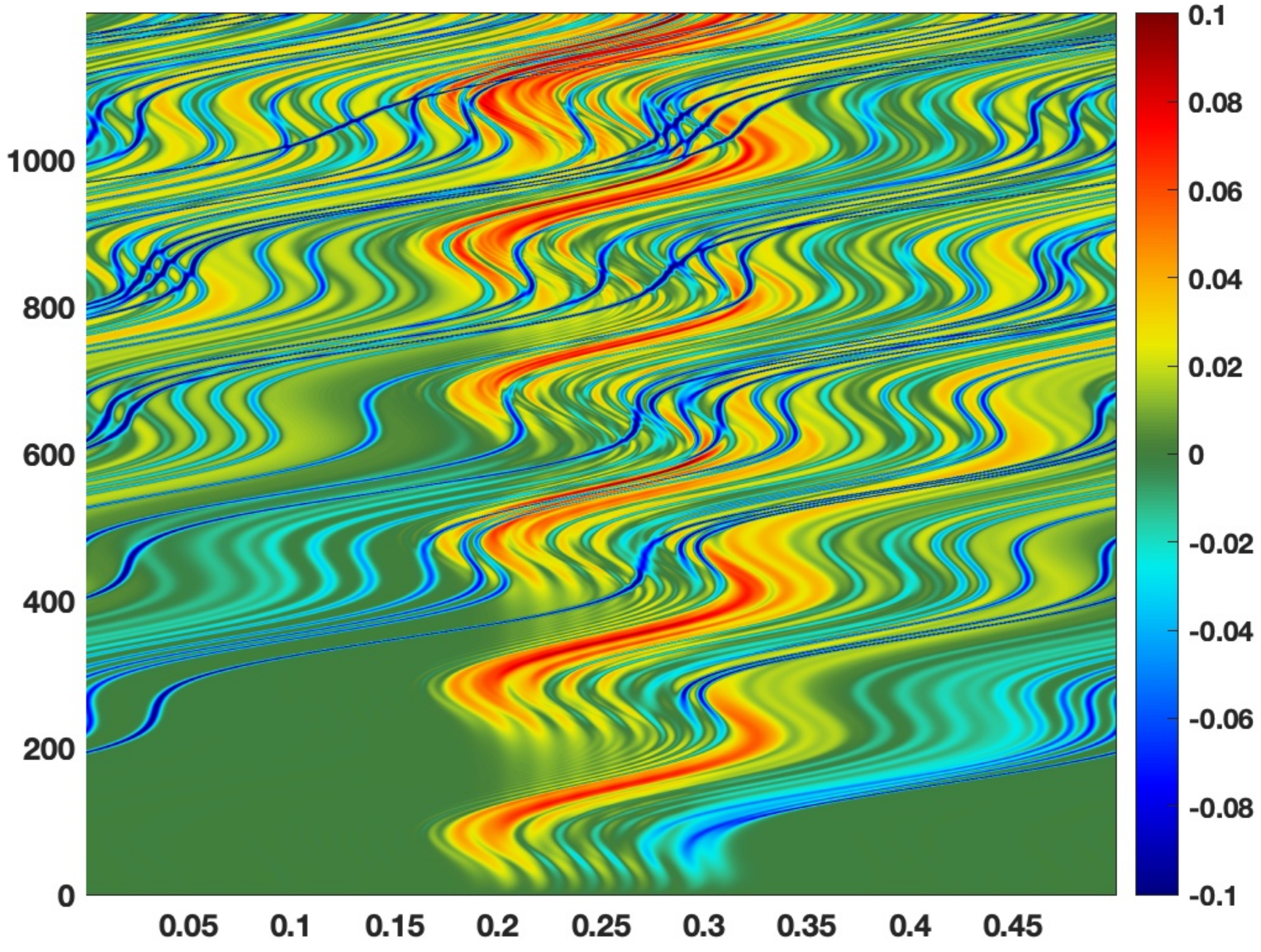
- That is not especially large, but it will take some time to find all those eigenvectors and that seems wasteful if we are only interested in say 10-20% of them.

