# Setting up TDA

#### Introduction

Recall the broad steps of TDA:

- 1. Start with the data. Apply a filter function.
- 2. Create overlapping bins of the data using the image of the filter function.
- 3. Cluster the data in the overlapping bins of the data (aka the pre-image).
- 4. Create a directed graph.

We must choose the following methods and parameters. These correspond to the first three steps of TDA.

- 1. The method for scaling the data and the filter function
- 2. Parameters or (a) number of bins and (b) percent overlap of the bins
- 3. The clustering algorithm and the parameters

We already decided on PCA2 for our filter function because...

#### Summary

This notebook is about selecting the methods and parameters within TDA. Specifically, we go through

- 1. Scaling the data -- we decide on Robust Scaling over Standard Scaling
- 2. Clustering -- we decide on DBscan clustering and the parameters epsilon = xx and min\_sample\_size = xx.
- 3. TDA parameters -- we decide on n\_cubes = xx and perc\_overlap = xx.

#### Heuristics of parameter and method selection

- 1. Each cluster has at most 10% of the data
- 2. The Mapper output represents at least 90% of the data (no more than 10% of the original data, aka 7600 data points, are lost as noise).

The print statements about the maximum data points in a node and number of unique samples address each of these heuristics, repsectively.

#### Notes

- · COND is removed in this analysis.

## **Load libraries**

```
In [1]:
         import kmapper as km
         # import sklearn
         from sklearn.cluster import DBSCAN # clustering algorithm
         from sklearn.decomposition import PCA # projection (lens) creation
         from sklearn.preprocessing import StandardScaler
         from sklearn.preprocessing import RobustScaler
         from sklearn.compose import ColumnTransformer
         import hdbscan
         # from sklearn import ensemble
         # from sklearn.manifold import MDS
         import plotly.graph_objs as go
         # from ipywidgets import interactive, HBox, VBox, widgets, interact # ?
         # import dash html components as html # ?
         # import dash_core_components as dcc # ?
         from kmapper.plotlyviz import * # static and interactive plots
         import psutil # for plotlyviz
         import kaleido # for plotlyviz
         # import networkx # ?
         # import dash # ?
         import warnings #?
         warnings.filterwarnings("ignore")
         import pandas as pd
         import numpy as np
         import matplotlib.pyplot as plt
```

## Read data

```
In [3]:
          water20 = pd.read_csv("../../LTRM data/RF interpolation/water_full.csv")
In [4]:
          water20.head()
            SHEETBAR
                            DATE LATITUDE LONGITUDE FLDNUM STRATUM LOCATCD
                                                                                         ΤN
                                                                                               TP TEMP DO TURB
                                                                                                                    COND
                                                                                                                            VEL
                                                                                                                                      WDP
                                                                                                                                             CH
Out[4]:
                                                            Lake
                                                                      Main
             41000065 07/26/1993
                                  44.571864
                                              -92.510970
                                                                             9312103 3.955 0.228
                                                                                                     23.0 6.6
                                                                                                                     550.0 0.50 42.3
                                                                                                                                        2.2
                                                                                                                                            9.4
                                                         City, MN
                                                                    channel
                                                            Lake
                                                                       Main
             41000066 07/26/1993 44.575497
                                              -92.518497
                                                                             9312002 4.876 0.229
                                                                                                    23.0 6.6
                                                                                                                     554.0 0.72 37.6
                                                                                                                                        8.2 8.2
                                                                                                                 28
                                                         City, MN
                                                            Lake
                                                                      Main
             41000067 07/26/1993 44.573718
                                             -92.523549
                                                                             9312102 3.955 0.220
                                                                                                    22.9 6.3
                                                                                                                 24
                                                                                                                     564.0 0.66
                                                                                                                                 34.1
                                                                                                                                        4.3 8.72
                                                         City, MN
                                                                    channel
                                                            Lake
                                                                      Main
             41000068 07/26/1993 44.566588
                                              -92.541238
                                                                             9312003 4.257
                                                                                             0.212
                                                                                                     22.9 6.4
                                                                                                                     563.0 0.69
                                                                                                                                33.4
                                                                                                                                        9.1 8.48
                                                         City, MN
                                                                    channel
                                                                       Main
             41000069 07/26/1993 44.568419 -92.548780
                                                                             9312104 4.030 0.237
                                                                                                    23.0 6.6
                                                                                                                 33
                                                                                                                     556.0 0.68 48.0
                                                                                                                                        6.7 9.5
                                                         City, MN
                                                                    channel
```

# Scaling

Standard scaling uses mean and standard deviation. Robust scaling uses median and IQR.

