Analysis of Spatio-Temporal Datasets

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1 The El-Niño Southern Oscillation

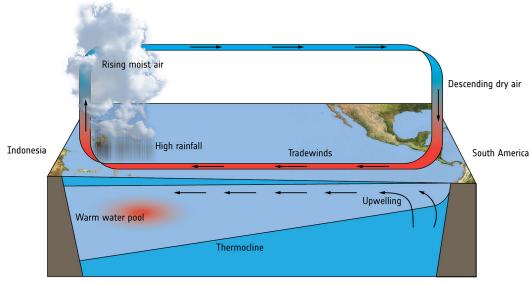
An example of a spatio-temporal climate oscillation pattern that can be summarized in a single time series.

"Experience precedes technical knowlegde." - W. Timothy Gallwey (*The Inner Game of Tennis*)

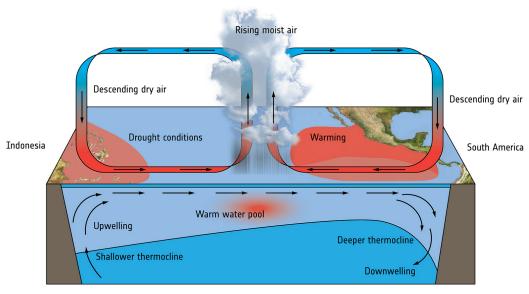
- a step-by-step guide for calculating the ENSO index based on SST data
- you will learn how to:
 - load a file
 - manipulate a dataset
 - apply a method (matrix factorization: SVD)
 - explore and interpret the results
 - perform a lead/lag correlation analysis
 - pretty plot the final results

1.1 What is ENSO?

- one of the largest modes of (internal) climate variability
- affects the climate of much of the tropics and subtropics
- comes in two phases: El $Ni\tilde{n}o$ and $La~Ni\tilde{n}a$
- both extremes can cause extreme weather (such as floods and droughts) in many regions of the world



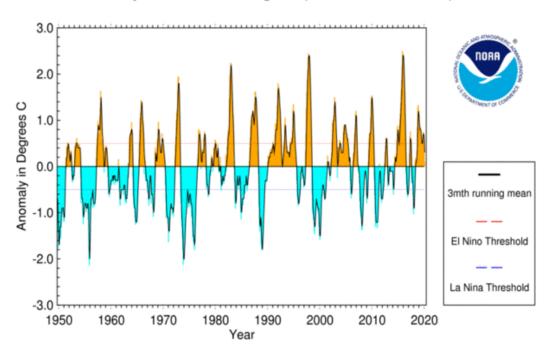
Normal conditions



El Niño conditions

The ENSO **index** is used to monitor the tropical Pacific and seasonal forecasting is a hot topic.

SST Anomaly in Nino 3.4 Region (5N-5S,120-170W)



National Centers for Environmental Information / NESDIS / NOAA

1.2 Why do we care?

```
[1]: from IPython.display import Video
# source: https://niwa.co.nz/climate/information-and-resources/elnino
Video("images/la_nina.mp4",width=800)
```

[1]: <IPython.core.display.Video object>

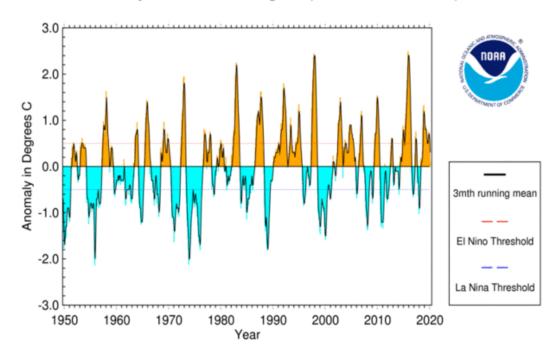
2 Can we come up with an ENSO index ourselves?

Or, getting from here...

```
[2]: import xarray as xr
ds = xr.open_dataset("sst.nc")
with xr.set_options(display_expand_attrs=False):
    display(ds)
```

```
* Y (Y) float32 -88.0 -86.0 -84.0 -82.0 -80.0 ... 82.0 84.0 86.0 88.0  
* zlev (zlev) float32 0.0  
* X (X) float32 0.0 2.0 4.0 6.0 8.0 ... 350.0 352.0 354.0 356.0 358.0  
Data variables:  
    sst (T, zlev, Y, X) float32 ...  
Attributes: (2)
```

SST Anomaly in Nino 3.4 Region (5N-5S,120-170W)



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...to here.

