# 2.0\_dcj\_explore\_all\_profiles

July 9, 2021

## 0.1 Exploratory clustering attempt: applying GMM to SO-CHIC data suite

In this exploratory notebook, I'll apply PCA and GMM to the SO-CHIC data suite that has been prepared by Shenjie Zhou (BAS). The results are reasonably distinct clusters, both in PC space and in lat-lon space. The i-metric highlights boundaries between the classes.

#### 0.1.1 Import modules

```
[1]: #import scikit-learn
     from sklearn import mixture
     from sklearn import preprocessing
     from sklearn.decomposition import PCA
     # import matplotlib
     import matplotlib.colors as colors
     import matplotlib.pyplot as plt
     import matplotlib.cm as cmx
     import matplotlib as mpl
     # pandas for just a couple things
     import pandas as pd
     # for label map
     import cartopy
     import cartopy.crs as ccrs
     import cartopy.feature as cfeature
     # pyxpcm, xarray, dask
     import numpy as np
     import xarray as xr
     import datetime as dt
     import random
     # import dask
     from dask.distributed import Client
     import dask
     # for 3D plotting
     from mpl_toolkits.mplot3d import Axes3D
     import matplotlib.cm as cm
     import seaborn as sns
```

#### Start Dask client

```
[2]: client = Client(n_workers=2, threads_per_worker=2, memory_limit='3GB')
client
```

[2]: <Client: 'tcp://127.0.0.1:60095' processes=2 threads=4, memory=6.00 GB>

#### 0.1.2 Subset parameters

These values indicate which lat-lon-depth range will be used in the clustering analysis. The first parameter, called "subset", is an arbitrary selection of profiles for quick plotting purposes. That parameter does not affect how many profiles are used in the clustering.

```
[3]: # name of file for saving output
fname = 'profiles_80W-80E_85-30S_100-900_labeled.nc'

# save the processed output as a NetCDF file?
saveOutput==True

# plotting subset
subset = range(1000,2000,1)

lon_min = -80
lon_max = 80
lat_min = -85
lat_max = -30

# depth range
zmin = 100.0
zmax = 900.0
```

#### 0.1.3 Import data

Shenjie Zhou (BAS) prepared these profiles using MITprof software, which produces a set of profiles that have been interpolated onto a specified set of depth levels. They are all in NetCDF format with standard names. I've decided to use xarray below for ease of use.

```
# select subset of data between 0-1000 dbar
     profiles = profiles.sel(iDEPTH=slice(zmin,zmax))
     # rename some of the variables
     profiles = profiles.rename({'iDEPTH':'depth',
                                  'iPROF': 'profile',
                                  'prof lon':'lon',
                                  'prof_lat':'lat'})
     # drop the "prof_depth" variable, because it's redundant
     profiles = profiles.drop_vars({'prof_depth'})
     # change lon and lat to coordinates
     profiles = profiles.set_coords({'lon','lat'})
     # only keep a subset of the data variables, as we don't need them all
     profiles = profiles.
      -get(['prof_date','prof_YYYYMDD','prof_HHMMSS','prof_T','prof_S'])
     # select lat/lon section using the subsetting parameters specified above
     profiles = profiles.where(profiles.lon<=lon_max,drop=True)</pre>
     profiles = profiles.where(profiles.lon>=lon_min,drop=True)
     profiles = profiles.where(profiles.lat<=lat_max,drop=True)</pre>
     profiles = profiles.where(profiles.lat>=lat_min,drop=True)
     # drop any remaining profiles with NaN values
     # the profiles with NaN values likely don't have measurements in the selected
     \rightarrow depth range
     profiles = profiles.dropna('profile')
     # exameine Dataset
     profiles
[4]: <xarray.Dataset>
     Dimensions:
                        (depth: 15, profile: 185612)
     Coordinates:
         lon
                        (profile) float64 dask.array<chunksize=(546,),
    meta=np.ndarray>
                        (profile) float64 dask.array<chunksize=(546,),
         lat
    meta=np.ndarray>
       * depth
                        (depth) float64 100.0 120.0 140.0 160.0 ... 640.0 730.0 820.0
```

profiles.coords['iDEPTH'] = profiles.prof\_depth[0,:].values

(profile) float64 dask.array<chunksize=(546,),

Dimensions without coordinates: profile

Data variables:

prof\_date
meta=np.ndarray>

```
prof_YYYYMMDD (profile) float64 dask.array<chunksize=(546,),
meta=np.ndarray>
    prof_HHMMSS (profile) float64 dask.array<chunksize=(546,),
meta=np.ndarray>
    prof_T (profile, depth) float64 dask.array<chunksize=(546, 15),
meta=np.ndarray>
    prof_S (profile, depth) float64 dask.array<chunksize=(546, 15),
meta=np.ndarray>
```