The motivation for scaling the data prior to running TDA is that the units of each continuous variable is different. Thus, the ranges are different. For example, SECCHI and SS have ranges from 0 to 120, while VEL and TP all have values less than 20.

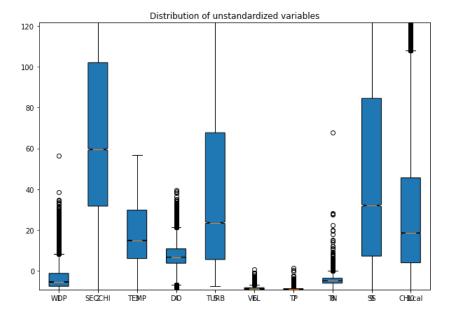
It is beneficial to have continuous variables in the same "units" by subtracting the mean or median and dividing by the standard deviation or IQR.

First, it is beneficial for PCA, which finds axes of maximum variance. Without standardizing the variables, SECCHI was consistently a PCA... xx.

Clustering algorithms use some form of distance metric, so standardizing is also helpful here. "If one of your features has a range of values much larger than the others, clustering will be completely dominated by that one feature." from this Stack Overflow thread. (If we were to cluster data on weight and height, we would want to cluster by kilograms and meters but not grams and meters.)

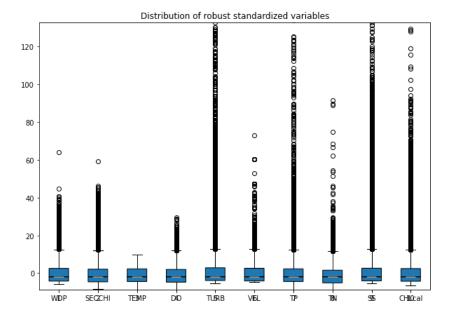
We let X denote the data with robust scaling and Z denote the data with standard scaling.

We choose robust scaling over standard scaling because the distributions among the continuous variables are more similar with robust scaling.



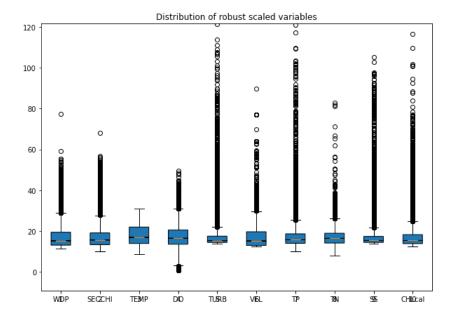
## Robust scaling

```
ct = ColumnTransformer([
     ('somename', RobustScaler(), ["WDP", "SECCHI", "TEMP", "DO", "TURB", "VEL", "TP", "TN", "SS", "CHLcal"])
   ], remainder='passthrough')
fig = plt.figure(figsize =(10, 7))
# Creating plot
plt.boxplot(X)
ax = fig.add_subplot(111)
bp = ax.boxplot(X, patch_artist = True,
           notch ='True', vert = 1)
ax.set_ylim(-1, 20)
ax.get_yaxis().set_visible(False)
#ax.set_yticklables([-5, 0, 5, 10, 15, 20])
plt.title("Distribution of robust standardized variables")
# show plot
plt.show(bp)
```



# Standard scaling

```
In [56]:
      ct = ColumnTransformer([
            ('somename', StandardScaler(), ["WDP", "SECCHI", "TEMP", "DO", "TURB", "VEL", "TP", "TN", "SS", "CHLcal"])
         |, remainder='passthrough')
      fig = plt.figure(figsize =(10, 7))
       # Creating plot
      plt.boxplot(Z)
       ax = fig.add_subplot(111)
       bp = ax.boxplot(Z, patch_artist = True,
                 notch ='True', vert = 1)
      ax.set_ylim(-5, 20)
       ax.get_yaxis().set_visible(False)
       #ax.set_yticklables([-5, 0, 5, 10, 15, 20])
       plt.title("Distribution of robust scaled variables")
       # show plot
      plt.show(bp)
```