3 What we want to do

- 1. Prepare Sea Surface Temperature (SST) for the NINO3.4 region
- 2. Decompose spatio-temporal SST dataset into principal components
- 3. Create spatial correlation maps using principal components

4 Prepare Sea Surface Temperature (SST) for the NINO3.4 region

• ERSSTv5 sea surface temperature dataset (find it on the OSF repository)

wget https://iridl.ldeo.columbia.edu/SOURCES/.NOAA/.NCDC/.ERSST/.version5/sst/data.nc -0 sst_or

- In this specific dataset the calendar attribute of the time dimension T is set to 360 but xarray expects 360_day instead (Bummer!).
- Use NCO attribute editor ncatted (part of nco toolbox):

```
ncatted -a calendar, T, o, c, "360_day" sst_orig.nc sst.nc
```

4.1 Interactive notebook(s)

Requirements: To run this and other Jupyter notebooks, you need to have a few Python packages pre-installed. For package management, we recommend using conda, so you can set up different environments for different projects, without worrying about incompatibility issues.

We use xarray to do the heavy-lifting of reading NetCDF files. Making nice geographic maps is relatively easy with cartopy. The other (standard) packages are matplotlib for plotting, numpy numerical manipulation of numbers, vectors, and arrays, scipy for detrending, and pandas for time series analysis (and plotting as well).

Import all packages and click on (Run)

```
[3]: %matplotlib inline
import xarray as xr
import cartopy.crs as ccrs
import numpy as np
import pandas as pd
import imageio
from scipy.signal import detrend
import matplotlib.pyplot as plt
import matplotlib.dates as mdates
import matplotlib.ticker as ticker
import warnings
warnings.filterwarnings('ignore')

plt.rcParams['figure.figsize'] = (9, 5)
plt.rcParams['font.size'] = 18
```

4.2 detrending and removing climatology

After loading our data, we need to remove the trend and subtract the monthly climatologies for our analysis. For the de-trending we use scipy's detrend function. As it doesn't like NaN's, we fill them with zeros. For the climatologies, we make use of the apply method which applies our custom-made subtract method to all monthly values (groubby creates unique labels along a dimension, e.g., 1, 2, 3, ... 12, for all the months).

We can double-check if the climatologies have been removed, by picking a random location and plotting the long-term monthly mean values (i.e., climatologies) before and after apply.

```
[4]: # load SST file into data sets
ds_sst = xr.open_dataset("sst.nc").squeeze("zlev").drop("zlev")

# we give the dimensions a standard name, e.g., "T" -> "time", etc.
```

```
new_dims = {'T': 'time', 'Y': 'latitude', 'X': 'longitude'}
ds_sst = ds_sst.rename(new_dims).set_coords(['longitude', 'latitude', 'time'])

# select a time period using ".sel()"
# and "slice" the time for the period between 1950 and 2021
ds_sst = ds_sst.sel(time=slice("1949-10","2021"))
## define a function that subtmasts the mean along the "time" dimension
```

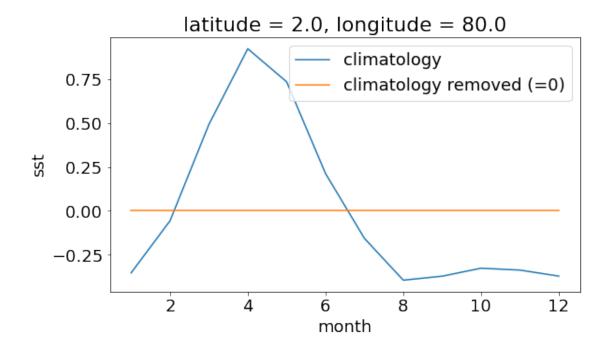
```
[5]: # define a function that subtracts the mean along the "time" dimension
def subtract(x):
    return x - x.mean(dim="time")

# define our custom detrend function that also fills NaNs with Os
def detrend_(x):
    return detrend(x.fillna(0),axis=0)
```

```
[6]: # we'll keep a copy after each step as reference ("ds0", "ds1", "ds2")
# but override "ds_sst"
ds0 = ds_sst*1.0

# apply the detrending
ds_sst = ds_sst.apply(detrend_)
ds1 = ds_sst*1.0

# apply the subtraction of the monthly means, using "groupby"
ds_sst = ds_sst.groupby("time.month").apply(subtract)
ds2 = ds_sst*1.0
```



4.3 Picking the region

Niño 1+2 (0-10S, 90W-80W): The Niño 1+2 region is the smallest and eastern-most of the Niño SST regions, [...]