### 0.1.4 Time and date handling (currently broken)

```
[5]: # select MITprof values
     ntime_array_ymd = profiles.prof_YYYYMMDD.values
     ntime_array_hms = profiles.prof_HHMMSS.values
     # select size
     nsize = ntime_array_ymd.size
     # create array of zeros
     time = np.zeros((nsize,), dtype='datetime64[s]')
     # loop over all values, convert do datetime64[s]
     for i in range(nsize):
         # extract strings for ymd and hms
         s_ymd = str(ntime_array_ymd[i]).zfill(8)
         # hms doesn't matter and has errors.
         # set to noon and ignore it
         #s_hms = str(ntime_array_hms[i]).zfill(8)
         s_hms = '120000'
         # problem with 24:00:00
         #if s_hms=='240000.0':
             s_hms = '235959.0'
         # format into yyyy-mm-dd hh:mm:ss
         date_str_ymd = s_ymd[0:4] + '-' + s_ymd[4:6] + '-' + s_ymd[6:8]
         date_str_hms = s_hms[0:2] + ':' + s_hms[2:4] + ':' + s_hms[4:6]
         date_str = date_str_ymd + ' ' + date_str_hms
         # convert to datetime64 (the 's' stands for seconds)
         time[i] = np.datetime64(date_str,'s')
     # convert to pandas datetime (may not may not end up using this)
     time_pd = pd.to_datetime(time)
     # convert time array into a DataArray
     da = xr.DataArray(time, dims=['profile'])
     # add DataArray as new data variable to DataSet
     profiles['time'] = da
```

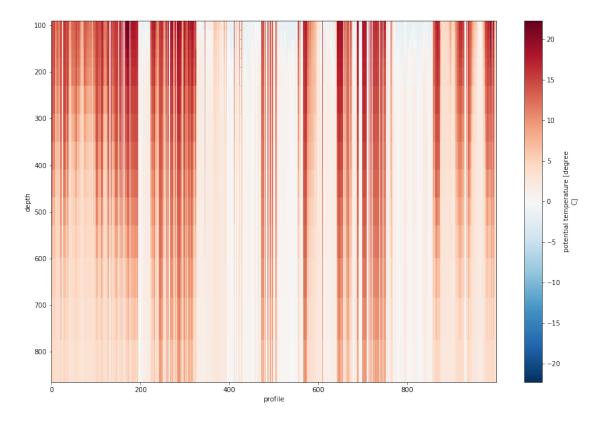
```
# set time as a coordinate
profiles = profiles.set_coords('time')
# examine Dataset again
#profiles
```

### 0.1.5 Plot subset of temperature profiles

This is an arbitrary subset of the profiles, just for data visualization purposes.

```
[6]: fig, ax = plt.subplots(figsize=(15,10))
profiles.prof_T[subset].plot(y='depth', yincrease=False)
```

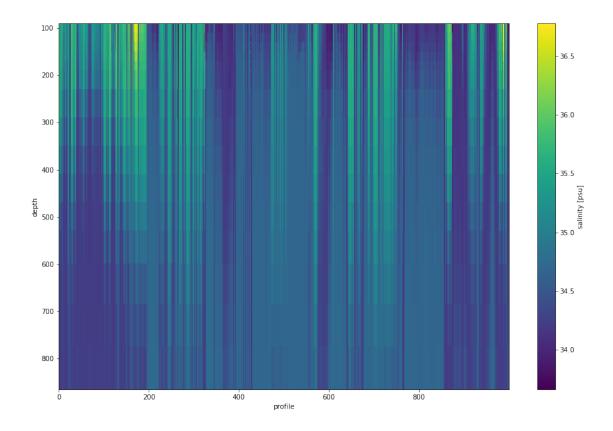
[6]: <matplotlib.collections.QuadMesh at 0x7fbc245b38d0>