## Filter function: PCA2 projection

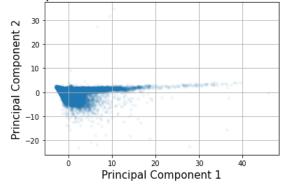
We can see that the ranges of PCA1 and PCA2 are within much more reasonable ranges after scaling. The unscaled PCA has

```
In [57]: pca = PCA(n_components = 2)
lens = pca.fit_transform(X)

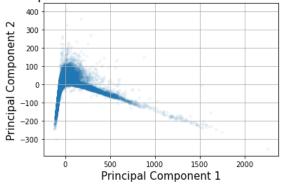
fig, ax = plt.subplots()
    ax.scatter(lens[:,0], lens[:,1], s = 10, alpha = 0.047)
    ax.set_xlabel('Principal Component 1', fontsize = 15)
    ax.set_ylabel('Principal Component 2', fontsize = 15)
    ax.set_title('2 component PCA of robust scaled LTRM data', fontsize = 20)
    ax.grid(True)

plt.show()
```

## 2 component PCA of robust scaled LTRM data



#### 2 component PCA of unstandardized LTRM data



# **Define mapper functions**

The first one uses DBscan as the clustering algorithm. The second one uses HDBscan as the clustering algorithm.

```
In [19]:
         def mapper_pca2_db(df, DBSCAN_EPSILON = 10, DBSCAN_MIN_SAMPLES = 20,
                         N_CUBES = [10,10], PERC_OVERLAP = [.25,.25], return_with_df = False, print_pca_info = False):
             ....
             X = df[["WDP", "SECCHI", "TEMP", "DO", "TURB",
                         "VEL", "TP", "TN", "SS", "CHLcal"]]
             # for discerning primary variables in PCA
             var_to_index = {continuous_variables[i] : i for i in range(len(continuous_variables))}
             projected vars = continuous variables
             projected_var_indices = [var_to_index[var] for var in projected_vars]
               if X.shape[0]<10:</pre>
                   #print(X)
                   print("Not enough data in ", title, "_size = ", X.shape[0])
                   return(X.shape[0])
             \# to match up indices in scomplex with the original dataframe X
             X.reset_index(drop = True, inplace = True)
             # create instance of clustering alg
             cluster_alg = DBSCAN(eps = DBSCAN_EPSILON, min_samples = DBSCAN MIN SAMPLES,
                                  metric='euclidean')
             # instantiate kepler mapper object
             mapper = km.KeplerMapper(verbose = 0)
             \# defining filter function as projection on to the first 2 component axis
             pca = PCA(n_components = 2)
             lens = pca.fit_transform(X)
             if print_pca_info:
                 for j in range(2):
                     pc_j = pca.components_[j]
                     largest_magnitude = max(abs(pc_j))
                     idx_magnitude = np.where(abs(pc_j) == largest_magnitude)[0][0]
                     print("*** PCA", j+1, " ***")
                     print("Primary variable: ", continuous_variables[idx_magnitude])
                     print("Corresponding component: ", pc_j[idx_magnitude])
                     print("Explained variance: ", pca.explained_variance_ratio_[j])
             summary_variable = mapper.project(np.array(X), projection=projected_var_indices, scaler=None)
             # similar to fit transform
             # Generate the simplicial complex
             scomplex = mapper.map(lens, X,
                                   cover=km.Cover(n cubes = N CUBES, perc overlap = PERC OVERLAP),
                                   clusterer = cluster alg)
             if return with df:
                 return(scomplex, X)
             return(scomplex)
```

```
N CUBES = [10,10], PERC OVERLAP = [.25,.25], return with df = False, print pca info = False):
var_to_index = {continuous_variables[i] : i for i in range(len(continuous_variables))}
projected_vars = continuous_variables
projected_var_indices = [var_to_index[var] for var in projected_vars]
  if X.shape[0]<10:</pre>
     #print(X)
     print("Not enough data in ", title, "_size = ", X.shape[0])
     return(X.shape[0])
\# to match up indices in scomplex with the original dataframe X
X.reset_index(drop = True, inplace = True)
# create instance of clustering alg
cluster_alg = hdbscan.HDBSCAN(min_cluster_size = HDB_MIN_CLUSTER, min_samples = HDB_MIN_SAMPLES,
                            cluster_selection_epsilon= HDB_EPSILON, cluster_selection_method = 'eom')
# instantiate kepler mapper object
mapper = km.KeplerMapper(verbose = 0)
# defining filter function as projection on to the first 2 component axis
pca = PCA(n_components = 2)
lens = pca.fit_transform(X)
if print_pca_info:
   for j in range(2):
       pc_j = pca.components_[j]
       largest_magnitude = max(abs(pc_j))
       idx_magnitude = np.where(abs(pc_j) == largest_magnitude)[0][0]
       print("*** PCA", j+1, " ***")
       print("Primary variable: ", continuous_variables[idx_magnitude])
       print("Corresponding component: ", pc_j[idx_magnitude])
       print("Explained variance: ", pca.explained variance ratio [j])
summary\_variable = mapper.project(np.array(X), projection=projected\_var\_indices, scaler=None)
# similar to fit transform
# Generate the simplicial complex
scomplex = mapper.map(lens, X,
                    cover=km.Cover(n_cubes = N_CUBES, perc_overlap = PERC_OVERLAP),
                    clusterer = cluster alg)
if return_with_df:
   return(scomplex, X)
return(scomplex)
```

