Temperature Profile Classification - 2 Class system

GMM classification of Southern Ocean Argo float temperature profile data. This notebook looks at automatic generation for PCA N values, with 2 classes.

Dask import

Choices for data

In [1]:

```
#Experiment data for analysis
dataVariableId = 'thetao'
dataExperimentId = 'historical'
dataSourceId = 'UKESM1-0-LL'
dataInstitutionId = 'MOHC'
approvedIds = ["r1i1p1f2", "r2i1p1f2", "r3i1p1f2"] #insert start of approved member_ids

#File imports
maskName = "OceanMaskVolcello"
modelName = "GMM_UK_2Class_R1"

#Data definitions
startDate = '1980-01'
endDate = '2009-12'
timeRange = slice(startDate, endDate)
levSel = slice(0, 2000) #Selected levels to be investigated
maxLat = -30 #Selected latitude to be investigated
runIdSel = 0

#Custom GMM variables
saveModel = True #if true saves a model under model name. To work createModel has to be en
pcaThreshold = 0.98
pcaNControl = 0 #set to int value to select, if set to 0 pcaThreshold is used to automatic
firstBicLoopControl = 10 #number of times bic value is calculated for each number of class
cvType = "full"
```

Libaries and Modules

Importing the necessary libaries and modules for the notebook.

In [2]:

```
#Import cell
import calendar
#import cartopy.crs as ccrs
#import cartopy.feature as cfeature
import dask.dataframe as dd
import fsspec
import matplotlib.dates as mdates
import matplotlib as mpl ###
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import pickle as pk
import matplotlib.ticker as ticker
import xarray as xr
```

```
import zarr

from dask import config
from dask import delayed
from joblib import dump, load
from matplotlib.pyplot import cm
from sklearn import mixture
from sklearn.decomposition import PCA
from sklearn import preprocessing

config.set(**{'array.slicing.split_large_chunks': True})
print("Imports complete")
```

```
Imports complete
```

Importing data sets

Importing the data for the models.

Import sample data set and corresponding time/geo data

In [3]:

```
#Importing UK ESM data cell

df = pd.read_csv('https://storage.googleapis.com/cmip6/cmip6-zarr-consolidated-stores.csv'
dfFilt = df[df.variable_id.eq(dataVariableId) & df.experiment_id.eq(dataExperimentId) & df

memberArr = np.empty(shape=(0), dtype=bool)
for i in dfFilt["member_id"]:
    rowSel = i[:] in approvedIds #adapt i[:] to match size of approvedIds
    memberArr = np.append(memberArr, rowSel)

memberSer = pd.Series(memberArr, name='bools')
dfFilt = dfFilt[memberSer.values]
dfFilt = dfFilt[:1]

fileSetList = []
for i in range(len(dfFilt)):
    zstore = dfFilt.zstore.values[i]
    mapper = fsspec.get_mapper(zstore)
    fileRaw = xr.open_zarr(mapper, consolidated=True)
    fileSetList.append(fileRaw)
fileCount = len(fileSetList)
if fileCount:
    print(str(fileCount)+" "+dataSourceId+" data sets opened")
else:
    print("No UKESM data sets opened")

for i in range(fileCount): #Formatting dates into np.datetime64 format
    startDateIterate = np.datetime64(fileSetList[i]['time'].values[0],'M')
    endDateIterate = np.datetime64(fileSetList[i]['time'].values[-1],'M') + np.timedelta64
    fileSetList[i]['time']=('time', np.arange(startDateIterate, endDateIterate, dtype='dat
    fileSetList[i]['time_bnds']=('time_bnds', np.arange(startDateIterate, endDateIterate,
fileSet = xr.combine_nested(fileSetList, concat_dim='RunId') #Combining data sets

dataRaw = fileSet.thetao

try:
    dataRaw = dataRaw.rename({"latitude":"lat", "longitude":"lon"})
except:
    pass

print("Data sets successfully merged and renamed into dataRaw.")
```

```
1 UKESM1-0-LL data sets opened
Data sets successfully merged and renamed into dataRaw.
```

In [4]:

```
#UK ESM raw processing cell
dfESMLev = dataRaw.sel(lev=levSel) #Selects level data down to 2k
dfESMLevT = dfESMLev.sel(time=timeRange)
dfESMLatLevT = dfESMLevT.where(dfESMLevT.lat < maxLat, drop=True) #Selection of latitude
dfESMLatLevT = dfESMLatLevT.squeeze()

globalStartDate = dfESMLatLevT["time"][0].values
globalDateInc = dfESMLatLevT["time"][1].values - globalStartDate
globalEndDateIn = dfESMLatLevT["time"][-1].values
globalEndDateOut = globalEndDateIn + globalDateInc

globalStartDateStr = str(globalStartDate)[:7]
globalEndDateInStr = str(globalEndDateIn)[:7]
globalEndDateOutStr = str(globalEndDateOut)[:7]

print("UKESM data loaded and stored in dfESMLatLevT")
```

```
UKESM data loaded and stored in dfESMLatLevT
```

Loading ocean Masks

In [5]:

```
#Ocean mask import cell
maskFile = xr.open_dataset(maskName)
oceanMask = maskFile.to_array()
maskFile = xr.open_dataset("OceanMaskUKESM1")
oceanMask2 = maskFile.to_array()
print("Mask Loaded and stored in oceanMask and oceanMask2 (volcello and UKESM).")
```

```
Mask Loaded and stored in oceanMask and oceanMask2 (volcello and UKESM).
```

Unpacking ocean masks

In [6]:

```
#Mask unpacking cell
geoRange = oceanMask #copying mask
geoRange = geoRange.rename({"variable":"cleanMe"}) #Dimension removal
geoRange = geoRange.sel(cleanMe = geoRange.cleanMe.values[0]) #Dimension removal
geoRange = geoRange.reset_coords("cleanMe", drop=True) #Dimension removal
geoRangeS = geoRange.stack(ij =("i", "j")) #Stacking
geoRangeFilt = geoRangeS.dropna("ij")
print("Ocean mask unpacked into geoRangeFilt.")

geoRange2 = oceanMask2 #copying mask
geoRange2S = geoRange2.stack(ij =("i", "j")) #Stacking
geoRangeFilt2 = geoRange2S.dropna("ij")
print("UKESM Ocean mask unpacked into geoRangeFilt2.")
```

```
Ocean mask unpacked into geoRangeFilt.
UKESM Ocean mask unpacked into geoRangeFilt2.
```

Date Calculations

In [7]:

```
#Date calculation cell
startDateNp = np.datetime64(startDate, 'M')
endDateNp = np.datetime64(endDate, 'M')

timeDiff = endDateNp - startDateNp
```

```
timeDiff = timeDiff.astype(int) + 1
print("Calculated date range.")
```

```
Calculated date range.
```

Calculation functions

Functions:

- pickRand - Takes in data frame and returns sampled data frame with a randomly selected number of rows from the input data frame, controled by the second input variable to the function.
- storeMeta - Returns a np array containing the latitude and longitude data for an input xarray and associated ij.
- loadModel - loadeds and returns GMM model named in input.
- saveModel - saves input GMM model to provided name, if no name provided default is GMMGenerated.