### 0.1.6 Plot subset of salinity profiles

```
[7]: fig, ax = plt.subplots(figsize=(15,10))
profiles.prof_S[subset].plot(y='depth', yincrease=False)
```

[7]: <matplotlib.collections.QuadMesh at 0x7fbc23f7c1d0>

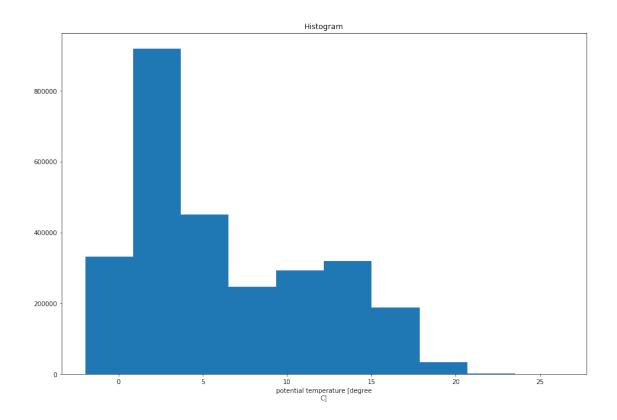


### 0.1.7 Plot histograms to get a sense of the data distribution

### First, plot the potential temperature histogram

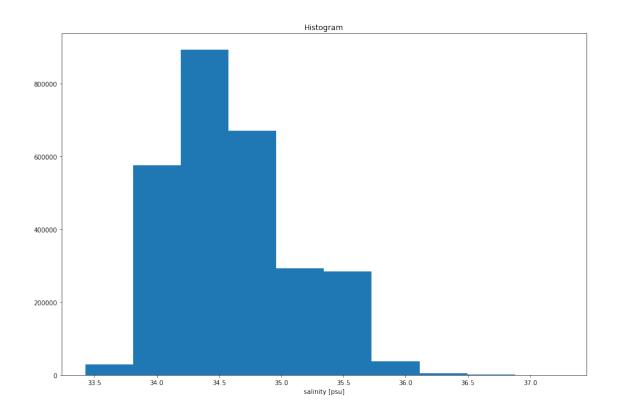
```
[8]: xr.plot.hist(profiles.prof_T,figsize=(15,10))
```

```
[8]: (array([3.31094e+05, 9.17855e+05, 4.50864e+05, 2.47243e+05, 2.92072e+05, 3.19577e+05, 1.88427e+05, 3.49050e+04, 2.08100e+03, 6.20000e+01]), array([-1.9605945, 0.8698903, 3.70037509, 6.53085988, 9.36134467, 12.19182947, 15.02231426, 17.85279905, 20.68328384, 23.51376864, 26.34425343]), <a list of 10 Patch objects>)
```



### Next, plot the salinity histogram

```
[9]: xr.plot.hist(profiles.prof_S,figsize=(15,10))
```



### 0.2 Clustering with GMM

### Preprocessing/scaling and dimensionality reduction via PCA

```
[10]: # scale salinity
X = profiles.prof_S
scaled_S = preprocessing.scale(X)
scaled_S.shape

# scale temperature
X = profiles.prof_T
scaled_T = preprocessing.scale(X)
scaled_T.shape

# concatenate
Xscaled = np.concatenate((scaled_T,scaled_S),axis=1)

# create PCA object
pca = PCA(n_components=3)

# fit PCA model
pca.fit(Xscaled)

# transform input data into PCA representation
```

```
Xpca = pca.transform(Xscaled)

# add PCA values to the profiles Dataset
PCA1 = xr.DataArray(Xpca[:,0],dims='profile')
PCA2 = xr.DataArray(Xpca[:,1],dims='profile')
PCA3 = xr.DataArray(Xpca[:,2],dims='profile')

# calculated total variance explained
total_variance_explained_ = np.sum(pca.explained_variance_ratio_)
total_variance_explained_
```