# Clustering in TDA

### Running DBScan and TDA

#### **TDA** parameters

#### **DBScan parameters**

```
In [22]: # dbscan parameters
                 eps_lst = [0.9, 1] # variables are standardized
                 min_samples_lst = [10]
                 print(eps_lst)
                 print(min samples lst)
                [0.8, 0.9, 1]
                [10]
In [75]:
                 db_params = []
                 db_scomplex = []
                  for epsilon in eps lst:
                        for min_samples in min_samples_lst: # min_samples = 10
                               for n cubes in n cubes 1st:
                                      for perc in perc_overlap_lst: # perc_overlap = [0.5, 0.5]
                                              db_params.append('epsilon = ' + str(epsilon) + ', min_samples = ' + str(min_samples) +
                                                                             , n cubes = ' + str(n cubes) + ", and perc overlap = " + str(perc))
                                              {\tt scomplex, \ df = mapper\_pca2\_db(X, \ DBSCAN\_EPSILON = epsilon, \ DBSCAN\_MIN\_SAMPLES = min\_samples, \ note that the sample of the sample o
                                                                                                 N_CUBES = n_cubes, PERC_OVERLAP = perc, return_with_df = True)
                                              db_scomplex.append(scomplex)
                                             idx = len(db params)-1
                                              print("*** ", idx, " ***")
                                             print(db_params[idx])
                                              all nodes = db scomplex[idx].get('nodes')
                                             obsv per node = []
                                              for node in all nodes:
                                                    obsv_per_node.append(len(all_nodes.get(node)))
                                             print("The maximum data points in a node is ", max(obsv_per_node))
print("The minimum data points in a node is ", min(obsv_per_node))
                                             print("The number of unique samples is ", get_mapper_graph(db_scomplex[idx])[1]["n_unique"])
                epsilon = 0.8, min_samples = 10, n_cubes = [100, 100], and perc_overlap = [0.4, 0.4]
                The maximum data points in a node is 10752
                The minimum data points in a node is 4
                The number of unique samples is 69065
                epsilon = 0.8, min samples = 10, n cubes = [100, 100], and perc overlap = [0.5, 0.5]
                The maximum data points in a node is 14690
                The minimum data points in a node is 4
                The number of unique samples is 69704
                *** 2 ***
                epsilon = 0.8, min_samples = 10, n_cubes = [125, 125], and perc_overlap = [0.4, 0.4]
                The maximum data points in a node is 7057
                The minimum data points in a node is 7
                The number of unique samples is 68265
                *** 3 ***
                epsilon = 0.8, min_samples = 10, n_cubes = [125, 125], and perc_overlap = [0.5, 0.5]
                The maximum data points in a node is 9873
                The minimum data points in a node is
                The number of unique samples is 69285
                *** 4 ***
                epsilon = 0.8, min_samples = 10, n_cubes = [150, 150], and perc_overlap = [0.4, 0.4]
                The maximum data points in a node is 5083
                The minimum data points in a node is 3
                The number of unique samples is 67227
                *** 5 ***
                epsilon = 0.8, min_samples = 10, n_cubes = [150, 150], and perc_overlap = [0.5, 0.5]
                The maximum data points in a node is 7021
                The minimum data points in a node is
                The number of unique samples is 68621
                *** 6 ***
                epsilon = 0.9, min_samples = 10, n_cubes = [100, 100], and perc_overlap = [0.4, 0.4]
                The maximum data points in a node is 10813
                The minimum data points in a node is
                The number of unique samples is 71149
                *** 7 ***
                epsilon = 0.9, min_samples = 10, n_cubes = [100, 100], and perc_overlap = [0.5, 0.5]
                The maximum data points in a node is 14757
                The minimum data points in a node is
```