In [8]:

```
#Calculation functions cell
def pickRand(dataArray, sampleFactor):
    '''Returns a sample of the input array, size of sampled array is based on sampleFactor
    arrLen = len(dataArray)
    if sampleFactor > 1:
        sampleSize = int(sampleFactor)
    elif sampleFactor > 0:
        sampleSize = int(sampleFactor*arrLen)
    else:
        return 1

    filtArr = np.zeros(arrLen, dtype=bool) # empty mask
    sampleId = np.random.choice(arrLen, sampleSize, False) # np array of randomly generate
    for i in sampleId:
        filtArr[i] = True # populating mask
    return dataArray[filtArr] # applies mask

def pickRandMask(maskLen, maskQuantity, sampleFactor):
    '''Returns a linear mask for the input dimensions, size of mask is based on sampleFact
    if sampleFactor > 1:
        sampleSize = int(sampleFactor)
    elif sampleFactor > 0:
        sampleSize = int(sampleFactor*maskLen)
    else:
        return 1

    globalArr = np.empty(shape=(0), dtype=bool)
    for i in range(maskQuantity):
        filtArr = np.zeros(maskLen, dtype=bool) # empty mask
        sampleId = np.random.choice(maskLen, sampleSize, False) # np array of randomly ge
        for j in sampleId:
            filtArr[j] = True # populating mask
        globalArr = np.append(globalArr, filtArr)
    return globalArr


def storeMeta(dataArray):
    '''Returns a np array containing the latitude and longitude data for the input xarray
    storeLen = len(dataArray["lat"]) # assumes each lat has a corresponding lon
    storage = np.empty(shape=(0,storeLen))
    storage = np.append(storage, [dataArray["lat"].values], axis = 0)
    storage = np.append(storage, [dataArray["lon"].values], axis = 0)
    #storage = np.append(storage, [dataArray["time"].values], axis = 0)
    #storage = np.append(storage, [dataArray["ij"].values], axis = 0)
```

```
    return storage


def loadModel(modelName:str):
    '''Loades the input GMM model named in the functions input. Returns loaded model.'''
    means = np.load(modelName + '_means.npy')
    covar = np.load(modelName + '_covariances.npy')
    GMModel = mixture.GaussianMixture(n_components = len(means), covariance_type='full')
    GMModel.precisions_cholesky_ = np.linalg.cholesky(np.linalg.inv(covar))
    GMModel.weights_ = np.load(modelName + '_weights.npy')
    GMModel.means_ = means
    GMModel.covariances_ = covar
    return GMModel


def saveModel(GMModel, modelName = "GMMGenerated"):
    '''Saves the input GMM model's weights, means and covariances. Assigns input name if p
    GMModel_name = str(modelName)
    np.save(modelName + '_weights', GMModel.weights_, allow_pickle=False)
    np.save(modelName + '_means', GMModel.means_, allow_pickle=False)
    np.save(modelName + '_covariances', GMModel.covariances_, allow_pickle=False)
    return 0

print("Calculation functions defined.")
```

```
Calculation functions defined.
```

Plotting functions

Functions:

- bicPlot - Plots BIC score array against component number.
- locationPlotGroup - plots location and classification of data points for an input numpy array.
- locationPlotGroupDF - plots location and classification of data points for an input data frame.
- locationPlotGroupDFMonthly - plots location and classification of data points for an input data frame in monthly subplots.
- locationPlotTime - plots locations of an input data array on a map with a colour scale for time.
- locationPlotUncertaintyDF - plots uncertainty in classification on a location plot.
- tempPointPlot - Plots the temperature profile of a single point against depth.
- tempGroupPlot - Plots the mean/+-1std temperature profiles of all classes in input dataArrays (seperate mean and std).