[10]: 0.9858584618007592

#### 0.2.1 Calculate BIC to inform selection of the number of clusters

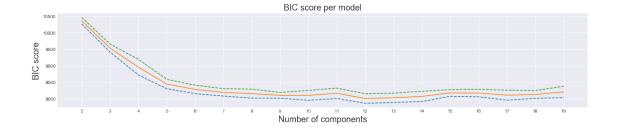
```
[11]: # select parameters
      max_N = 20 # the maximum number of classes to try
      max_bic_iter = 20 # the maximum number of iterations for BIC
      # for the BIC step, try using a subset of the profiles
      # you can change this 1000 value for different subsets
      \#Xpca\_for\_BIC = Xpca[::1000]
      # initialise, declare variables
      lowest_bic = np.infty
      bic_scores = np.zeros((2,max_bic_iter))
      # loop through the maximum number of classes, estimate BIC
      n_components_range = range(2, max_N)
      bic_iter_range = range(0,max_bic_iter)
      # iterate through all the covariance types (just 'full' for now)
      cv_types = ['full']
      for cv_type in cv_types:
          # iterate over all the possible numbers of components
          for n_components in n_components_range:
              bic one = []
              # repeat the BIC step for better statistics
              for bic_iter in bic_iter_range:
                  # select a new random subset
                  rows_id = random.sample(range(0, Xpca.shape[0]-1), 1000)
                  Xpca_for_BIC = Xpca[rows_id,:]
                  # fit a Gaussian mixture model
                  gmm = mixture.GaussianMixture(n_components=n_components,
                                                covariance_type=cv_type,
                                                random_state=42)
                  # uncomment for 'rapid' BIC fitting
```

```
gmm.fit(Xpca_for_BIC)
            # uncomment for 'full' BIC fitting
            #qmm.fit(Xpca)
            # append this BIC score to the list
            bic_one.append(gmm.bic(Xpca_for_BIC))
            Xpca_for_BIC = []
        # stack the bic scores into a single 2D structure
       bic_scores = np.vstack((bic_scores, np.asarray(bic_one)))
# the first two rows are not needed; they were only placeholders
bic_scores = bic_scores[2:,:]
# mean values for BIC
bic_mean = np.mean(bic_scores, axis=1)
# standard deviation for BIC
bic_std = np.std(bic_scores, axis=1)
# examine the mean bic values
#bic mean
```

#### 0.2.2 Plot the BIC scores

```
[12]: # plot the BIC scores
   plt.figure(figsize=(20, 8))
   plt.style.use('seaborn-darkgrid')
   spl = plt.subplot(2, 1, 1)
   plt.plot(n_components_range, bic_mean-bic_std, '--')
   plt.plot(n_components_range, bic_mean, '-')
   plt.plot(n_components_range, bic_mean+bic_std, '--')
   plt.xticks(n_components_range)
   #plt.ylim([bic.min() * 1.01 - .01 * bic.max(), bic.max()])
   plt.title('BIC score per model', fontsize=18)
   spl.set_xlabel('Number of components',fontsize=18)
   spl.set_ylabel('BIC score',fontsize=18)
   #plt.show()
```

[12]: Text(0, 0.5, 'BIC score')



As with many other oceanographic applications, there is not a clear minimum. Instead, the BIC curve flattens. We can opt for a smaller number of classes for ease of interpretation. Choosing a value of 5 is not quite the minimum, but after 5 the decrease in BIC is much more gradual, so it's still a reasonable choice.

#### 0.2.3 Select the actual GMM to be used in the analysis

```
[13]: # set variables
      n_components_selected = 5
      # establish qmm
      best_gmm = mixture.GaussianMixture(n_components=n_components_selected,
                                          covariance_type='full',
                                          random_state=42)
      # fit this GMM
      best_gmm.fit(Xpca)
      # check to make sure that n comp is as expected
      n_comp = gmm.n_components
      # select colormap
      colormap = plt.get_cmap('tab10', n_comp)
      # assign class labels ("predict" the class using the selected GMM)
      labels = best_gmm.predict(Xpca)
      # find posterior probabilities (the probabilities of belonging to each class)
      posterior_probs = best_gmm.predict_proba(Xpca)
      # maximum posterior probability (the class is assigned based on this value)
      max_posterior_probs = np.max(posterior_probs,axis=1)
      # put the labels and maximum posterior probabilities back in original dataframe
      #df.insert(3, 'label', labels, True)
      #df.insert(4, 'max posterior prob', max_posterior_probs, True)
```