The number of unique samples is 71721

epsilon = 0.9, min\_samples = 10, n\_cubes = [125, 125], and perc\_overlap = [0.4, 0.4]

\*\*\* 8 \*\*\*

```
The minimum data points in a node is
The number of unique samples is 70477
epsilon = 0.9, min samples = 10, n cubes = [125, 125], and perc overlap = [0.5, 0.5]
The maximum data points in a node is 9934
The minimum data points in a node is
The number of unique samples is 71267
*** 10 ***
epsilon = 0.9, min_samples = 10, n_cubes = [150, 150], and perc_overlap = [0.4, 0.4]
The maximum data points in a node is 5112
The minimum data points in a node is 5
The number of unique samples is 69565
*** 11 ***
epsilon = 0.9, min_samples = 10, n_cubes = [150, 150], and perc_overlap = [0.5, 0.5]
The maximum data points in a node is 7060
The minimum data points in a node is 4
The number of unique samples is 70743
*** 12 ***
epsilon = 1, min_samples = 10, n_cubes = [100, 100], and perc_overlap = [0.4, 0.4]
The maximum data points in a node is 10833
The minimum data points in a node is 8
The number of unique samples is 72428
*** 13 ***
epsilon = 1, min_samples = 10, n_cubes = [100, 100], and perc_overlap = [0.5, 0.5]
The maximum data points in a node is 14788
The minimum data points in a node is
The number of unique samples is 72981
epsilon = 1, \ min\_samples = 10, \ n\_cubes = [125, \ 125], \ and \ perc\_overlap = [0.4, \ 0.4]
The maximum data points in a node is 7116
The minimum data points in a node is
The number of unique samples is 71822
*** 15 ***
epsilon = 1, min_samples = 10, n_cubes = [125, 125], and perc_overlap = [0.5, 0.5]
The maximum data points in a node is 9949
The minimum data points in a node is 2
The number of unique samples is 72494
*** 16 ***
epsilon = 1, \; min\_samples = 10, \; n\_cubes = [150, \; 150], \; and \; perc\_overlap = [0.4, \; 0.4]
The maximum data points in a node is 5137
The minimum data points in a node is
The number of unique samples is 71106
*** 17 ***
epsilon = 1, \min_samples = 10, n_cubes = [150, 150], and perc_overlap = [0.5, 0.5]
The maximum data points in a node is 7075
The minimum data points in a node is 6
The number of unique samples is 71999
```

# Parameters for DBscan, TDA mapper

The maximum data points in a node is 7105

With these parameters,

- Epsilon = 1
- min\_samples = 10
- n\_cubes = [125, 125]
- perc\_overlap = [0.4, 0.4],

Each node represents at most 10% of the data, and about 5% of the data is lost as noise. The graph layout is one large connected component.

#### Running HDBScan and TDA

Use the cluster selection epsilon method so that it is a hybrid of DBscan and HDBscan. We will see that HDBscan graph outputs are not as desirable because xx.