In [9]:

```
#Plotting functions Cell
sampleDepthAxis = dfESMLatLevT["lev"]

def bicPlot(bicArray, startNo, endNo, skipNo, title, label, plotNo):
    '''Plots input BIC score array'''
    plt.figure(plotNo, figsize=(20, 8))
    plt.style.use("seaborn-darkgrid")
    componentRange = range(startNo, endNo, skipNo)
    plt.plot(componentRange, bicArray, label = str(label))

    bicArrayMax = np.max(bicArray)
    bicArrayMin = np.min(bicArray)
    bicRange = bicArrayMax-bicArrayMin
    if bicRange == 0:
        bicRange = 20 #provides border 1 if all bic values are identical
    plt.xticks(componentRange)
    plt.xlim([startNo-0.5, endNo+0.5])
```

```
    plt.ylim([bicArrayMin-0.05*bicRange, bicArrayMax+0.05*bicRange])

    plt.legend(bbox_to_anchor=(1.05, 1), loc='upper left')
    plt.xlabel("Number of components")
    plt.ylabel("BIC score")
    plt.title(title)


def locationPlotGroup(metaDataArray, size, plotNo):
    '''Plots locations of numpy arrays with group colour scheme'''
    plt.figure(plotNo, figsize=size)
    ax = plt.axes(projection=ccrs.SouthPolarStereo())
    ax.add_feature(cfeature.OCEAN)
    ax.add_feature(cfeature.COASTLINE)
    ax.coastlines()
    ax.gridlines()
    im = ax.scatter(metaDataArray[1], metaDataArray[0], transform=ccrs.PlateCarree(), c =
    cb = plt.colorbar(im)
    plt.plot(np.arange(0,361,1),np.ones(361)*-29.5, transform=ccrs.PlateCarree(), color="
    plt.title("Grouped Sample Locations ("+str(len(metaDataArray[0]))+")")


def locationPlotGroupDFTime(dataFrame, title, size, plotNo):
    '''Plots locations of data frame points with group colour scheme'''
    plt.figure(plotNo, figsize=size)
    ax = plt.axes(projection=ccrs.SouthPolarStereo())
    ax.add_feature(cfeature.OCEAN)
    ax.add_feature(cfeature.COASTLINE)
    ax.coastlines()
    ax.gridlines()
    im = ax.scatter(dataFrame["lon"], dataFrame["lat"], transform=ccrs.PlateCarree(), c =
    cb = plt.colorbar(im)
    loc = mdates.AutoDateLocator()
    cb.ax.yaxis.set_major_locator(loc)
    cb.ax.yaxis.set_major_formatter(mdates.ConciseDateFormatter(loc))
    plt.plot(np.arange(0,361,1),np.ones(361)*-29.5, transform=ccrs.PlateCarree(), color="
    plt.title(str(title))


def locationPlotGroupDFLab(dataFrame, title, size, plotNo):
    '''Plots locations of data frame points with group colour scheme'''
    plt.figure(plotNo, figsize=size)
    ax = plt.axes(projection=ccrs.SouthPolarStereo())
    ax.add_feature(cfeature.OCEAN)
    ax.add_feature(cfeature.COASTLINE)
    ax.coastlines()
    ax.gridlines()
    im = ax.scatter(dataFrame["lon"], dataFrame["lat"], transform=ccrs.PlateCarree(), c =
    cb = plt.colorbar(im)
    plt.plot(np.arange(0,361,1),np.ones(361)*-29.5, transform=ccrs.PlateCarree(), color="
    plt.title(str(title))


def locationPlotGroupDFMonthly(dataFrame, title, plotNo):
    '''Plots locations of dataframe points by monthly subplot with group colour scheme'''
    fig = plt.figure(plotNo, figsize=(30,42))
    plt.title(str(title))
    for i in range(1, 13):
        timeData = dataFrame.where(dataFrame["time"].dt.month==i)
        ax = plt.subplot(4, 3, i, projection=ccrs.SouthPolarStereo())
        ax.add_feature(cfeature.OCEAN)
        ax.add_feature(cfeature.COASTLINE)
        ax.coastlines()
        ax.gridlines()
        im = ax.scatter(timeData["lon"], timeData["lat"], transform=ccrs.PlateCarree(), c
        plt.plot(np.arange(0,361,1),np.ones(361)*-29.5, transform=ccrs.PlateCarree(), colo
```

```
        plt.title(calendar.month_abbr[i])
    plt.subplots_adjust(wspace=0, hspace=0.05)
    cb_ax = fig.add_axes([0.27, 0.1, 0.5, 0.02])
    cbar = fig.colorbar(im, cax=cb_ax, orientation="horizontal")


def locationPlotTime(dataArray, size, plotNo):
    '''Plots locations of numpy arrays with date colour scheme'''
    plt.figure(plotNo, figsize=size)
    ax = plt.axes(projection=ccrs.SouthPolarStereo())
    ax.add_feature(cfeature.OCEAN)
    ax.add_feature(cfeature.COASTLINE)
    ax.coastlines()
    ax.gridlines()
    im = ax.scatter(dataArray[1], dataArray[0], transform=ccrs.PlateCarree(), c= mdates.da
    cb = plt.colorbar(im)
    loc = mdates.AutoDateLocator()
    cb.ax.yaxis.set_major_locator(loc)
    cb.ax.yaxis.set_major_formatter(mdates.ConciseDateFormatter(loc))
    plt.plot(np.arange(0,361,1),np.ones(361)*-29.5, transform=ccrs.PlateCarree(), color="
    plt.title("Sample Locations ("+str(len(dataArray[0]))+")")


def locationPlotUncertaintyDF(dataFrame, title, size, plotNo):
    '''Plots input data array classification uncertainties'''
    plt.figure(plotNo, figsize=size)
    ax = plt.axes(projection=ccrs.SouthPolarStereo())
    ax.add_feature(cfeature.OCEAN)
    ax.add_feature(cfeature.COASTLINE)
    ax.coastlines()
    ax.gridlines()
    im = ax.scatter(dataFrame["lon"], dataFrame["lat"], transform=ccrs.PlateCarree(), c =
    cb = plt.colorbar(im)
    plt.plot(np.arange(0,361,1),np.ones(361)*-29.5, transform=ccrs.PlateCarree(), color="
    plt.title(str(title))


def locationPlotUncertaintyDFMonthly(dataFrame, title, plotNo):
    '''Plots locations of dataframe points by monthly subplot with group colour scheme'''
    fig = plt.figure(plotNo, figsize=(30,42))
    plt.title(str(title))
    for i in range(1, 13):
        timeData = dataFrame.where(dataFrame["time"].dt.month==i)
        ax = plt.subplot(4, 3, i, projection=ccrs.SouthPolarStereo())
        ax.add_feature(cfeature.OCEAN)
        ax.add_feature(cfeature.COASTLINE)
        ax.coastlines()
        ax.gridlines()
        im = ax.scatter(timeData["lon"], timeData["lat"], transform=ccrs.PlateCarree(), c
        #cb = plt.colorbar(im, fraction=0.046, pad=0.04)
        plt.plot(np.arange(0,361,1),np.ones(361)*-29.5, transform=ccrs.PlateCarree(), colo
        plt.title(calendar.month_abbr[i])
    plt.subplots_adjust(wspace=0, hspace=0.05)
    cb_ax = fig.add_axes([0.27, 0.1, 0.5, 0.02])
    cbar = fig.colorbar(im, cax=cb_ax, orientation="horizontal")


def locationPlotXr(dataArray, size, plotNo):
    '''Plots locations of numpy arrays with date colour scheme'''
    plt.figure(plotNo, figsize=size)
    ax = plt.axes(projection=ccrs.SouthPolarStereo())
    ax.add_feature(cfeature.OCEAN)
    ax.add_feature(cfeature.COASTLINE)
    ax.coastlines()
    ax.gridlines()
    im = ax.scatter(dataArray["lon"], dataArray["lat"], transform=ccrs.PlateCarree())
```

```
    plt.plot(np.arange(0,361,1),np.ones(361)*-29.5, transform=ccrs.PlateCarree(), color="B
    plt.title("Sample Locations ("+str(len(dataArray["lat"]))+")")


def tempPointPlot(dataArray, label, title, plotNo):
    '''Displays temperature profile plot for a given data set, singular point'''
    plt.figure(plotNo)
    plt.plot(dataArray, sampleDepthAxis, label = label)
    plt.legend(bbox_to_anchor=(1.05, 1), loc='upper left')
    plt.title(str(title))
    plt.gca().invert_yaxis()


def tempGroupProfile(dataArrayMean, dataArrayStd, plotNo):
    '''Displays mean /+-1 std temperature profiles for classes in dataArrayMean and dataAr
    dataCompNo = len(dataArrayMean)
    columnNames = sampleDFSortMeans.columns.values
    dataStart = np.where(columnNames == sampleDepthAxis[0].values)[0][0]
    subPlotX = int(np.ceil(dataCompNo/5))

    plt.figure(plotNo, figsize=(35, 10*subPlotX))
    plt.style.use("seaborn-darkgrid")
    palette = cm.coolwarm(np.linspace(0,1, dataCompNo))

    for i in range(dataCompNo):
        meanT = dataArrayMean.iloc[i, dataStart:].to_numpy()
        stdT = dataArrayStd.iloc[i, dataStart:].to_numpy()

        plt.subplot(subPlotX, 5, i+1)
        plt.plot(meanT, sampleDepthAxis, marker='', linestyle="solid", color=palette[i], l
        plt.plot(meanT+stdT, sampleDepthAxis, marker='', linestyle="dashed", color=palette
        plt.plot(meanT-stdT, sampleDepthAxis, marker='', linestyle="dashed", color=palette

        plt.xlim([-2,20])
        plt.ylim([0,1000])
        ax = plt.gca()
        ax.invert_yaxis()
        ax.grid(True)

        fs = 16 #font size
        plt.xlabel("Temperature (°C)", fontsize=fs)
        plt.ylabel("Depth (m)", fontsize=fs)
        plt.title("Class = "+str(i), fontsize=fs)
        mpl.rc("xtick", labelsize=fs)
        mpl.rc("ytick", labelsize=fs)

        '''
        textstr = '\n'.join((
            r'N profs. = %i' % (nprofs[nrow], ),
            r'Mean lon = %i' % (meanLon, ),
            r'Mean lat = %i' % (meanLat, ),
            r'Post. = %i' % (meanMaxPP, )))
        props = dict(boxstyle="round", facecolor="wheat", alpha=0.8)
        ax.text(0.45, 0.25, textstr, transform=ax.transAxes, fontsize=fs, verticalalignmen
        '''


print("Plotting functions defined.")
```

```
Plotting functions defined.
```

