# 3.0_dcj_explore_antarctic_profiles

July 9, 2021

# 1 Examine Antarctic profiles

Here, we take the output of the "whole domain" classification notebook (2.0) and look for classes within the Antarctic group of profiles.

## 1.1 Initial setup

### 1.1.1 Load 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
```

### 1.1.2 Start Dask client

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

[2]:
```
<Client: 'tcp://127.0.0.1:61952' processes=2 threads=4, memory=6.00 GB>
```

### 1.1.3 Select subsetting parameters

Check for consistency with the input file

[3]:
```
# 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
```

### 1.1.4 Import data

[4]:
```
profiles = xr.open_dataset('processed_data/
 ↪profiles_80W-80E_85-30S_100-900_labeled.nc')
profiles
```

[4]:
```
<xarray.Dataset>
Dimensions:        (CLASS: 5, depth: 15, profile: 185612)
Coordinates:
  * profile        (profile) int64 0 1 2 3 4 … 185608 185609 185610 185611
    lon            (profile) float64 …
    lat            (profile) float64 …
  * depth          (depth) float64 100.0 120.0 140.0 160.0 … 640.0 730.0 820.0
    time           (profile) datetime64[ns] …
  * CLASS          (CLASS) int64 0 1 2 3 4
Data variables:
    prof_date      (profile) float64 …
    prof_YYYYMMDD  (profile) float64 …
    prof_HHMMSS    (profile) float64 …
    prof_T         (profile, depth) float64 …
    prof_S         (profile, depth) float64 …
    label          (profile) int64 …
    posteriors     (profile, CLASS) float64 …
```

### 1.1.5 Select Antarctic profiles

Check for consistency with notebook 2.0

[5]:
```
profiles_antarctic = profiles.where(profiles.label==int(4)).dropna('profile')
profiles_antarctic
```

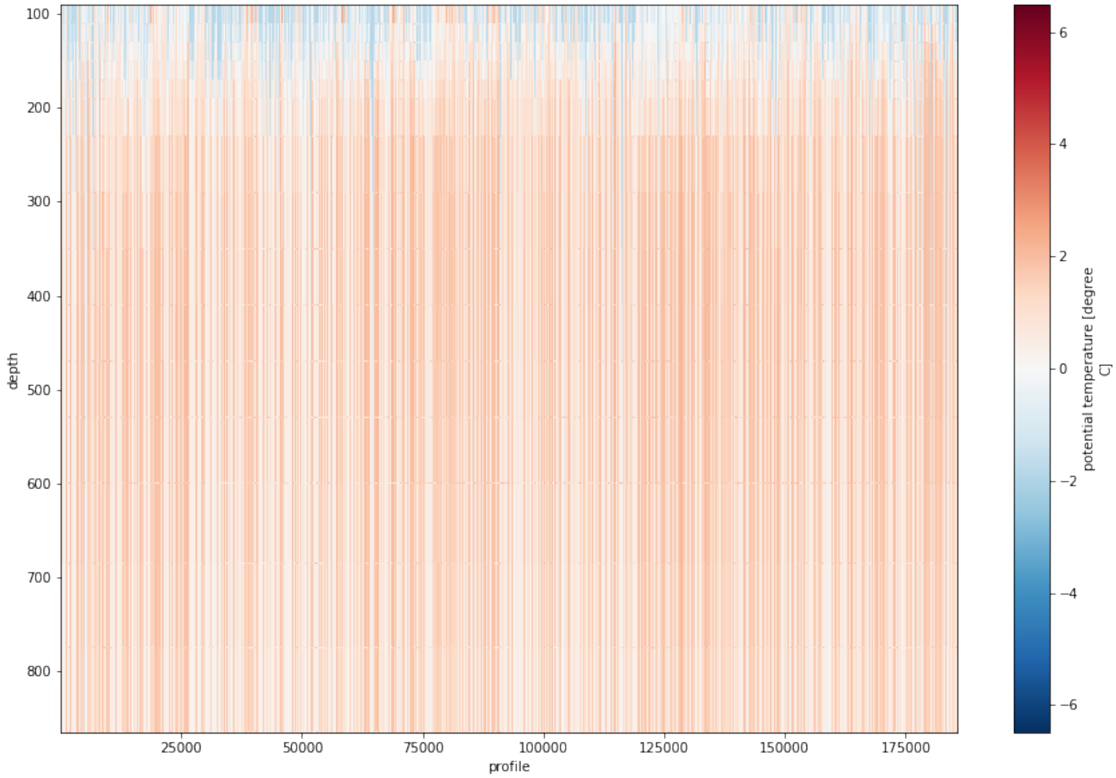
[5]:
```
<xarray.Dataset>
Dimensions:         (CLASS: 5, depth: 15, profile: 35709)
Coordinates:
  * profile         (profile) int64 14 15 16 17 … 185602 185603 185609 185610
    lon             (profile) float64 -26.44 -22.37 -17.38 … 51.89 64.79 35.28
    lat             (profile) float64 -55.98 -56.81 -57.51 … -58.72 -60.98
  * depth           (depth) float64 100.0 120.0 140.0 160.0 … 640.0 730.0 820.0
    time            (profile) datetime64[ns] 1973-01-11T12:00:00 … 2017-08-2…
  * CLASS           (CLASS) int64 0 1 2 3 4
Data variables:
    prof_date       (profile) float64 7.206e+05 7.206e+05 … 7.369e+05 7.369e+05
