# Somoclu Python Documentation

***Release 1.7.5***

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CHAPTER 1

# Introduction

Somoclu is a massively parallel implementation of self-organizing maps. It relies on OpenMP for multicore execution and it can be accelerated by CUDA. The topology of map is either planar or toroid, the grid is rectangular or hexagonal. Currently a subset of the command line version is supported with this Python module.

Key features of the Python interface:

- Fast execution by parallelization: OpenMP and CUDA are supported.
- Multi-platform: Linux, macOS, and Windows are supported.
- Planar and toroid maps.
- Rectangular and hexagonal grids.
- Gaussian or bubble neighborhood functions.
- Visualization of maps, including those that were trained outside of Python.
- PCA initialization of codebook.

The documentation is available online. Further details are found in the following paper:

Peter Wittek, Shi Chao Gao, Ik Soo Lim, Li Zhao (2017). Somoclu: An Efficient Parallel Library for Self-Organizing Maps. Journal of Statistical Software, 78(9), pp.1–21. DOI:10.18637/jss.v078.i09. arXiv:1305.1422.

## 1.1 Copyright and License

## 1.2 Acknowledgment

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CHAPTER 2

# Download and Installation

The package is available in the Python Package Index, containing the source, documentation, and examples. The latest development version is available on GitHub.

## 2.1 Dependencies

The module requires Numpy and matplotlib. The code is compatible with both Python 2 and 3.

On Linux and macOS, you need a standard C++ compile chain, for instance, GCC, ICC and clang are known to work.

On Windows, having `MSVCP90.DLL` and `VCOMP90.DLL` is usually sufficient. See this issue if you have problems.

### 2.1.1 Installation

The code is available on PyPI, hence it can be installed by

```
$ pip install somoclu
```

Alternatively, it is also available on [conda-forge](https://github.com/conda-forge/somoclu-feedstock):

```
$ conda install somoclu
```

If you want the latest git version, clone the repository, make the Python target, and follow the standard procedure for installing Python modules:

```
$ git clone https://github.com/peterwittek/somoclu.git
$ cd somoclu
$ ./autogen.sh
$ ./configure
$ make python
$ cd src/Python
$ sudo python setup.py install
```

### 2.1.2 Build with CUDA support on Linux and macOS:

If the `CUDAHOME` variable is set, the usual install command will build and install the library:

```
$ sudo python setup.py install
```

### 2.1.3 Build with CUDA support on Windows:

You should first follow the instructions to build the Windows binary with MPI disabled with the same version Visual Studio as your Python is built with.(Since currently Python is built by VS2008 by default and CUDA v6.5 removed VS2008 support, you may use CUDA 6.0 with VS2008 or find a Python prebuilt with VS2010. And remember to install VS2010 or Windows SDK7.1 to get the option in Platform Toolset if you use VS2013.) Then you should copy the .obj files generated in the release build path to the Python/src folder.

Then modify the win_cuda_dir in setup.py to your CUDA path and run the install command

```
$ sudo python setup.py install
```

Then it should be able to build and install the module.