Niño 3 (5N-5S, 150W-90W): This region was once the primary focus for monitoring and predicting El Niño, but researchers later learned that the key region for coupled ocean-atmosphere interactions for ENSO lies further west [...]

Niño 3.4 (5N-5S, 170W-120W): The Niño 3.4 anomalies may be thought of as representing the average equatorial SSTs across the Pacific [...]

Niño 4 (5N-5S, 160E-150W): The Niño 4 index captures SST anomalies in the central equatorial Pacific. This region tends to have less variance than the other Niño regions.

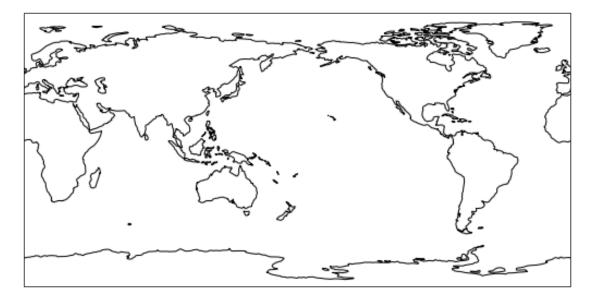
 $(source: \ https://climatedataguide.ucar.edu/climate-data/nino-sst-indices-nino-12-3-34-4-oni-and-tni)$

```
[8]: # define Nino3.4 region boundaries
lon1 = 360-170; lon2 = 360-120
lat1 = -5; lat2 = 5
# also the other NINO regions
# Nino1.2
lon1_12 = 360-90; lon2_12 = 360-80
lat1_12 = -10; lat2_12 = 0
# Nino3
lon1_3 = 360-150; lon2_3 = 360-90
```

```
lat1_3 = -5; lat2_3 = 5
# Nino4
lon1_4 = 160; lon2_4 = 360-150
lat1_4 = -5; lat2_4 = 5
```

```
[9]: # define projection of SST data: lonlat grid -> "PlateCarree()"
    data_proj = ccrs.PlateCarree()
    # define projection for maps
    proj = ccrs.PlateCarree(central_longitude=180)

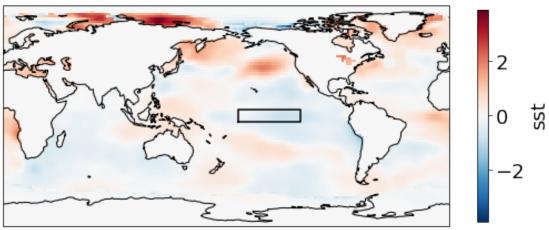
# create figure and axis with map projection
    fig, ax = plt.subplots(1,1,subplot_kw={'projection':proj})
    # draw some coastlines
    ax.coastlines();
```



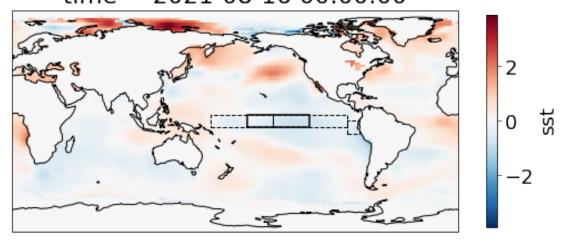
```
[10]: # plot SST anomalies for last month,
    # i.e, the last time index, -1
    ds_sst["sst"][-1].plot(ax=ax,transform=data_proj,cbar_kwargs={"shrink": 0.7})
    # plot extend of Nino3.4
    nino34 = [lon1,lon2,lon2,lon1,lon1],[lat1,lat1,lat2,lat2,lat1]
    ax.plot(*nino34,'k-',transform=data_proj)
    fig
[10]:
```

8





time = $2021-08-16\ 00:00:00$



```
[12]: # slice dataset along Nino3.4 boundaries
      # i.e., between "lon1" and "lon2",
      # and between "lat1" and "lat2"
      sst = ds_sst["sst"].loc[{
          'latitude': slice(lat1,lat2),
          'longitude': slice(lon1,lon2)
      }]
      # fill all masked values (land) with Os
      x = sst.fillna(0).values
      # print dimensions of Nino3.4 SST data
      print("Original dimensions:", x.shape)
      # save the dimensions
      nt, ny, nx = x.shape
      # reshape array into matrix with time and space dimension, only
      # i.e, nt, nx*ny
      x = np.reshape(x,(nt,ny*nx))
      print("New dimensions: ",x.shape)
      # store number of principipal components (for later)
     n_components = nx*ny
```