    prof_YYYYMMDD   (profile) float64 1.973e+07 1.973e+07 … 2.017e+07 2.017e+07
    prof_HHMMSS     (profile) float64 1.2e+05 1.2e+05 1.2e+05 … 8.4e+04 1.4e+04
    prof_T          (profile, depth) float64 -1.228 -0.9877 … 1.167 1.067
    prof_S          (profile, depth) float64 34.2 34.25 34.33 … 34.73 34.72
    label           (profile) float64 4.0 4.0 4.0 4.0 4.0 … 4.0 4.0 4.0 4.0 4.0
    posteriors      (profile, CLASS) float64 1.969e-45 3.878e-168 … 1.0
```

## 1.2 Data visualization and exploration

### 1.2.1 Plot temperature profiles

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

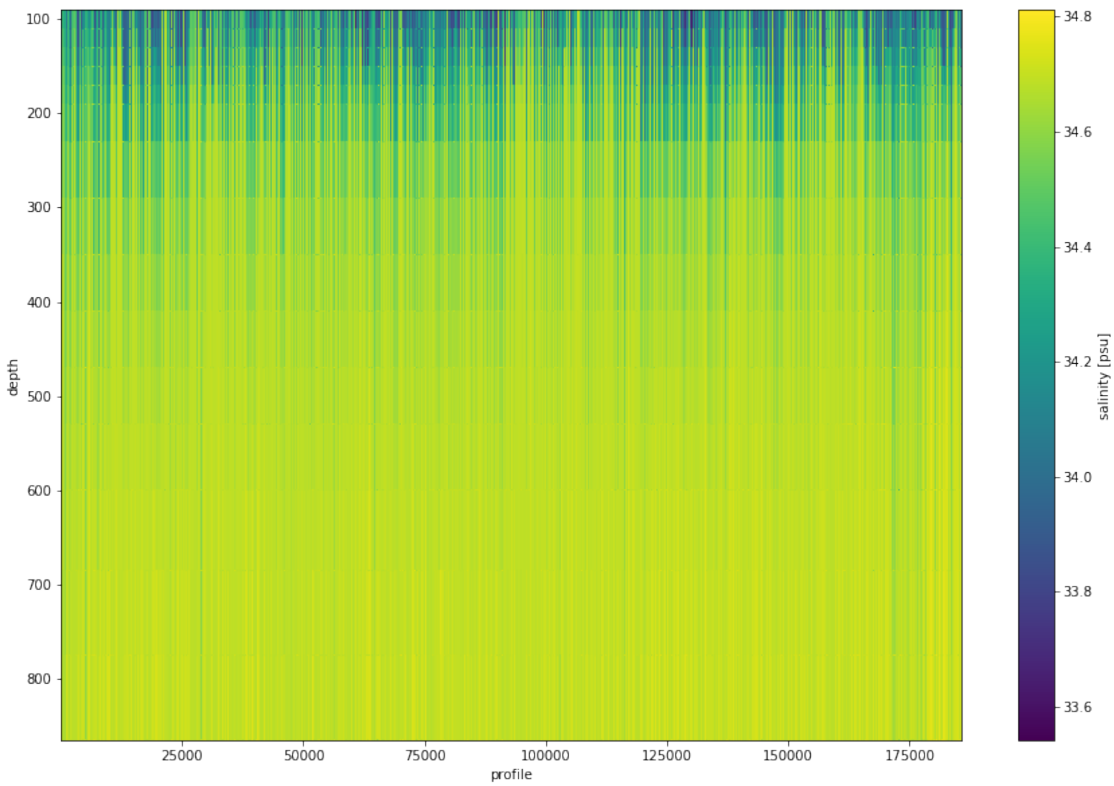
[6]:
```
<matplotlib.collections.QuadMesh at 0x7fa89bc44690>
```




### 1.2.2 Plot salinity profiles

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

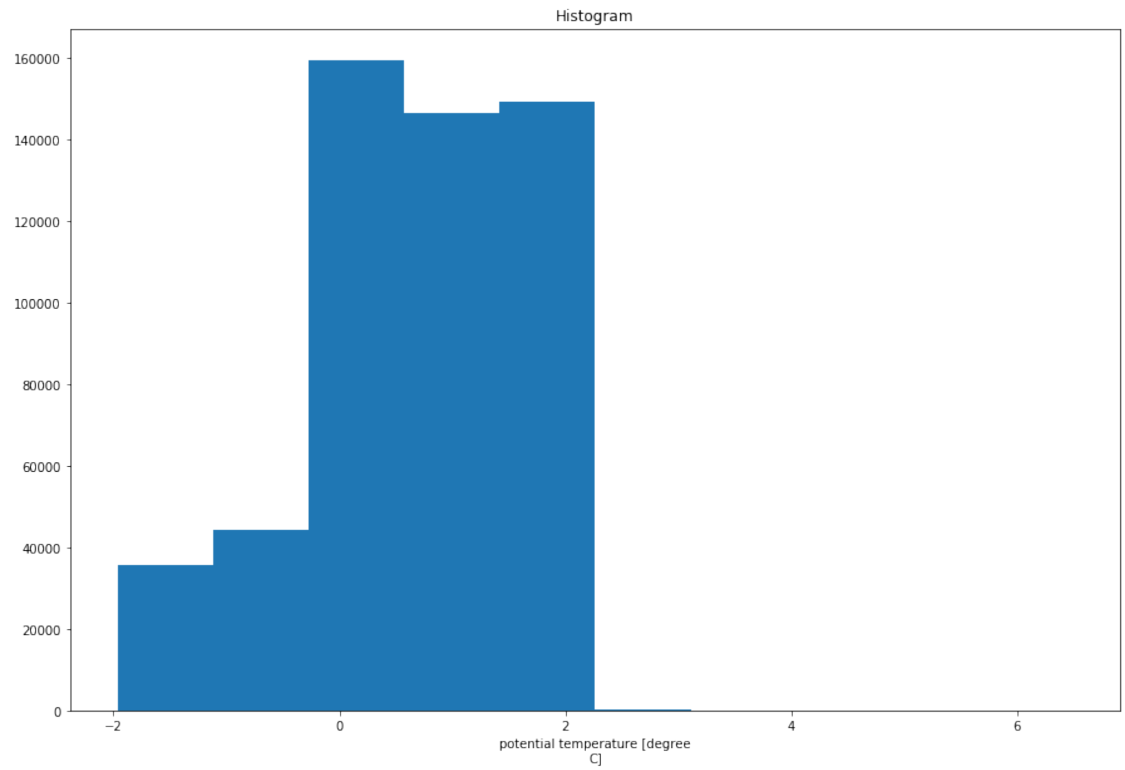
[7]: <matplotlib.collections.QuadMesh at 0x7fa89d0e1310>




### 1.2.3 Plot temperature histogram

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

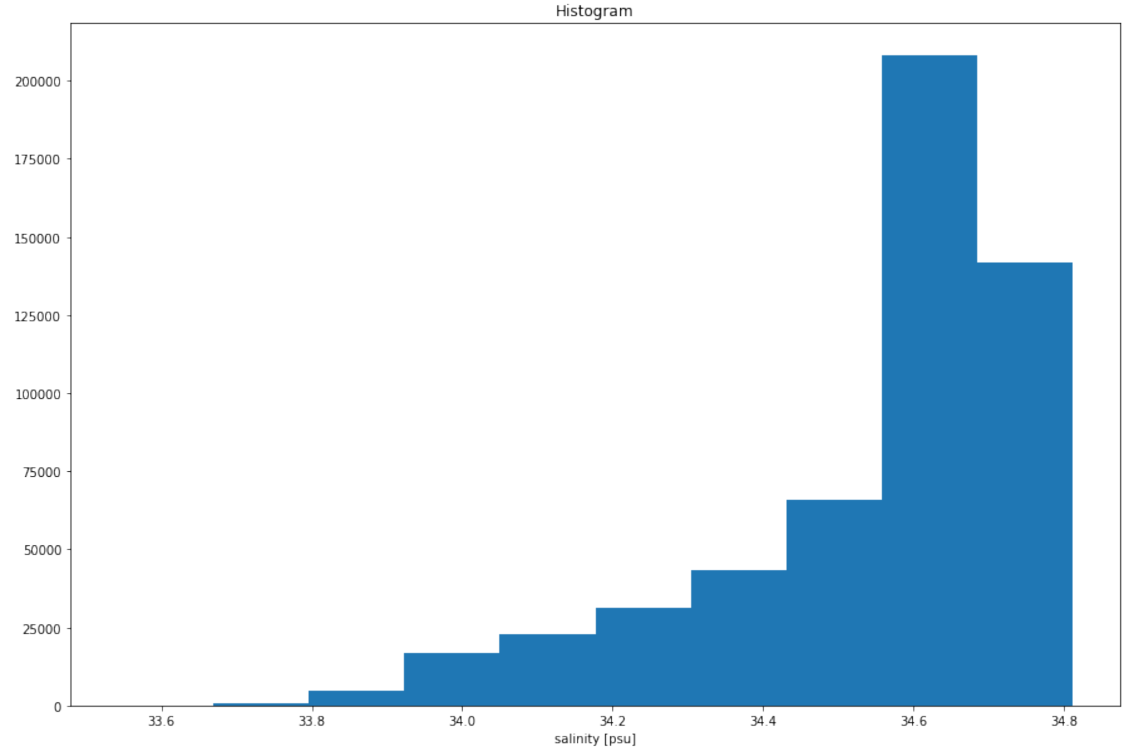
[8]:
```
(array([3.57350e+04, 4.43950e+04, 1.59234e+05, 1.46523e+05, 1.49330e+05,
        4.02000e+02, 1.00000e+01, 4.00000e+00, 0.00000e+00, 2.00000e+00]),
 array([-1.9605945 , -1.11570456, -0.27081462,  0.57407532,  1.41896526,