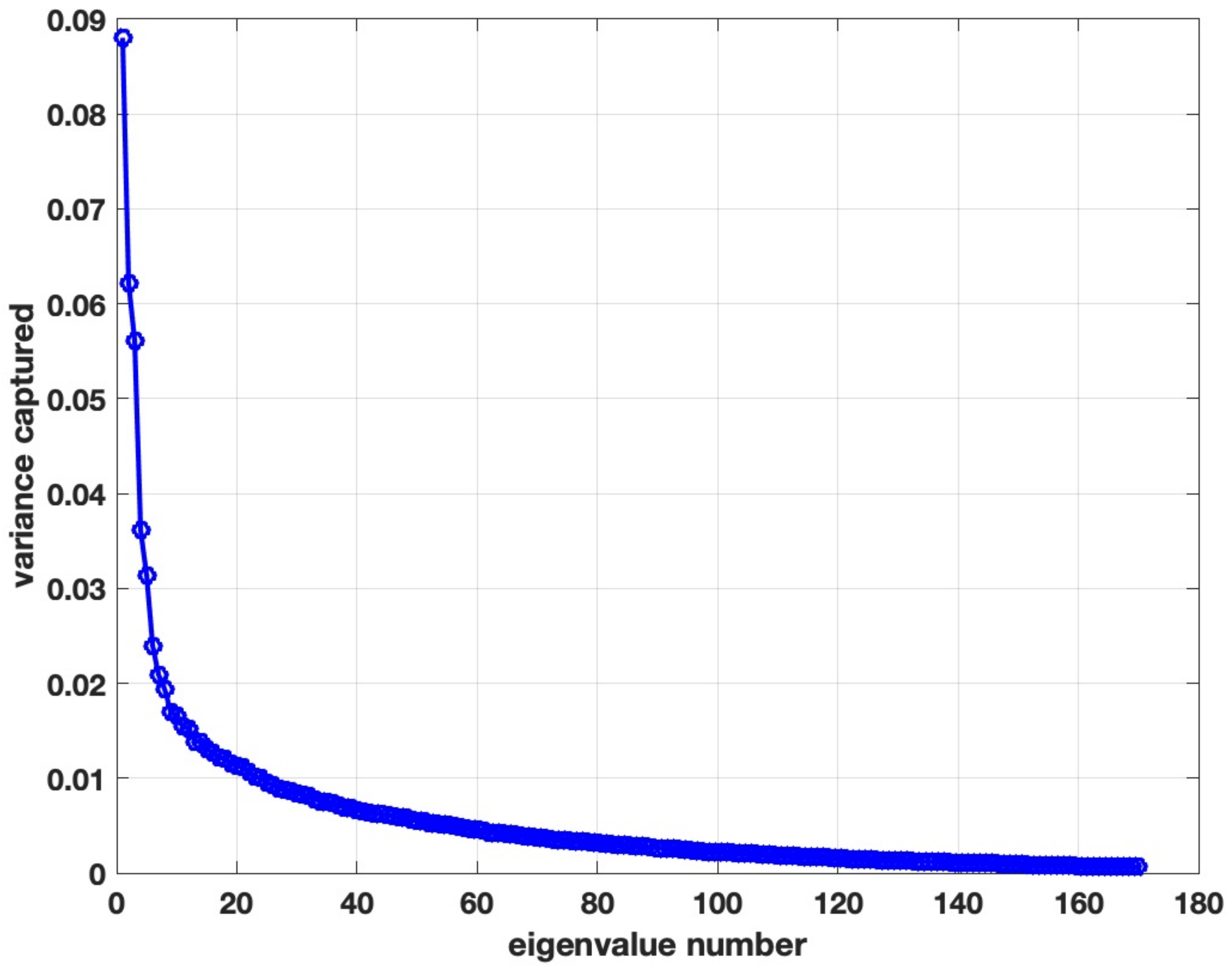
- In the next lecture we will take a bit of a side tour into eigenvalue/singular value calculations in Matlab when only a subset of eigenvalues is desired.