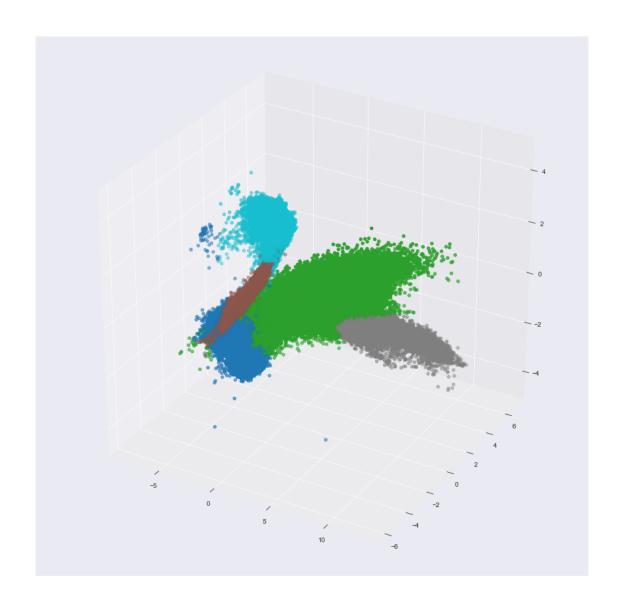
### 0.2.4 Visualise clustering in PC space

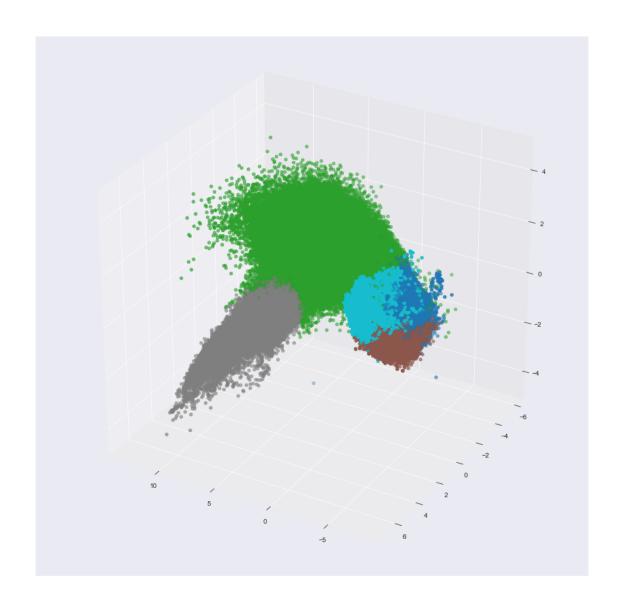
```
[14]: # initial view
fig = plt.figure(figsize=(15,15))
ax = fig.add_subplot(projection='3d')
ax.scatter(PCA1.values, PCA2.values, PCA3.values, c=labels, cmap=cm.tab10)

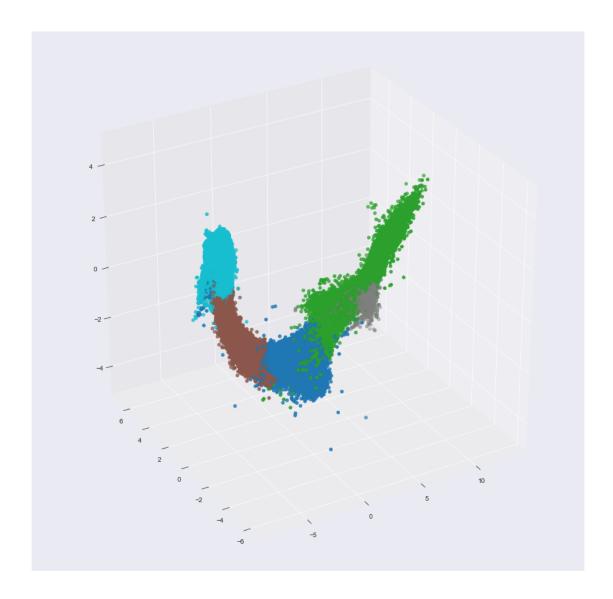
# new view
fig = plt.figure(figsize=(15,15))
ax = fig.add_subplot(projection='3d')
ax.view_init(30, 120)
ax.scatter(PCA1.values, PCA2.values, PCA3.values, c=labels, cmap=cm.tab10)

# new view
fig = plt.figure(figsize=(15,15))
ax = fig.add_subplot(projection='3d')
ax.view_init(30, 240)
ax.scatter(PCA1.values, PCA2.values, PCA3.values, c=labels, cmap=cm.tab10)
```

[14]: <mpl\_toolkits.mplot3d.art3d.Path3DCollection at 0x7fbc12e5edd0>







The classes look reasonably distinct in PCA space. There are some subtle oddities that might be better captured by a different clustering method; we'll explore later.