         2.2638552 ,  3.10874514,  3.95363508,  4.79852502,  5.64341496,
         6.4883049 ]),
 <a list of 10 Patch objects>)
```




### 1.2.4 Plot salinity histogram

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

[9]:
```
(array([5.70000e+01, 8.04000e+02, 4.81400e+03, 1.67650e+04, 2.29790e+04,
        3.11940e+04, 4.32740e+04, 6.58410e+04, 2.08047e+05, 1.41860e+05]),
 array([33.54245915, 33.66937578, 33.7962924 , 33.92320903, 34.05012566,
        34.17704228, 34.30395891, 34.43087553, 34.55779216, 34.68470879,
        34.81162541]),
 <a list of 10 Patch objects>)
```




#### 1.2.5 Apply unsupervised classification method

#### 1.2.6 Preprocessing, scaling, and dimensionality reduction

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

# scale temperature
X = profiles_antarctic.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=8)

# 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]: 0.9848536571195076

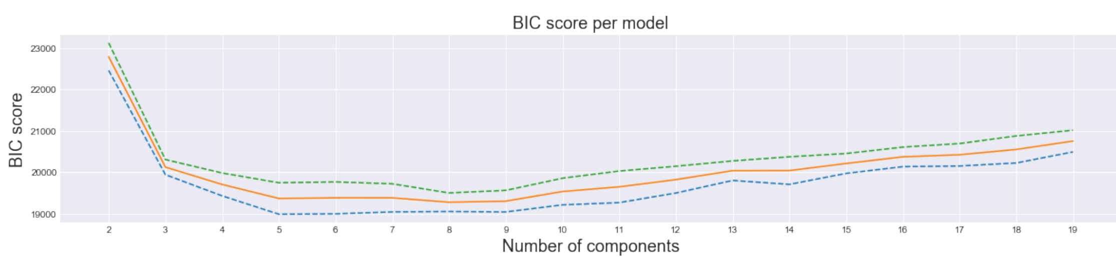
### 1.2.7 Use BIC to inform number of classes

[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
                #gmm.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
```