Plotting Ocean Mask

In [10]:
```
#Mask plotting cell
#locationPlotXr(geoRangeFilt, (10,10), 1)
#locationPlotXr(geoRangeFilt2, (10,10), 2)
plt.show()
```

Generating Data Samples

In [11]:
```
#Identifying, masking and stacking raw data cell
dfESMLatLevTStack = dfESMLatLevT.stack(ij =("i", "j"))
dfESMLatLevTStack = dfESMLatLevTStack.transpose('time', 'ij', 'lev')
dfESMLatLevTStackFilt = dfESMLatLevTStack.sel(ij = geoRangeFilt.ij.values) #Produces 2219
print("Raw data identified, stacked and stored in dfESMLatLevTStackFilt. Data dimensions:
```

```
Raw data identified, stacked and stored in dfESMLatLevTStackFilt. Data dimensions: Frozen
({'time': 360, 'ij': 22194, 'lev': 54}).
```

In [12]:
```
#Sample mask creation cell
ijLen = len(dfESMLatLevTStackFilt["ij"])
timeLen = len(dfESMLatLevTStackFilt["time"])
mask = pickRandMask(ijLen, timeLen, 0.34)
print("Data mask calculated")
```

```
Data mask calculated
```

In [13]:
```
#Sample selection cell
sampleDataRaw = dfESMLatLevTStackFilt.reset_index('ij')
sampleDataRaw = sampleDataRaw.stack(ijT = ('time', 'ij'))
sampleData = sampleDataRaw[:,mask]
sampleData = sampleData.transpose('ijT', 'lev')
print("Sample data calculated and stored in sampleData. Sample data dimensions: "+str(samp
```

```
Sample data calculated and stored in sampleData. Sample data dimensions: Frozen({'ijT': 27
16200, 'lev': 54}).
```

Placing sample data into tables

In [14]:
```
#Location and time data to table cell
metaData = {"lat":sampleData["lat"], "lon":sampleData["lon"], "time":sampleData["time"]}
sampleMetaDF = pd.DataFrame(metaData, columns=["lat", "lon", "time"])
print("Sample lat, lon and time converted to datafile (sampleMetaDF). "+str(len(sampleMeta
sampleMetaDF.head()
```

```
Sample lat, lon and time converted to datafile (sampleMetaDF). 2716200 samples identified.
```

Out[14]:

	lat	lon	time
0	-65.703316	73.5	1980-01-01
1	-65.288567	73.5	1980-01-01
2	-63.562469	73.5	1980-01-01
3	-60.270821	73.5	1980-01-01
4	-59.771149	73.5	1980-01-01

In [15]:
```
#Temperature data to table and table merging cell
```

```
#Generating surface temperature level value and column name
surfaceTemp = sampleData["lev"][0].values
surfaceData = sampleData.sel(lev = surfaceTemp)
surfaceTempName = "Surface Temp ("+str(np.round(surfaceTemp,2))+")"

#Exporting sample data into pandas
if True:
    sampleDataDF = sampleData.to_pandas()

    sampleDataDFClean = sampleDataDF.reset_index()
    sampleDataDFClean = sampleDataDFClean.drop(columns=['ij'])
    sampleDF = pd.concat([sampleMetaDF, sampleDataDFClean.drop(columns=["time"])], axis=1)
else:
    sampleDF = sampleMetaDF

sampleDF["time"] = pd.to_datetime(sampleDF["time"])
print("SampleData converted to datafile (sampleDataDF). Datafiles combined into sampleDF.
sampleDF.head()
```

```
SampleData converted to datafile (sampleDataDF). Datafiles combined into sampleDF. 2716200
samples identified.
```

Out[15]:

	lat	lon	time	0.5057600140571594	1.5558552742004395	2.6676816940307617	3.8562798500061035
0	-65.703316	73.5	1980-01-01	-1.632348	-1.632239	-1.635037	-1.637914
1	-65.288567	73.5	1980-01-01	-1.604592	-1.609563	-1.617265	-1.624262
2	-63.562469	73.5	1980-01-01	-1.370728	-1.381026	-1.394235	-1.404338
3	-60.270821	73.5	1980-01-01	-1.064825	-1.071327	-1.076603	-1.082442
4	-59.771149	73.5	1980-01-01	-0.885555	-0.895390	-0.903586	-0.914104

5 rows × 57 columns

In [16]:

```
#Location Plotting Cell
#locationPlotGroupDFTime(sampleDF, "Sample locations", (10,10), 1) #Should match mask
plt.show()
```

Scaling

Scaling Implementation

Applying scaling to the data set, ensuring all levels have same influence over data.