#### 0.2.5 Calculate class means and standard deviations

```
[15]: # create grouped object using the labels
grouped = profiles.groupby("label")

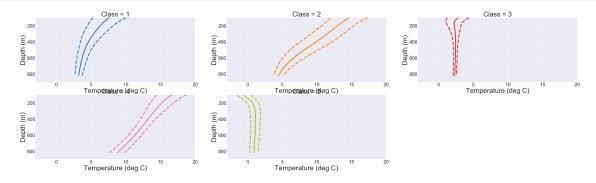
# class means and standard deviations
class_means = grouped.mean()
class_stds = grouped.std()

# visualize grouped dataset
#class_means
```

#### 0.2.6 Plot vertical T and S structure of the classes

```
[16]: cNorm = colors.Normalize(vmin=0, vmax=n_components_selected)
      scalarMap = cmx.ScalarMappable(norm=cNorm, cmap=colormap)
      # initialize the figure
      plt.figure(figsize=(60, 60))
      plt.style.use('seaborn-darkgrid')
      #palette = cmx.Paired(np.linspace(0,1,n_comp))
      # vertical coordinate
      z = profiles.depth.values
      # iterate over groups
      num = 0
      for nrow in range(0,n_components_selected):
          num += 1
          colorVal = scalarMap.to_rgba(nrow)
          # extract means
          mean_T = class_means.prof_T[nrow,:].values
          # extract stdevs
          std_T = class_stds.prof_T[nrow,:].values
          # select subplot
          ax = plt.subplot(np.ceil(n_comp/3),3,num)
          plt.plot(mean_T, z, marker='', linestyle='solid', color=colorVal,_
       \rightarrowlinewidth=6.0, alpha=0.9)
          plt.plot(mean_T+std_T, z, marker='', linestyle='dashed', color=colorVal,u
       \rightarrowlinewidth=6.0, alpha=0.9)
          plt.plot(mean_T-std_T, z, marker='', linestyle='dashed', color=colorVal,_
       \rightarrowlinewidth=6.0, alpha=0.9)
          # custom grid and axes
          plt.ylim([zmin,zmax])
          plt.xlim([-3, 20])
         #text box
          fs = 42 \# font size
          plt.xlabel('Temperature (deg C)', fontsize=fs)
          plt.ylabel('Depth (m)', fontsize=fs)
          plt.title('Class = ' + str(num), fontsize=fs)
          # font and axis stuff
          plt.gca().invert_yaxis()
          ax.tick_params(axis='x', labelsize=30)
```

#### ax.tick\_params(axis='y', labelsize=30)

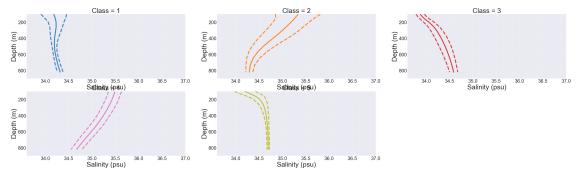


```
[17]: cNorm = colors.Normalize(vmin=0, vmax=n_components_selected)
      scalarMap = cmx.ScalarMappable(norm=cNorm, cmap=colormap)
      # initialize the figure
      plt.figure(figsize=(60, 60))
      plt.style.use('seaborn-darkgrid')
      #palette = cmx.Paired(np.linspace(0,1,n_comp))
      # vertical coordinate
      z = profiles.depth.values
      # iterate over groups
      num = 0
      for nrow in range(0,n_components_selected):
          num += 1
          colorVal = scalarMap.to rgba(nrow)
          # extract means
          mean_S = class_means.prof_S[nrow,:].values
          # extract stdevs
          std_S = class_stds.prof_S[nrow,:].values
          # select subplot
          ax = plt.subplot(np.ceil(n_comp/3),3,num)
          plt.plot(mean_S, z, marker='', linestyle='solid', color=colorVal,_
       \rightarrowlinewidth=6.0, alpha=0.9)
          plt.plot(mean_S+std_S, z, marker='', linestyle='dashed', color=colorVal,_
       \rightarrowlinewidth=6.0, alpha=0.9)
          plt.plot(mean_S-std_S, z, marker='', linestyle='dashed', color=colorVal,
       \rightarrowlinewidth=6.0, alpha=0.9)
          # custom grid and axes
```

```
plt.ylim([zmin, zmax])
plt.xlim([33.6, 37.0])

#text box
fs = 42 # font size
plt.xlabel('Salinity (psu)', fontsize=fs)
plt.ylabel('Depth (m)', fontsize=fs)
plt.title('Class = ' + str(num), fontsize=fs)

# font and axis stuff
plt.gca().invert_yaxis()
ax.tick_params(axis='x', labelsize=30)
ax.tick_params(axis='y', labelsize=30)
```