[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')



Interestingly, there is a minimum between 5-9. We'll opt for the smaller number for ease of interpretation.

#### 1.2.8 Apply selected GMM

[13]:
```
# set variables
n_components_selected = 5

# establish gmm
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)

# print out best_gmm parameters
#posterior_probs.shape

# convert labels into xarray format
xlabels = xr.DataArray(labels, coords=[profiles_antarctic.profile],␣
↪dims='profile')

# convert posterior probabilities into xarray format
gmm_classes = [b for b in range(0,n_components_selected,1)]
xprobs = xr.DataArray(posterior_probs,
```

```
                      coords=[profiles_antarctic.profile, gmm_classes],
                      dims=['profile', 'CLASS'])

# add label DataArray to Dataset
profiles_antarctic = profiles_antarctic.assign({'label':xlabels})
profiles_antarctic = profiles_antarctic.assign({'posteriors':xprobs})
```

### 1.3 Plot GMM results

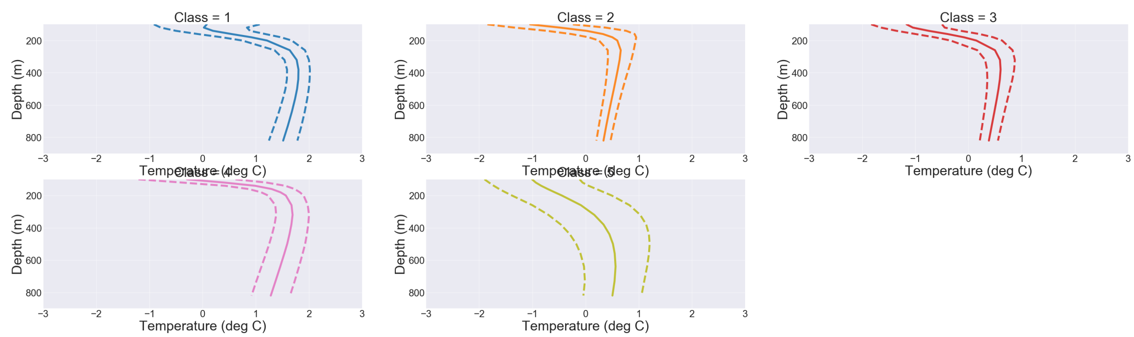
#### 1.3.1 Calculate class means

[14]:
```
# create grouped object using the labels
grouped = profiles_antarctic.groupby("label")

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

# visualize grouped dataset
#class_means
```