In [17]:

```
#Scaler calculation cell
scalerUK = preprocessing.StandardScaler().fit(sampleData)
print("Scaler calculated for data, stored in scalerUK.")
```

```
Scaler calculated for data, stored in scalerUK.
```

In [18]:

```
#Scaler application cell
sampleDataScaled = scalerUK.transform(sampleData)
print("Sample data scaled and stored in sampleDataScaled.")
```

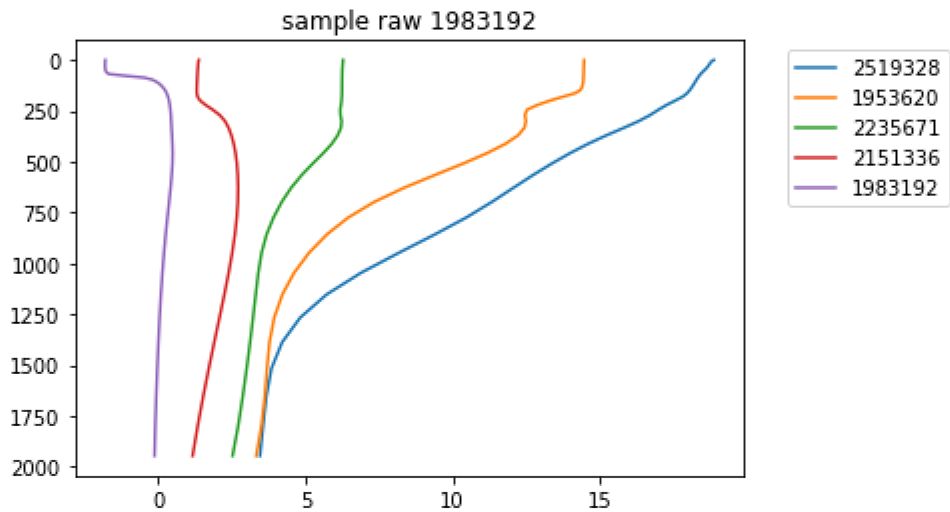
```
Sample data scaled and stored in sampleDataScaled.
```

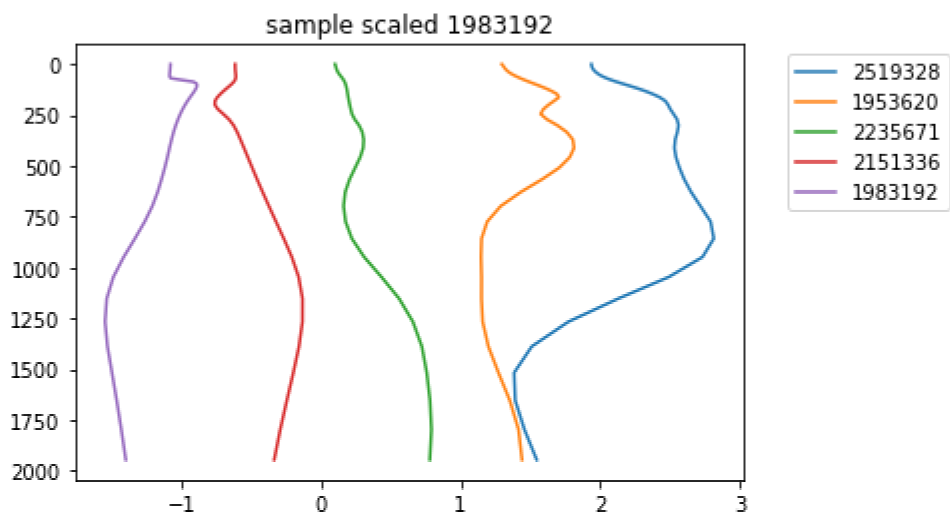
Scaling comparison

Comparing raw temperature profiles with their scaled equivalent. To show individual plots set solo to True.

In [19]:

```
#Scaled temperature profile plotting cell
solo = False #Set to true for seperate plots, false for combined plots.
for i in range(5):
    x = np.random.randint(len(sampleMetaDF))
    tempPointPlot(sampleData[x], x, "sample raw "+str(x), solo*2*i)
    tempPointPlot(sampleDataScaled[x], x, "sample scaled "+str(x), solo*2*i+1)
plt.show()
```





Principle Component Analysis

This process is performed to reduce the number of dimensions of the the data, as well as to improve overall model performance.

In [20]:

```
#PCA component setting cell
for i in range(1,8):
    pca = PCA(n_components=i) #initialising PCA
    pca.fit(sampleDataScaled) #fitting model to data
    totalVarianceExplained = np.sum(pca.explained_variance_ratio_)
    print("For "+str(i)+" PCA components, "+str(totalVarianceExplained)+" is explained.")
    if not(pcaNControl) and (totalVarianceExplained > pcaThreshold):
        pcaNControl = i
```

```
        print("Threshold of "+str(pcaThreshold)+" exceeded, pcaNControl assigned a value c
print("\nAssigned value of pcaNcontrol = "+str(pcaNControl))
```

```
For 1 PCA components, 0.9483991898349492 is explained.
For 2 PCA components, 0.9765474669586303 is explained.
For 3 PCA components, 0.9910479725748748 is explained.
Threshold of 0.98 exceeded, pcaNControl assigned a value of 3
For 4 PCA components, 0.9972582961167935 is explained.
For 5 PCA components, 0.9990374603828521 is explained.
For 6 PCA components, 0.9998315607910341 is explained.
For 7 PCA components, 1.0002645752377928 is explained.

Assigned value of pcaNcontrol = 3
```

In [21]:

```
#PCA fitting cell
pca = PCA(n_components=pcaNControl) #initialising PCA
pca.fit(sampleDataScaled) #fitting model to data
sampleDataScaledPCA = pca.transform(sampleDataScaled) #converting input data into PCA repi
print("Data passed through PCA to sampleDataPCA.")
```

```
Data passed through PCA to sampleDataPCA.
```

Model generation/BIC score calculation

To identify the best fitting models a BIC score metric is used, with a lower BIC score indicating a better model. BIC scores for each number of classes will differ based on starting values used in the modelling, so repeated runs of the BIC scoring helps to provide a more overall score for each number of classes.

The number of iterations for each quantity of classes can be controlled by modifying the bicLoopControl variable at the top of the notepad in Choices for data.