Original dimensions: (863, 5, 26) New dimensions: (863, 130)

Let's now apply a Singular Value Decomposition to the matrix x

```
[13]: # THIS LINE HERE IS WHERE THE WHOLE ACTION IS!
u, s, vh = np.linalg.svd(x, full_matrices=False)

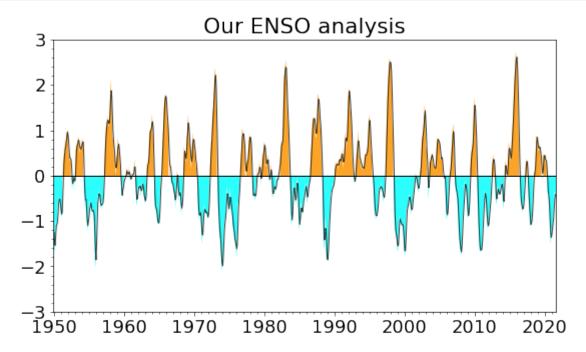
# print dimensions of returned matrices
print(u.shape, s.shape, vh.shape)
```

(863, 130) (130,) (130, 130)

- u contains the temporal representation (time series) of the principal components
- s contains the eigenvalues of the principal components
- vh contains the spatial representation (spatial maps) of of the **principal components**

```
pc_3m = pc.rolling(3).mean()
# get the time stamps for the x-axis dates
time = pc.index.to_datetimeindex()
time_3m = pc_3m.index.to_datetimeindex()
```

```
[15]: # and plot it all
plt.fill_between(time,pc[1],0,where=(pc[1] > 0), lw=0, color='#fca428')
plt.fill_between(time,pc[1],0,where=(pc[1] < 0), lw=0, color='#2cfefe')
plt.plot(time_3m,pc_3m[1],'k-',lw=1,alpha=0.75)
plt.axhline(0,c='k',zorder=1,lw=1)
plt.xlim(time[0],time[-1])
plt.title("Our ENSO analysis")
plt.gca().xaxis.set_minor_locator(mdates.YearLocator())
plt.gca().yaxis.set_minor_locator(ticker.FixedLocator(np.arange(-3,3.1,0.2)))
plt.ylim(-3,3)
plt.savefig("images/our_enso.png",dpi=300)</pre>
```



And here's how it compares to NOAA's NINO3.4 index

5 What just happened?

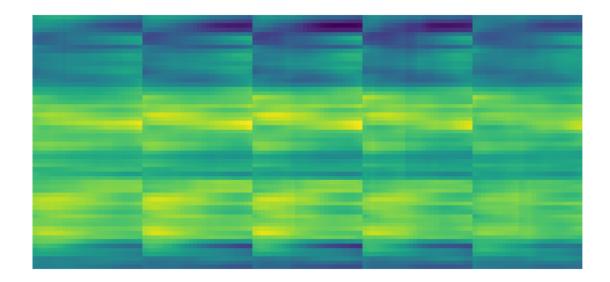
[16]: # fill all masked values (land) with Os

6 Decompose spatio-temporal SST dataset into principal components

The SST (or any spatio-temporal) dataset can be re-arranged into a matrix, M, with rows representing the time series of each location (columns)

$$M = \begin{bmatrix} x_{11} & x_{12} & x_{13} & \dots & x_{1n} \\ x_{21} & x_{22} & x_{23} & \dots & x_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{t1} & x_{t2} & x_{t3} & \dots & x_{tn} \end{bmatrix}$$

```
x = sst.fillna(0).values
      # print dimensions of Nino3.4 SST data
      print(x.shape)
      # save the size of each dimension
      nt, ny, nx = x.shape
      # reshape array into matrix with time and space dimension, only
      # i.e, nt,nx*ny
      x = np.reshape(x,(nt,ny*nx))
      print(x.shape)
     (863, 5, 26)
     (863, 130)
[17]: print(x.shape)
      # plot matrix for last 5 years (=60 months)
      plt.matshow(x[:60,:])
      plt.gca().set_axis_off()
     (863, 130)
```



Before we get back to this high-dimensional example, let's have a look at a simpler 2D case with a matrix of shape (nt,2), so we get a feeling of what's going on.