#### 1.3.2 Plot vertical structure of class means: temperature

[15]:
```
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
```

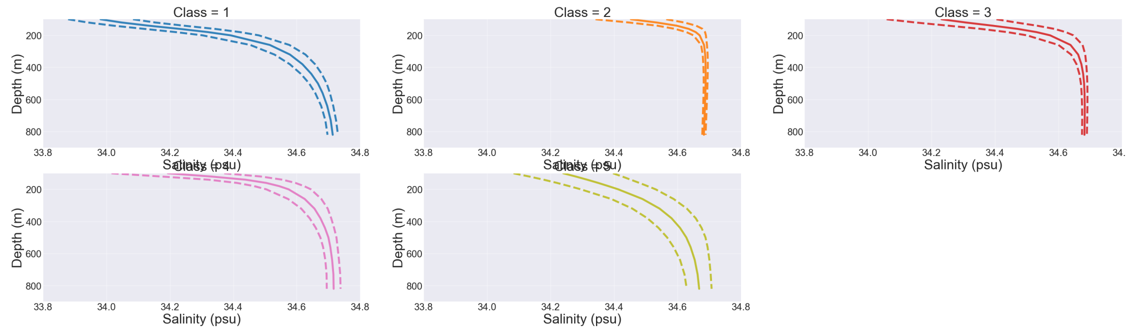
```
    ax = plt.subplot(np.ceil(n_comp/3),3,num)
    plt.plot(mean_T, z, marker='', linestyle='solid', color=colorVal,␣
↪linewidth=6.0, alpha=0.9)
    plt.plot(mean_T+std_T, z, marker='', linestyle='dashed', color=colorVal,␣
↪linewidth=6.0, alpha=0.9)
    plt.plot(mean_T-std_T, z, marker='', linestyle='dashed', color=colorVal,␣
↪linewidth=6.0, alpha=0.9)

    # custom grid and axes
    plt.ylim([zmin,zmax])
    plt.xlim([-3, 3])

   #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)
```




### 1.3.3 Plot vertical structure of class means: salinity

[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_antarctic.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,␣
↪linewidth=6.0, alpha=0.9)
    plt.plot(mean_S+std_S, z, marker='', linestyle='dashed', color=colorVal,␣
↪linewidth=6.0, alpha=0.9)
    plt.plot(mean_S-std_S, z, marker='', linestyle='dashed', color=colorVal,␣
↪linewidth=6.0, alpha=0.9)

    # custom grid and axes
    plt.ylim([zmin, zmax])
    plt.xlim([33.8, 34.8])

   #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)
```

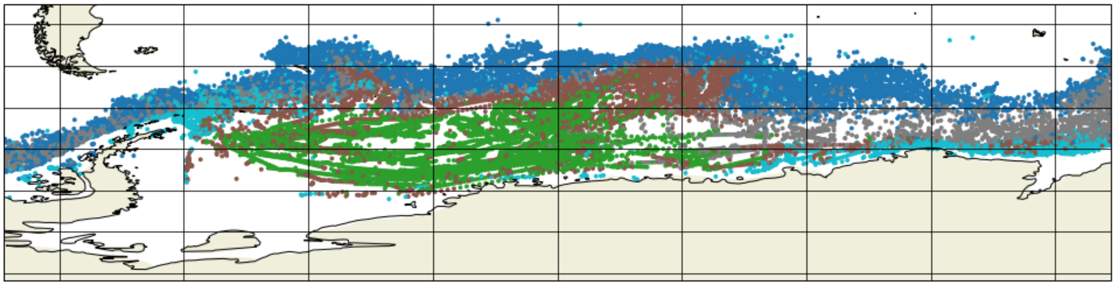



### 1.3.4 Plot label map

[17]:
```
# extract values as new DataArrays
df1D = profiles_antarctic.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 (all profiles by now)
random_sample_size = int(np.ceil(0.99*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]
clabels_random_sample = clabels[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, -45], ccrs.PlateCarree())
CS = plt.scatter(lons_random_sample-360,
                 lats_random_sample,
                 c=clabels_random_sample,
                 marker='o',
                 cmap= colormap,
                 s=8.0,
                 transform=ccrs.Geodetic(),
                 )
ax.coastlines(resolution='50m')
```

```
ax.gridlines(color='black')
ax.add_feature(cartopy.feature.LAND)
```

[17]: <cartopy.mpl.feature_artist.FeatureArtist at 0x7fa8a51299d0>



## 1.4 Calculate i-metric

### 1.4.1 Define function

[18]:
```
# 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()
```

### 1.4.2 Iterate through profiles, calculate i-metric

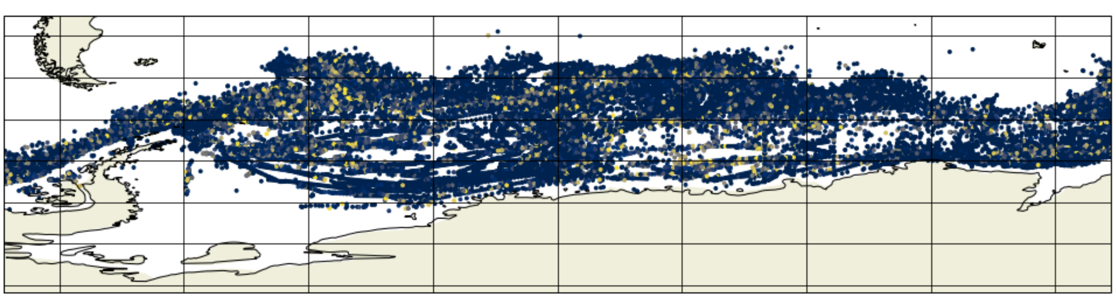
[19]:
```
# declare variables
i_metric = np.zeros(df1D.profile.size)
a_b = np.zeros((df1D.profile.size,2))