## 0.2.7 Label map of the classes

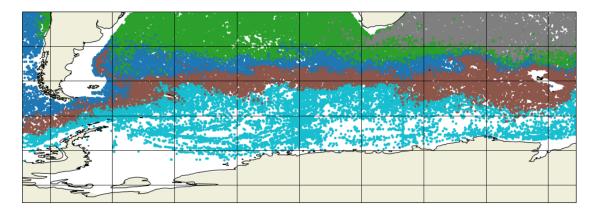
```
[18]: # extract values as new DataArrays
df1D = profiles.isel(depth=0)
da_lon = df1D.lon
da_lat = df1D.lat
da_label = df1D.label

# extract values
lons = da_lon.values
lats = da_lat.values
clabels = da_label.values

# size of random sample
random_sample_size = int(np.ceil(0.30*df1D.profile.size))

# random sample for plotting
rows_id = random.sample(range(0,clabels.size-1), random_sample_size)
lons_random_sample = lons[rows_id]
lats_random_sample = lats[rows_id]
```

[18]: <cartopy.mpl.feature\_artist.FeatureArtist at 0x7fbc283dd190>



Note the emergence of the near-Antarctic class. One idea would be to take only those profiles and re-apply a clustering algorithm to them in order to capture finer-scale structure.

### 0.2.8 Calculate the i-metric

https://os.copernicus.org/preprints/os-2021-40/

```
[19]: # function to calculate the i_metric, label, and runner-up label

def get_i_metric(posterior_prob_list):
    sorted_posterior_list = sorted(posterior_prob_list)
    ic_metric = 1 - (sorted_posterior_list[-1] - sorted_posterior_list[-2])
    runner_up_label = posterior_prob_list.index(sorted_posterior_list[-2])
    label = posterior_prob_list.index(sorted_posterior_list[-1])
    return ic_metric, np.array([label, runner_up_label]) # np.sort()
```

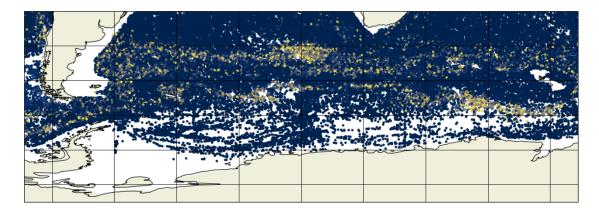
### Loop through profiles (this may take a few minutes)

```
[20]: # declare variables
      i_metric = np.zeros(df1D.profile.size)
      a b = np.zeros((df1D.profile.size,2))
      # loop through the profiles, calculate the i_metric for each one
      for i in range(df1D.profile.size):
            i_metric[i], a_b[i,:] = get_i_metric(df1D.posteriors[i, :].values.
       →tolist())
     distributed.comm.tcp - WARNING - Closing dangling stream in <TCP
     local=tcp://127.0.0.1:60178 remote=tcp://127.0.0.1:60095>
     distributed.comm.tcp - WARNING - Closing dangling stream in <TCP
     local=tcp://127.0.0.1:60181 remote=tcp://127.0.0.1:60095>
     distributed.comm.tcp - WARNING - Closing dangling stream in <TCP
     local=tcp://127.0.0.1:60246 remote=tcp://127.0.0.1:60095>
[21]: # convert i metric numpy array to xarray DataArray
      i_metric = xr.DataArray(i_metric, coords=[profiles.profile], dims='profile')
      # add i_metric DataArray to Dataset
      df1D = df1D.assign({'i_metric':i_metric})
```