7 SVD explained

```
[18]: rng = np.random.default_rng(1234) # random number generator instance

C = np.array([[1,0],[0,1]])
Z = rng.multivariate_normal(mean=[0,0],cov=C,size=(nt))

plt.figure(figsize=(10,2))
plt.plot(Z[:,0])
plt.plot(Z[:,1]);
```

```
2.5

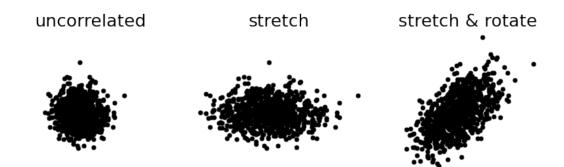
0.0

-2.5

0 200 400 600 800
```

```
[19]: # rotation matrix R
    np.set_printoptions(precision=4)
    theta = np.pi/4
    print(f" = {np.degrees(theta)} ")
```

```
R = np.array([[np.cos(theta),-np.sin(theta)],[np.sin(theta),np.cos(theta)]])
     print("R=")
     print(R)
     # inverse of rotation matrix R
     R_inv = np.linalg.inv(R)
     print("R_inv=")
     print(R inv)
     # stretch matrix S
     S = np.diag([2**0.5,1])
     print("S=")
     print(S)
      = 45.0^{\circ}
     R=
     [[ 0.7071 -0.7071]
     [ 0.7071 0.7071]]
     R inv=
     [[ 0.7071  0.7071]
      [-0.7071 0.7071]]
     [[1.4142 0.
                   1
                   11
      ГО.
             1.
[20]: # define method to create a phase plot of two timeseries
      ax.plot(x,y,ls='',marker='o',mew=0,color=color)
         ax.set_aspect("equal")
         ax.set_xlabel(xlab); ax.set_ylabel(ylab)
         ax.set_title(title)
         if off: ax.set_axis_off()
         if grid: ax.grid()
[21]: fig, ax = plt.subplots(1,3,figsize=(10,4),sharex=True,sharey=True)
     # raw, uncorrelated
     plot_xy(Z[:,0],Z[:,1],ax[0],title="uncorrelated",off=True)
     # stretch
     Zs = np.dot(Z,S@S)
     plot_xy(Zs[:,0],Zs[:,1],ax[1],title="stretch",off=True)
     # stretch & rotate
     Zsr = np.dot(Z,R@S@S@R_inv)
     plot_xy(Zsr[:,0],Zsr[:,1],ax[2],title="stretch & rotate",off=True)
     fig.tight_layout()
     print(np.cov(Zsr.T))
     [[2.4384 1.4093]
      [1.4093 2.4533]]
```



```
[22]: # Let's create two new time series with the same covariance as the
      # "stretched & rotated" dataset
      M = R@S@S@R inv
      print(M@M)
      Z2 = rng.multivariate_normal(mean=[0,0],cov=M@M,size=(nt//10)) # use fewer_
      \rightarrowpoints
      plot_xy(Z2[:,0],Z2[:,1],ax[2],title="stretch &__
      →rotate", off=True, color='lightgrey')
      Z2r = Z20R
      plot_xy(Z2r[:,0],Z2r[:,1],ax[1],title="stretch",off=True,color='lightgrey')
      Z2u = Z2@np.linalg.inv(M)
      plot_xy(Z2u[:,0],Z2u[:,1],ax[0],title="uncorrelated",off=True,color='lightgrey')
      fig.tight_layout()
      fig
     [[2.5 1.5]
      [1.5 2.5]]
[22]:
              uncorrelated
                                           stretch
                                                               stretch & rotate
```

```
[23]: # Now let's do a SVD and compare
u, s, vh = np.linalg.svd(Z2, full_matrices=False)
print(u.shape,s.shape,vh.shape)
```

```
Z3 = u@np.diag(s)
plot_xy(Z3[:,0],Z3[:,1],ax[1],title="stretch",off=True,color='dodgerblue')

fig.tight_layout()
fig

(86, 2) (2,) (2, 2)

[23]:

uncorrelated stretch stretch & rotate
```

7.1 Interactive session (20min)

Break out into groups of 2 or 3 and work through notebook O1-SVD.ipynb.