# 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())

# convert i_metric numpy array to xarray DataArray
i_metric = xr.DataArray(i_metric, coords=[profiles_antarctic.profile],␣
 ↪dims='profile')

# add i_metric DataArray to Dataset
df1D = df1D.assign({'i_metric':i_metric})
```

### 1.4.3 Plot i-metric by class

[20]:
```
# 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, -45], ccrs.PlateCarree())
CS = plt.scatter(lons_random_sample-360,
                 lats_random_sample,
                 c=clabels_random_sample,
                 marker='o',
                 cmap= plt.get_cmap('cividis'),
                 s=8.0,
                 transform=ccrs.Geodetic(),
                 )
ax.coastlines(resolution='50m')
ax.gridlines(color='black')
ax.add_feature(cartopy.feature.LAND)
```

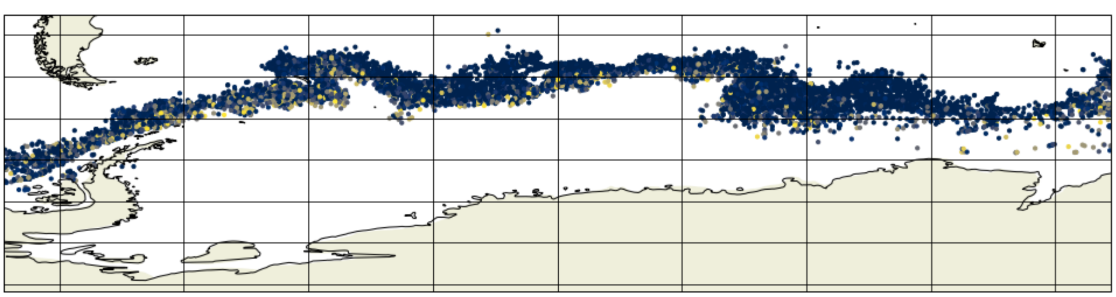
```
distributed.comm.tcp - WARNING - Closing dangling stream in <TCP
local=tcp://127.0.0.1:62038 remote=tcp://127.0.0.1:61952>
```

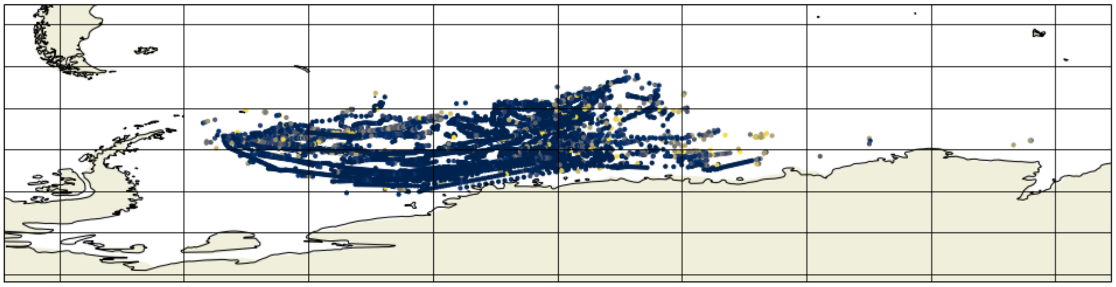
[20]:
```
<cartopy.mpl.feature_artist.FeatureArtist at 0x7fa8a0ea1bd0>
```

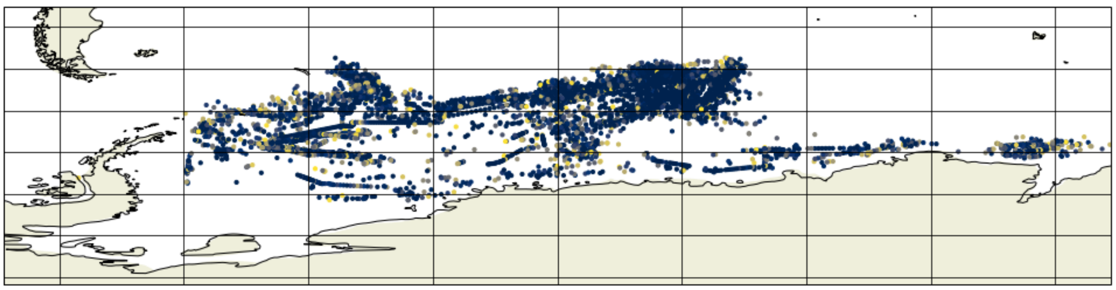


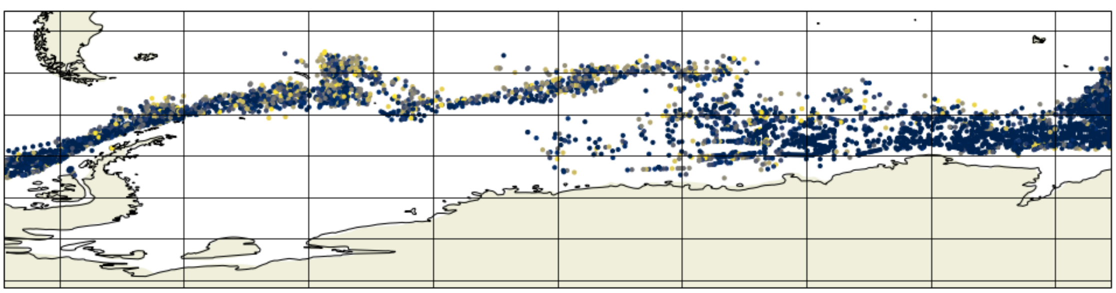