#### 0.2.9 Plot i-metric map

```
[22]: # extract values as new DataArrays
      da lon = df1D.lon
      da_lat = df1D.lat
      da_i_metric = df1D.i_metric
      # extract values
      lons = da_lon.values
      lats = da_lat.values
      c = da_i_metric.values
      # random sample for plotting
      rows_id = random.sample(range(0,c.size-1), random_sample_size)
      lons random sample = lons[rows id]
      lats_random_sample = lats[rows_id]
      clabels_random_sample = c[rows_id]
      #colormap with Historical data
      plt.figure(figsize=(17, 13))
      ax = plt.axes(projection=ccrs.PlateCarree())
      ax.set_extent([lon_min, lon_max, lat_min, lat_max], ccrs.PlateCarree())
      CS = plt.scatter(lons_random_sample-360,
                       lats_random_sample,
```

### [22]: <cartopy.mpl.feature\_artist.FeatureArtist at 0x7fbc28ba7ad0>



Darker shading indicates that the profile is *less* likely to be near a boundary between classes. Ligher shading indicates that the profile is *more* likely to be near a boundary between classes.

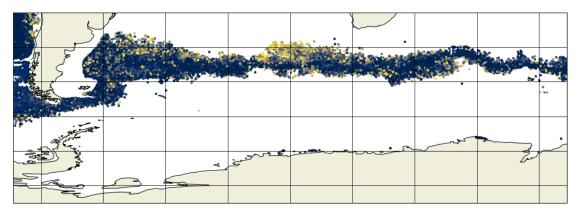
#### 0.2.10 Plot i-metric by class

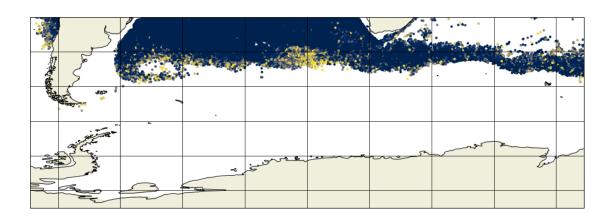
```
[23]: # extract values as new DataArrays
da_lon = df1D.lon
da_lat = df1D.lat
da_i_metric = df1D.i_metric

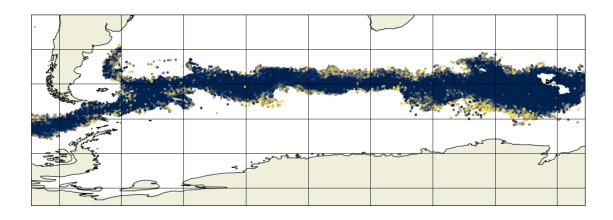
# extract values
lons = da_lon.values
lats = da_lat.values
c = da_i_metric.values

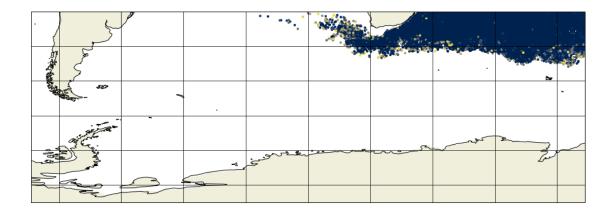
for iclass in range(n_components_selected):

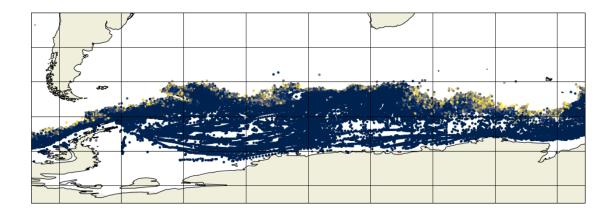
# random sample for plotting
lons_random_sample = lons[labels==iclass]
lats_random_sample = lats[labels==iclass]
clabels_random_sample = c[labels==iclass]
```











This view makes it easier to see that the classes are reasonably spatially distinct, with "fuzzy" boundaries in the expected locations.

# Save this dataset for further processing

```
[30]: if saveOutput==True:
    profiles.chunk().compute().to_netcdf(path='processed_data/' + fname,
    →engine='netcdf4')
```