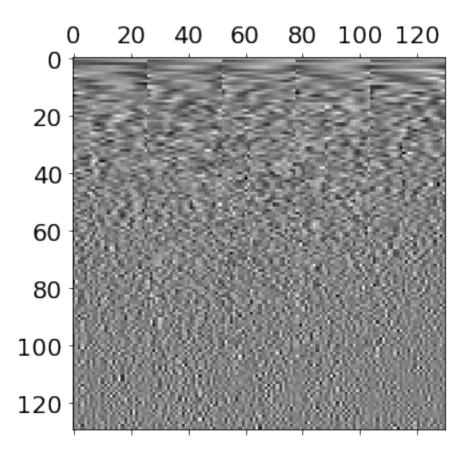
Back to our SST dataset...

```
[24]: # store number of principipal components (for later)
      n_components = nx*ny
      # decompose SST data into spatial and temporal components
      # using numpy's linear algebra method "svd":
      # Singular Value Decomposition
      # THIS LINE HERE IS WHERE THE WHOLE ACTION IS!
      u, s, vh = np.linalg.svd(x, full_matrices=False)
      # print dimensions of returned matrices
      print(u.shape, s.shape, vh.shape)
     (863, 130) (130,) (130, 130)
[25]: # inspect (transposed) matrix u
      plt.matshow(u.T,cmap="gray");
                    100
                             200
                                     300
                                             400
                                                      500
                                                              600
                                                                      700
                                                                               800
           20
           40
           60
           80
          100
          120
```

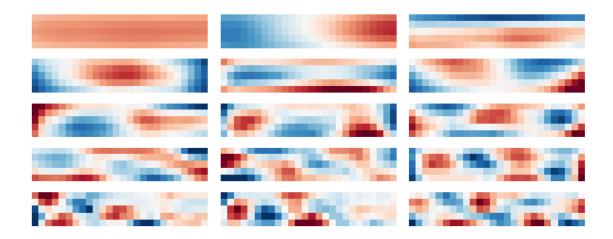
```
[26]: # inspect first 15 elements of "u"
fig, axes = plt.subplots(5,3,sharex=True,sharey=True,figsize=(15,5))
for i,ax in enumerate(axes.flat):
    ax.plot(u[:,i])
    ax.set_axis_off()
fig.tight_layout()
```

```
months of the contraction of the
```

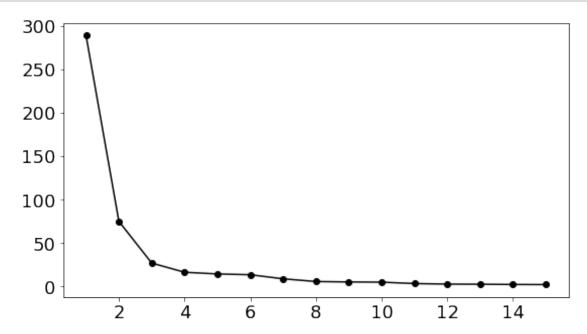
```
[27]: # inspect (already transposed) matrix v
plt.matshow(vh,cmap="gray");
```



```
[28]: # inspect first 15 elements of "vh"
fig, axes = plt.subplots(5,3,sharex=True,sharey=True,figsize=(12,5))
for i,ax in enumerate(axes.flat):
    # reshape into orginal (ny,nx) shape, i.e., the NINO3.4 region
    im = ax.matshow(np.reshape(vh[i,:],(ny,nx)),cmap="RdBu_r",vmin=-0.2,vmax=0.
    \_2)
    ax.set_axis_off()
fig.tight_layout()
```



[29]: # inspect first 15 (diagonal) elements of matrix "s"
plt.plot(range(1,16),s[:15],'ko-');

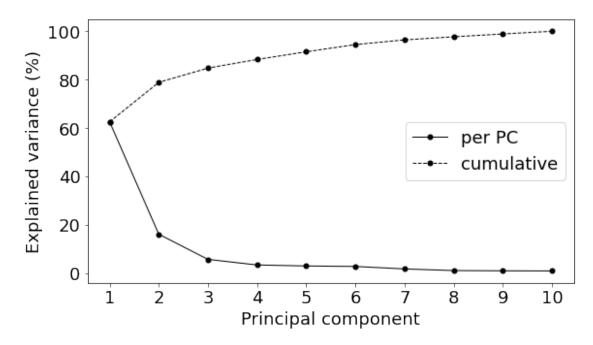


Let's tidy everything up a little bit, here.

```
[30]: X = s[:10]/np.sum(s[:10])*100
    plt.plot(range(1,len(X)+1),X,'ko-',lw=1,mew=0,label='per PC')
    plt.xlabel("Principal component")
    plt.ylabel("Explained variance (%)")
    plt.xticks(range(1,len(X)+1))
```

```
plt.plot(range(1,len(X)+1),np.cumsum(X),'ko--',lw=1,mew=0,label='cumulative')
plt.legend();
print("Total variance of SST data: %f"%x.var())
```