# CHAPTER 3

# Examples

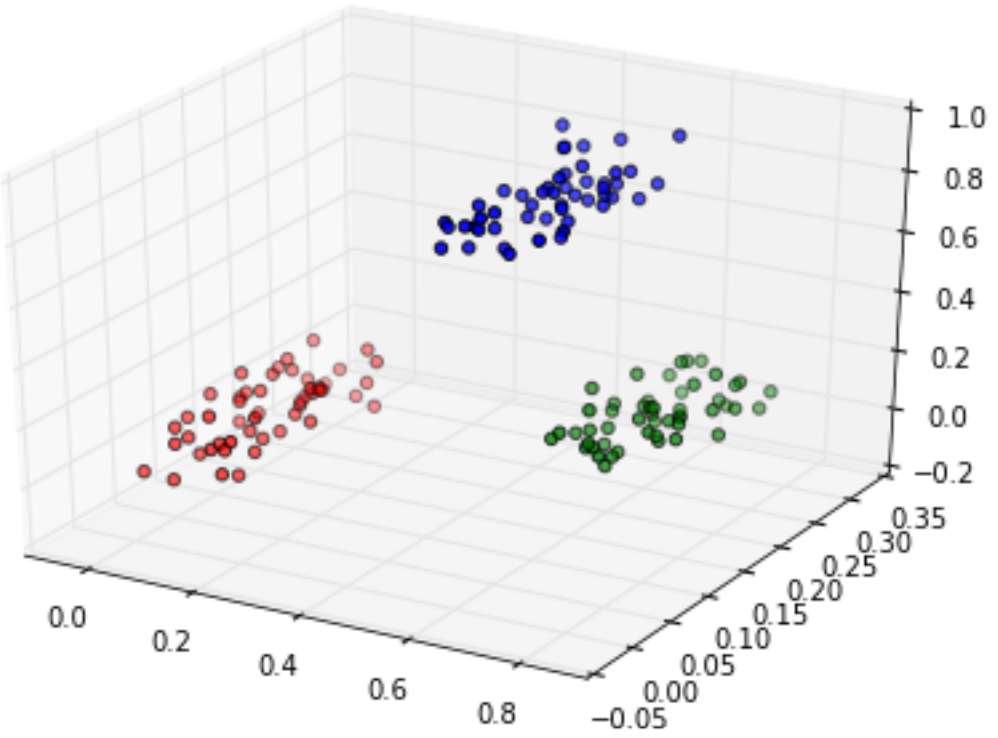
Self-organizing maps are computationally intensive to train, especially if the original space is high-dimensional or the map is large. Very large maps where the number of neurons is at least five times the number of data points are sometimes called emergent-self organizing maps – these are especially demanding to train. Somoclu is a highly efficient, parallel and distributed algorithm to train such maps, and its Python interface was recently updated. This enables fast training of self-organizing maps on multicore CPUs or a GPU from Python, albeit only on dense data, and the distributed computing capability is also not exposed. The Python interface also lets you process the output files of the command-line version, so if the data is sparse or the map was trained on a cluster, you can still use the module for visualization. Here we take a quick look at how to train and visualize a small map.

First, we import the necessary modules:

```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
import somoclu
%matplotlib inline
```

Then we generate and plot some random data in three categories:

```
c1 = np.random.rand(50, 3)/5
c2 = (0.6, 0.1, 0.05) + np.random.rand(50, 3)/5
c3 = (0.4, 0.1, 0.7) + np.random.rand(50, 3)/5
data = np.float32(np.concatenate((c1, c2, c3)))
colors = ["red"] * 50
colors.extend(["green"] * 50)
colors.extend(["blue"] * 50)
fig = plt.figure()
ax = Axes3D(fig)
ax.scatter(data[:, 0], data[:, 1], data[:, 2], c=colors)
labels = range(150)
```




## 3.1 Planar maps

We train Somoclu with default parameter settings, asking for a large map that qualifies as an emergent self-organizing map for this data:

```
n_rows, n_columns = 100, 160
som = somoclu.Somoclu(n_columns, n_rows, compactsupport=False)
%time som.train(data)
```

```
CPU times: user 6.99 s, sys: 3.33 ms, total: 6.99 s
Wall time: 5.21 s
```

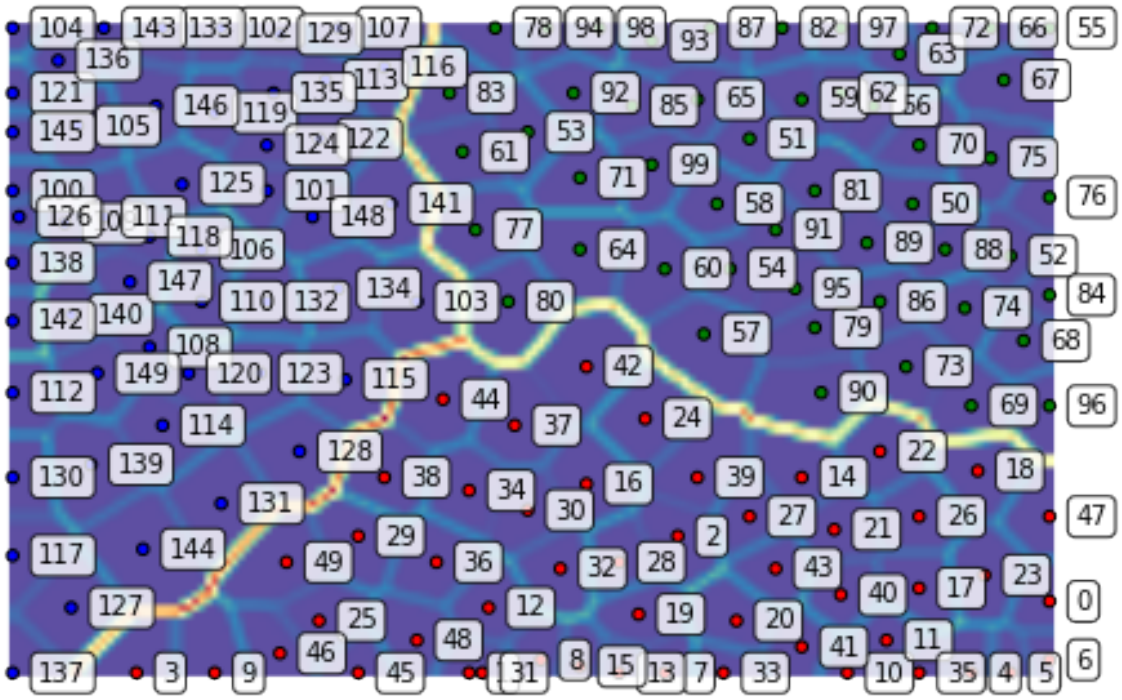
We plot the component planes of the trained codebook of the ESOM:

```
som.view_component_planes()
```

```
<module 'matplotlib.pyplot' from '/usr/lib/python3.5/site-packages/matplotlib/pyplot.
↪py'>
```