[21]:

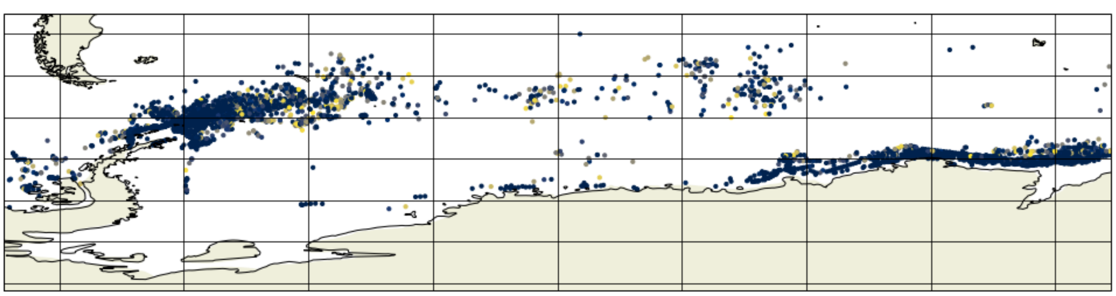
```
# extract values as new DataArrays
da_lon = df1D.lon
da_lat = df1D.lat
da_i_metric = df1D.i_metric

# 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]

    #colormap with Historical data
    plt.figure(figsize=(17, 13))
    ax = plt.axes(projection=ccrs.PlateCarree())
    ax.set_extent([-80, 80, -85, -45], ccrs.PlateCarree())
    CS = plt.scatter(lons_random_sample-360,
                     lats_random_sample,
                     c=clabels_random_sample,
                     marker='o',
                     cmap= plt.get_cmap('cividis'),
                     s=10.0,
                     transform=ccrs.Geodetic(),
                     )
    ax.coastlines(resolution='50m')
    ax.gridlines(color='black')
    ax.add_feature(cartopy.feature.LAND)
```











Notably, we do seem to have what could be called a “Weddell Gyre class”, sort of. It’s roughly in the right place; in the core of where the gyre circulation is expected to be.

Caveats: this is sort of a climatological picture, so to speak. It will be biased towards more recent times, where the density of observations is higher.