Total variance of SST data: 0.809341



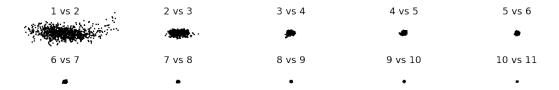
Let's put the resulting data back into a useful xarray data structure

```
[31]: # we refer to the spatial component of the decomposition as EOF
eofs = np.reshape(vh,(n_components,ny,nx))
coords = [
          ("n",range(1,n_components+1)),
          ("latitude", sst["latitude"].data),
          ("longitude", sst["longitude"].data)
]
# turn the eofs into an xarray DataArray
eof = xr.DataArray(eofs, coords=coords)
```

```
pc = ds_pc.to_dataframe()
```

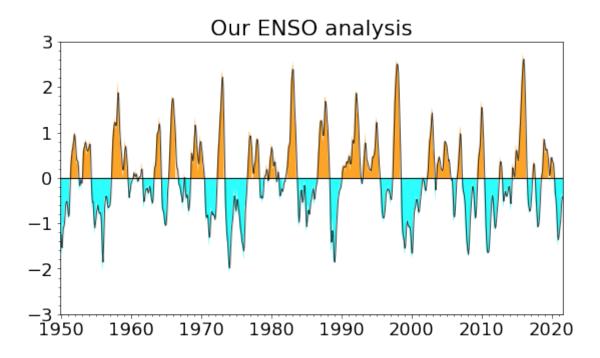
```
fig, axes = plt.subplots(2,5,sharex=True,sharey=True,figsize=(15,3))
for i,ax in enumerate(axes.flat):
    x = i+1
    y = i+2
    xt,yt = 0,1.1
    ax.plot(pc.loc[x],pc.loc[y],'k.',mew=0)
    ax.text(xt,yt,"%d vs %d"%(x,y),ha='center',va='center')
    ax.set_aspect('equal')
    ax.set_axis_off()
fig.tight_layout()
fig.suptitle("Explained Variance of PCs visualized",y=1.2);
```

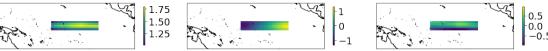
Explained Variance of PCs visualized



```
[34]: # extract the 1st PC, and scale it
pc1 = pc.loc[1]
pc1.index = pd.to_datetime([t.strftime() for t in sst["time"].data])
# a 3-month running mean using "rolling(3)"
pc1_3m = pc1.rolling(3).mean()
# get the time stamps for the x-axis dates
time = pc1.index
time_3m = pc1_3m.index
```

```
pc1 = pc1.values.flatten()
  plt.fill_between(time,pc1,0,where=(pc1 > 0), lw=0, color='#fca428')
  plt.fill_between(time,pc1,0,where=(pc1 < 0), lw=0, color='#2cfefe')
  plt.plot(time_3m,pc1_3m,'k-',lw=1,alpha=0.75)
  plt.axhline(0,c='k',zorder=1,lw=1)
  plt.xlim(time[0],time[-1])
  plt.title("Our ENSO analysis")
  plt.gca().xaxis.set_minor_locator(mdates.YearLocator())
  plt.gca().yaxis.set_minor_locator(ticker.FixedLocator(np.arange(-3,3.1,0.2)))
  plt.ylim(-3,3)
  plt.savefig("images/our_enso.png",dpi=300)</pre>
```