In [22]:

```
#GMM modelling cell
bicMin = np.infty
bicComponentMin = 2
bicRaw = np.empty(shape=(0))

bicCurrentArray = np.empty(shape=(0))
for i in range(firstBicLoopControl):     #Number of iterations for each number of componen
    GMModel = mixture.GaussianMixture(n_components = 2, covariance_type = cvType) #Run moc
    GMModel.fit(sampleDataScaledPCA)

    bicCurrent = GMModel.bic(sampleDataScaledPCA)
    bicCurrentArray = np.append(bicCurrentArray, bicCurrent)
    if bicCurrent < bicMin:   #if latest BIC score is lowest, update and save model
        bicMin = bicCurrent
        bicComponentMin = 2
        bestGMModel = GMModel
        GMMRunId = i

bicRaw = np.append(bicRaw, bicCurrentArray)
componentNo = bestGMModel.n_components

if componentNo != bicComponentMin:
    print("Warning, error with assigning optimum GMM. The model was unable to be saved.")
elif saveModel:
    saveModel(bestGMModel, modelName)
    print("Best GMM from training saved to "+modelName+".")

print("Modelling and scoring complete. The lowest bicScore was "+str(np.round(bicMin, 2))+
print("BIC values are stored in bicRaw, with lowest stored in bicMin and model in bestGGMc
```

```
Best GMM from training saved to GMM_UK_2Class_R1.
Modelling and scoring complete. The lowest bicScore was 28871166.75 for 2 from run 6.
BIC values are stored in bicRaw, with lowest stored in bicMin and model in bestGGModel.
```

BIC score calculations

The average and minimum BIC scores for each number of components are calculated and stored in the corresponding arrays.

In [23]:

```
#BIC score sorting cell
bicAvg = np.infty
bicAvg = np.mean(bicRaw)
print("BIC score sorting finished. Lowest scores for each component value stored in bicMi
```

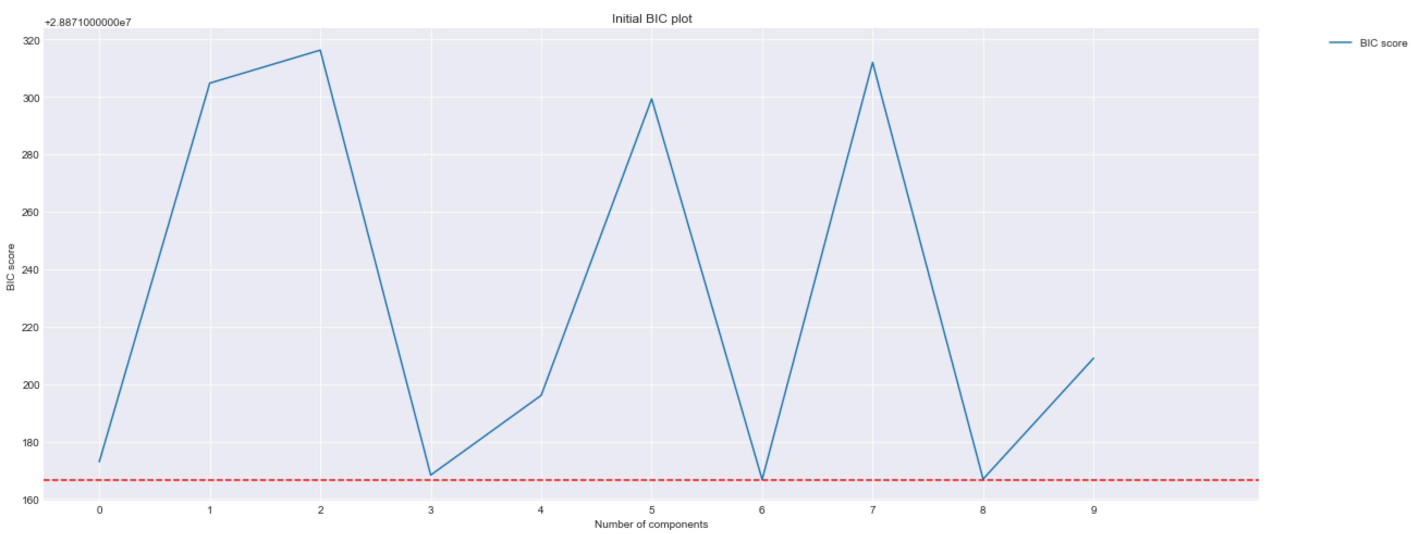
```
BIC score sorting finished. Lowest scores for each component value stored in bicMin, with
average BIC scores stored in bicAvg.
```

BIC score plotting

Plotting the BIC scores from the modelling. The minimum BIC score indicates the ideal number of classes to be used in the model.

In [24]:

```
#BIC curve plotting cell
bicPlot(bicRaw, 0, firstBicLoopControl, 1, "Initial BIC plot", "BIC score", 1)
plt.axhline(bicMin, color = "Red", ls="--")
plt.show()
print("Component number with minimum BIC score: "+str(componentNo)+" with a score of "+st
```




```
Component number with minimum BIC score: 2 with a score of 28871166.74876448 from run 6.
```

Assigning class labels to each profile using the best GMM

Implementation of classification.

In [25]:

```
#Classification and classification probability cell
labels = bestGMModel.predict(sampleDataScaledPCA) #assignment of class labels from best G
posteriorProbs = bestGMModel.predict_proba(sampleDataScaledPCA) #probability of profile b
maxPosteriorProbs = np.max(posteriorProbs, axis=1)
```

```
classUncertainty = 2 - 2*maxPosteriorProbs
print("Labels, posterior probabilities and class uncertainties identified.")
```

```
Labels, posterior probabilities and class uncertainties identified.
```

In [26]:

```
#Initial class labels to sampleDF table cell
try:
    sampleDF = sampleDF.drop(columns=["label", "max posterior prob", "classUncertainty"])
except:
    pass
sampleDF.insert(3, "label", labels, True)
sampleDF.insert(4, "max posterior prob", maxPosteriorProbs, True)
sampleDF.insert(5, "classUncertainty", classUncertainty, True)
print("Labels identified for model ("+str(componentNo)+" components) and added to sampleDF
```

```
Labels identified for model (2 components) and added to sampleDF with associated probabili
ty.
```

Calculating properties of profiles based on class assignment

In [27]:

```
#Class Mean Calculation Cell
sampleDFGrouped = sampleDF.groupby("label") #group profiles according to label
sampleDFMeans = sampleDFGrouped.mean() #calculate mean of all profiles in each class
print("Sample dataframe grouped by label (sampleDFGrouped) and means taken (sampleDFMeans)
```

```
Sample dataframe grouped by label (sampleDFGrouped) and means taken (sampleDFMeans).
```