### **HDBScan parameters**

```
min_cluster_lst = [10]
print(min_cluster_lst)
print(min_samples_lst)

[10]
[10]
```

```
In [63]:
           # hdbscan
           hdb_params = []
           hdb_scomplex = []
           for min_clust in min_cluster_lst: # min_clust = 10
               min_clust = int(min_clust)
               for min_samples in min_samples_lst: # min_samples = 10
                    min_samples = int(min_samples)
                    for n cubes in n cubes 1st:
                        for perc in perc_overlap_lst: # perc_overlap = [0.5, 0.5]
                             hdb_params.append('min_clust = ' + str(min_clust) + ', min_samples = ' + str(min_samples) +
                                                , n cubes = ' + str(n cubes) + ", and perc overlap = " + str(perc))
                            hdb_scomplex.append(mapper_pca2_hdb(X, HDB_MIN_CLUSTER = min_clust, HDB_MIN_SAMPLES = min_samples,
                                                                    HDB_EPSILON = 1,N_CUBES = n_cubes, PERC_OVERLAP = perc,
                                                                    return_with_df = False))
                            idx = len(hdb params)-1
                            print("*** ", idx, " ***")
                            print(hdb_params[idx])
                             all nodes = hdb scomplex[idx].get('nodes')
                            obsv_per_node = []
                             for node in all nodes:
                                 obsv_per_node.append(len(all_nodes.get(node)))
                            print("The maximum data points in a node is ", max(obsv_per_node))
                             print("The minimum data points in a node is ", min(obsv_per_node))
                            print("The number of unique samples is ", get_mapper_graph(hdb_scomplex[idx])[1]["n_unique"])
          *** () ***
          min_clust = 10, min_samples = 10, n_cubes = [100, 100], and perc_overlap = [0.5, 0.5]
          The maximum data points in a node is 12639 The minimum data points in a node is 10
          The number of unique samples is 67094
          \min_{\text{clust}} = 10, \min_{\text{samples}} = 10, n_{\text{cubes}} = [125, 125], and \text{perc\_overlap} = [0.5, 0.5]
The maximum data points in a node is 8491
          The minimum data points in a node is \ 10
          The number of unique samples is 63616
          *** 2 ***
          min_clust = 10, min_samples = 10, n_cubes = [150, 150], and perc_overlap = [0.5, 0.5]
          The maximum data points in a node is 6458 The minimum data points in a node is 10
          The number of unique samples is 63490
         Deciding not to use HDBscan
```

```
XX.
```

# Save selected parameters into .html and .json

### Old

```
In [ ]:
                # the rest of this is for coloring
               pl_brewer = [[0.0, '#006837'],
          #
                         [0.1, '#1a9850'],
                         [0.2, '#66bd63'],
[0.3, '#a6d96a'],
[0.4, '#d9ef8b'],
                          [0.5, '#ffffbf'],
                          [0.6, '#fee08b'],
                         [0.0, #feeoob],
[0.7, '#fdae61'],
[0.8, '#f46d43'],
[0.9, '#d73027'],
[1.0, '#a50026']]
          #
               color_values = lens[:,0] - lens[:,0].min() # changes if PCA1 or PCA1 and PCA2
               # can change to other variables
               color_function_name = ['Distance to x-min'] # set name of color function
          #
               my\_colorscale = pl\_brewer
          #
               kmgraph, mapper_summary, colorf_distribution = get_mapper_graph(scomplex,
                                                                                     color_values,
                                                                                    color_function_name=color_function_name,
                                                                                    colorscale=my colorscale)
          #
               plotly_graph_data = plotly_graph(kmgraph, graph_layout='fr', colorscale=my_colorscale,
                                                   factor_size=2.5, edge_linewidth=0.5)
               plot_title = str(DBSCAN_EPSILON) + str(DBSCAN_EPSILON) + ', MIN_SAMPLES ' + str(DBSCAN_MIN_SAMPLES)
          #
                layout = plot_layout(title=plot_title,
                                      width=620, height=570,
          #
                                       annotation_text=get_kmgraph_meta(mapper_summary))
          #
                # FigureWidget is responsible for event listeners
                fw_graph = go.FigureWidget(data=plotly_graph_data, layout=layout)
                fw_summary = summary_fig(mapper_summary, height=300)
                dashboard = hovering_widgets(kmgraph, fw_graph, member_textbox_width=600)
                # DESIRED FILE PATH, CHANGE TO FIT YOUR LOCAL MACHINE
                directory_path = "mapper outputs"
                #Update the fw_graph colorbar, setting its title:
                fw graph.data[1].marker.colorbar.title = 'dist to<br>x-min'
                html_output_path = directory_path + 'Eps_' + str(DBSCAN_EPSILON) +'_Mins_' + str(DBSCAN_MIN_SAMPLES) + '_NCubes_' +
          #
          #
                mapper.visualize(scomplex, color_values=color_values, color_function_name=color_function_name,
                                  path_html=html_output_path, lens = summary_variable, lens_names = projected_vars)
               return scomplex, X
```