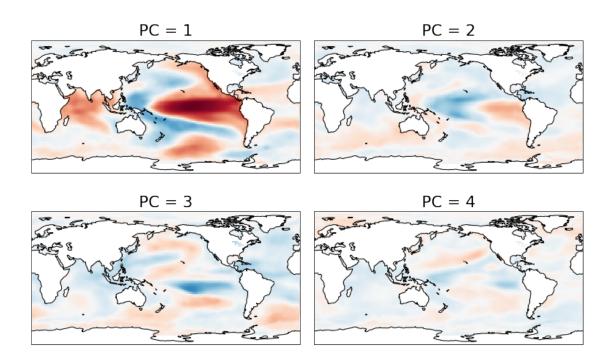


8 Create spatial correlation maps using principal components

- correlation between two random variables X and Y is expressed as $\rho_{X,Y} = \frac{Cov(X,Y)}{\sigma_X \sigma_Y}$
- if X, Y are two random variables with zero mean, then the covariance $Cov(X, Y) = E[X \cdot Y]$ is the dot product of X and Y

8.1 Correlation with Sea Surface Temperature

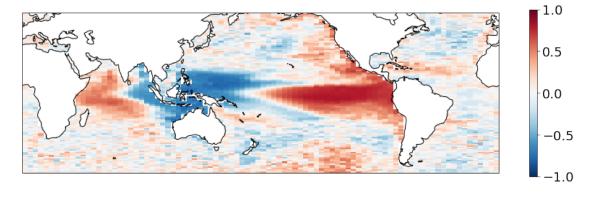
```
[37]: sst_all = ds_sst["sst"].fillna(0).values
      nt, ny, nx = sst_all.shape
      print(sst_all.shape)
      sst_all = np.reshape(sst_all,(nt,ny*nx))
      print(sst_all.shape)
      print(u.shape)
      # this is the "matrix" way of doing a regression
      X = np.dot((u/u.std(axis=0)).T,sst_all/sst_all.std(axis=0))/nt
      sst_eof_corr = np.reshape(X,(n_components,ny,nx))
      print(sst_eof_corr.shape)
      coords = [("PC",range(1,n_components+1)),
                ("latitude", ds_sst["latitude"].data),
                ("longitude", ds_sst["longitude"].data)]
      eof_maps = xr.DataArray(sst_eof_corr, coords=coords)
     (863, 89, 180)
     (863, 16020)
     (863, 130)
     (130, 89, 180)
[38]: fig, axes = plt.subplots(2,2,subplot_kw={'projection':proj},figsize=(11,7))
      for i,ax in enumerate(axes.flat):
          ax.coastlines()
          eof_maps[i].plot(ax=ax,transform=data_proj,
                           cmap='RdBu_r',vmin=-1,vmax=1,add_colorbar=False)
      fig.tight_layout()
```

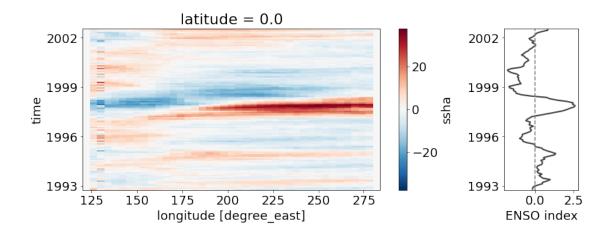


8.2 Correlation with Sea Surface Height

```
[39]: ds ssh = xr.open dataset("ssha.nc")
      ds_ssh = ds_ssh.rename({'T': 'time', 'Y': 'latitude', 'X': 'longitude'}).
      set_coords(['longitude', 'latitude', 'time'])
      \# ds0\_ssh = ds\_ssh*1.0
      ds_ssh = ds_ssh.apply(detrend_)
      # ds1_ssh = ds_ssh*1.0
      ds_ssh = ds_ssh.groupby("time.month").apply(subtract)
      \# ds2\_ssh = ds\_ssh*1.0
      \# ds1\_ssh["ssha"].groupby("time.month").mean().sel(longitude=82,latitude=2).
      \rightarrow plot(label="climatology")
      # ds2_ssh["ssha"].groupby("time.month").mean().sel(longitude=82,latitude=2).
       ⇒plot(label="climatology removed (=0)")
      # plt.legend();
[40]: ssh_all = ds_ssh["ssha"].fillna(0).values
      nt, ny, nx = ssh_all.shape
      ssh_all = np.reshape(ssh_all,(nt,ny*nx))
      print(ssh_all.shape)
      t1 = ds_ssh["time"].data[0].strftime()
      t2 = ds_ssh["time"].data[-1].strftime()
      pc = ds_pc.sel(time=slice(t1,t2)).sel(n=1)
```

(118, 10890)





8.3 Interactive session (30min)

Break out into groups of 2 or 3 and work through notebook 02-Correlation.ipynb.