Sort the labels based on mean near-surface temperatures

In [28]:

```
#Sorted Dictionary creation cell
surfaceMeans = sampleDFMeans[surfaceTemp].to_numpy() #Takes first temperature data column
surfaceMeansOrder = np.argsort(surfaceMeans)
di = dict(zip(surfaceMeansOrder, range(0, componentNo)))
print("Surface temperature means taken and sorted. Label dictionary created and stored in
```

```
Surface temperature means taken and sorted. Label dictionary created and stored in di.
```

In [29]:

```
#Sorted label column to tables cell
try: #Removing labelSorted column from tables
    sampleMetaDF = sampleMetaDF.drop(columns = "labelSorted")
except:
    pass
try:
    sampleDF = sampleDF.drop(columns = "labelSorted")
except:
    pass

#Adding sorted label information to sampleMetaDF and sampleDF
sampleMetaDF.insert(3, "labelSorted", sampleDF["label"].map(di))
sampleDF.insert(5, "labelSorted", sampleDF["label"].map(di))
print("Sorted labels assigned to sampleDF based on surface temperature, coldest to warmest
```

```
Sorted labels assigned to sampleDF based on surface temperature, coldest to warmest.
```

In [30]:

```
#Probability and uncertainty adition to sampleMetaDF (cell)
try:
    sampleMetaDF = sampleMetaDF.drop(columns = ["max posterior prob", "classUncertainty"])
```

```
except:
    pass

sampleMetaDF.insert(4, "max posterior prob", maxPosteriorProbs, True)
sampleMetaDF.insert(5, "classUncertainty", classUncertainty, True)
sampleMetaDF.head()
```

Out[30]:

	lat	lon	time	labelSorted	max posterior prob	classUncertainty
0	-65.703316	73.5	1980-01-01	0	1.0	1.517286e-09
1	-65.288567	73.5	1980-01-01	0	1.0	3.287965e-10
2	-63.562469	73.5	1980-01-01	0	1.0	2.375877e-12
3	-60.270821	73.5	1980-01-01	0	1.0	1.288398e-09
4	-59.771149	73.5	1980-01-01	0	1.0	6.863701e-10

Use pandas to calculate the properties of the profiles by sorted label

In [31]:

```
#Class temperature means and stds cell
sampleDFSortGrouped = sampleDF.groupby("labelSorted")
sampleDFSortMeans = sampleDFSortGrouped.mean()
sampleDFSortStds = sampleDFSortGrouped.std()
profileCount = sampleDFSortGrouped[sampleDF.columns[0]].count().to_numpy()
print("sampleDF grouped by sorted label (sampleDFSortGrouped), with means and standard dev
print("Number of samples in each group calculated and stored in profileCount.")
```

```
sampleDF grouped by sorted label (sampleDFSortGrouped), with means and standard deviations
calculated for each group (sampleDFSortMeans, sampleDFSortStd).
Number of samples in each group calculated and stored in profileCount.
```

Confirmation of sorting

The means printed below should be ordered, going from coldest to warmest.

In [32]:

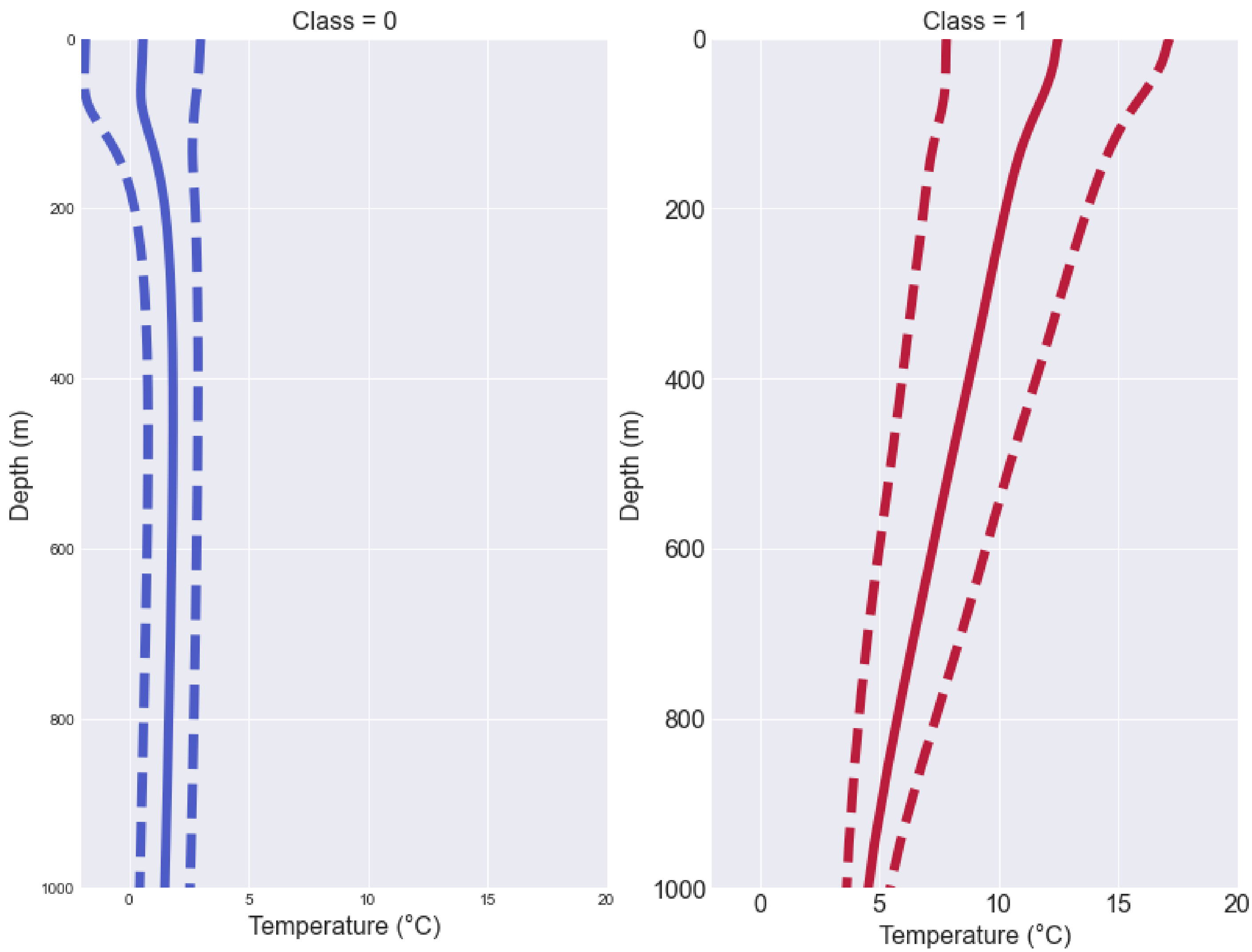
```
#Temperature display cell
print(sampleDFSortMeans[sampleDataDF.columns[0]])
```

```
labelSorted
0     0.594839
1    12.487027
Name: 0.5057600140571594, dtype: float32
```