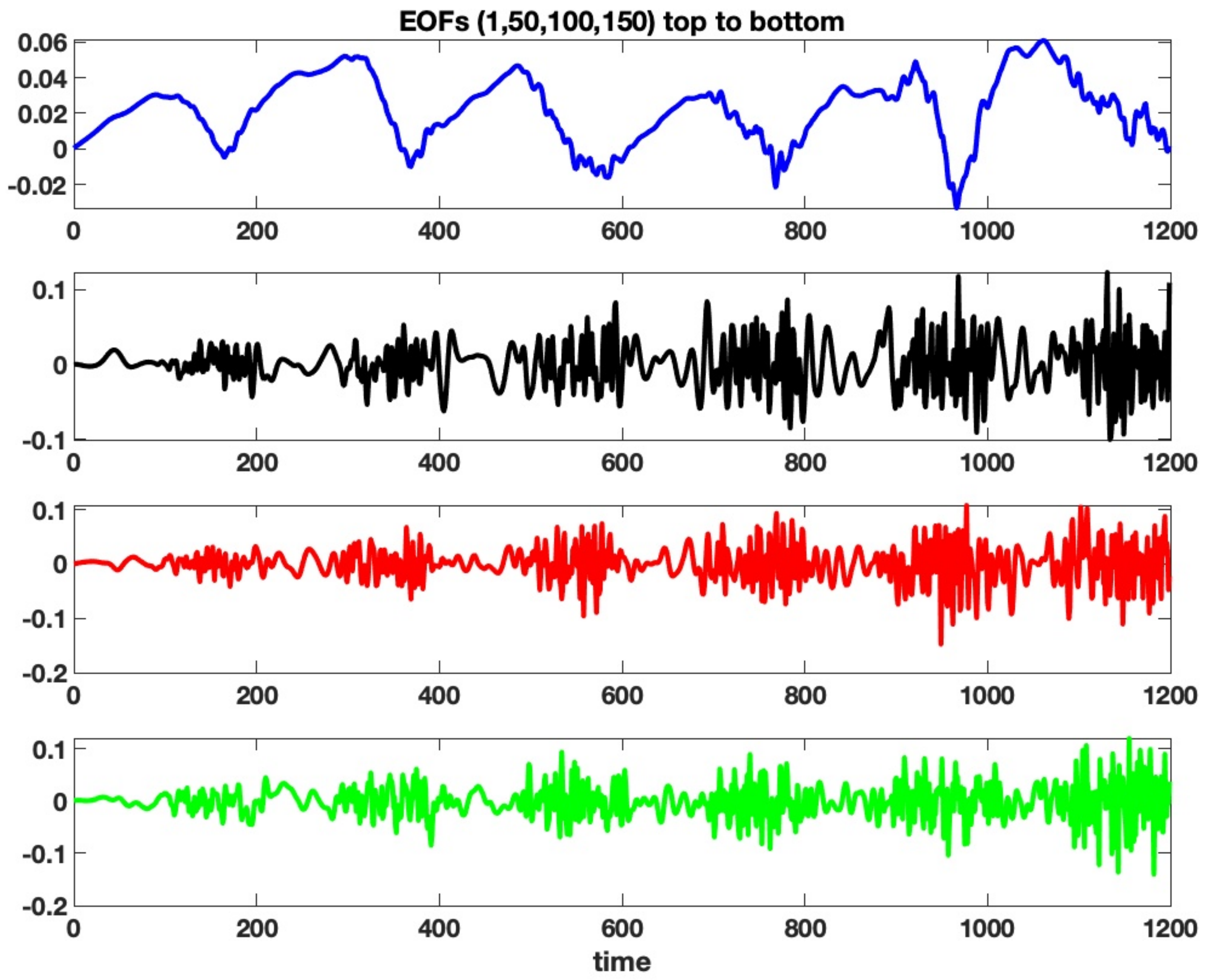
- But to assure the readers, on the next slide we show the successful use of EOFs for our data set.



EOF results 1







- The scree plot shows that only the first ten eigenvalues or so contribute strongly.
- But in contrast to the field data example, the subsequent drop off is gradual.
- The first EOF captures, mostly, the periodic oscillations do the flow back and forth across the topography.
- The waves that dominate the space-time plot aren’t really clear.
- They are quite clear in all of the 50th, 100th and 105th EOFs.
- So basically the EOFs tend to find the larger scale features first and then focus on the details of the others.