Plotting the means and standard deviations of the classes by profile

In [33]:

```
#Plotting mean and std profiles cell
tempGroupProfile(sampleDFSortMeans, sampleDFSortStds, 1)
plt.show()
```



Plotting location and cluster

In [34]:

```
#Surface Temperature Plotting Cell
if False:
    plt.figure(1, figsize=(20,20))
    ax = plt.axes(projection=ccrs.SouthPolarStereo())
    ax.add_feature(cfeature.OCEAN)
    ax.add_feature(cfeature.COASTLINE)
    ax.coastlines()
    ax.gridlines()
    im = ax.scatter(sampleDF["lon"], sampleDF["lat"], transform=ccrs.PlateCarree(), c =  s
    cb = plt.colorbar(im)
    plt.plot(np.arange(0,361,1),np.ones(361)*-29.5, transform=ccrs.PlateCarree(), color="F
    plt.title("Surface Temperature of Samples")
    plt.show()
```

In [35]:

```
#locationPlotGroupDFLab(sampleDF, "Location plot of grouping", (25,25), 1)
```

In [36]:

```
#locationPlotGroupDFMonthly(sampleDF, "Monthly summaries for training data set", 1)
print("Classifications, grouped by month.")
```

```
Classifications, grouped by month.
```

In [37]:

```
#locationPlotUncertaintyDFMonthly(sampleDF, "Monthly uncertainty", 1)
```

```
print("Uncertainty in classifications, grouped by month.")
```

```
Uncertainty in classifications, grouped by month.
```

Exporting Meta Data

In [38]:

```
#Meta data export cell
exportName = modelName + "_Meta"
sampleMetaDF.to_csv(exportName) #Exporting meta data
exportName = modelName + "_Mask"
np.save(exportName, mask)
print("Meta data and mask exported to "+modelName+" _Meta.csv and _Mask.npy respectively")
```

```
Meta data and mask exported to GMM_UK_2Class_R1 _Meta.csv and _Mask.npy respectively
```

In [39]:

```
#Meta data reload cell
importName = modelName + "_Meta"
sampleMetaReload = pd.read_csv(importName)
print("Meta data reloaded from "+ importName +". "+str(len(sampleMetaReload))+" samples ic
sampleMetaReload.head()
```

```
Meta data reloaded from GMM_UK_2Class_R1_Meta. 2716200 samples identified.
```

Out[39]:

	Unnamed: 0	lat	lon	time	labelSorted	max posterior prob	classUncertainty
0	0	-65.703316	73.5	1980-01-01	0	1.0	1.517286e-09
1	1	-65.288570	73.5	1980-01-01	0	1.0	3.287965e-10
2	2	-63.562470	73.5	1980-01-01	0	1.0	2.375877e-12
3	3	-60.270820	73.5	1980-01-01	0	1.0	1.288398e-09
4	4	-59.771150	73.5	1980-01-01	0	1.0	6.863701e-10

Exporting Scaler

In [40]:

```
#Exporting scaler cell
exportName = modelName + "_Scaler"
dump(scalerUK, exportName, compress=True) #Saves
print("Scaler exported to "+ exportName +".")
```

```
Scaler exported to GMM_UK_2Class_R1_Scaler.
```

Exporting PCA

In [41]:

```
#Exporting PCA cell
exportName = modelName + "_PCA.pkl"
pk.dump(pca, open(exportName, "wb"))
print("PCA exported to "+ exportName + ".")
```

```
PCA exported to GMM_UK_2Class_R1_PCA.pkl.
```

In [43]:

```
#Reloading PCA cell
importName = modelName + "_PCA.pkl"
pca_reload = pk.load(open(importName, "rb"))
```

```
totalVarianceExplainedOg = np.sum(pca.explained_variance_ratio_)
pca_reload.fit(sampleDataScaled)
totalVarianceExplainedRe = np.sum(pca_reload.explained_variance_ratio_)
print("PCA reloaded. Original total variance was: "+str(totalVarianceExplainedOg)+". Reloa
```

```
PCA reloaded. Original total variance was: 0.99104792822321. Reloaded total variance was:
0.9910479657515417.
```

Single Point investigation

In [44]:

```
#Initial anomalous data point df creation cell
labelAnomDF = sampleDF[np.logical_or(np.logical_and(sampleDF["lat"]<-60, sampleDF["labelSc
print("Class 0 above -45 and Class 1 below -60 lat. Stored in labelAnomDF. "+str(len(label
```

```
Class 0 above -45 and Class 1 below -60 lat. Stored in labelAnomDF. 1334 anomalous points
detected.
```

In [45]:

```
#High confidence anomalous data point df creation cell
labelAnomConDF = labelAnomDF[labelAnomDF["classUncertainty"]<0.25]
print("High Classification Confidence DF of labelAnomDF (<0.25). "+str(len(labelAnomConDF)
```

```
High Classification Confidence DF of labelAnomDF (<0.25). 81 anomalous points detected.
```

In [48]:

```
antarcticAnomDF = labelAnomDF[np.logical_and(labelAnomDF["label"]==1, labelAnomDF["lat"]<-
#antarcticAnomDF
for i in range(5):
    x = np.random.randint(len(antarcticAnomDF))
    tempProfile = np.array(antarcticAnomDF.iloc[x, 7:])
    tempPointPlot(tempProfile, x, "Antarctic Anomalous Classification Temperature Profiles

    #tempProfileScaled = scalerUK.transform(tempProfile)
    #tempPointPlot(tempProfileScaled, x, "Antarctic Anomalous Classification Temperature P
plt.show()
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
~\AppData\Local\Temp/ipykernel_10072/2837525228.py in <module>
      2 #antarcticAnomDF
      3 for i in range(5):
----> 4     x = np.random.randint(len(antarcticAnomDF))
      5     tempProfile = np.array(antarcticAnomDF.iloc[x, 7:])
      6     tempPointPlot(tempProfile, x, "Antarctic Anomalous Classification Temperature
 Profiles", 1)

mtrand.pyx in numpy.random.mtrand.RandomState.randint()

_bounded_integers.pyx in numpy.random._bounded_integers._rand_int32()

ValueError: low >= high
```