We can plot the U-Matrix, together with the best matching units for each data point. We color code the units with the classes of the data points and also add the labels of the data points.

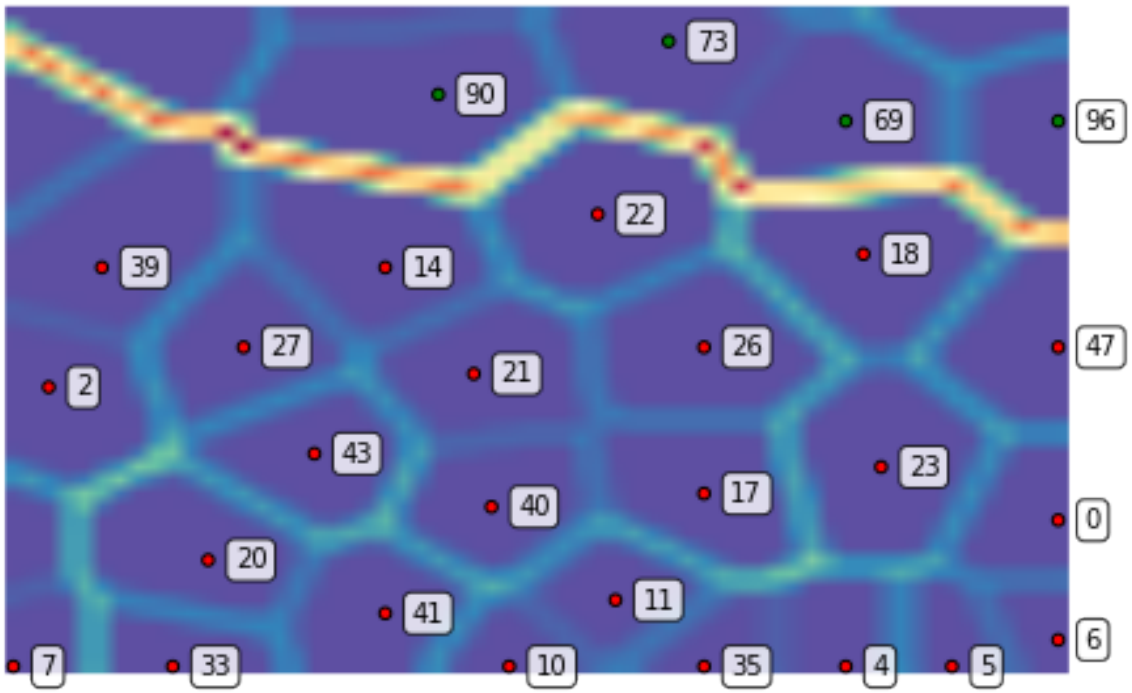
```
som.view_umatrix(bestmatches=True, bestmatchcolors=colors, labels=labels)
```




```
<module 'matplotlib.pyplot' from '/usr/lib/python3.5/site-packages/matplotlib/pyplot.
↪py'>
```

We can also zoom into a region of interest, for instance, the dense lower right corner:

```
som.view_umatrix(bestmatches=True, bestmatchcolors=colors, labels=labels,
                 zoom=((50, n_rows), (100, n_columns)))
```

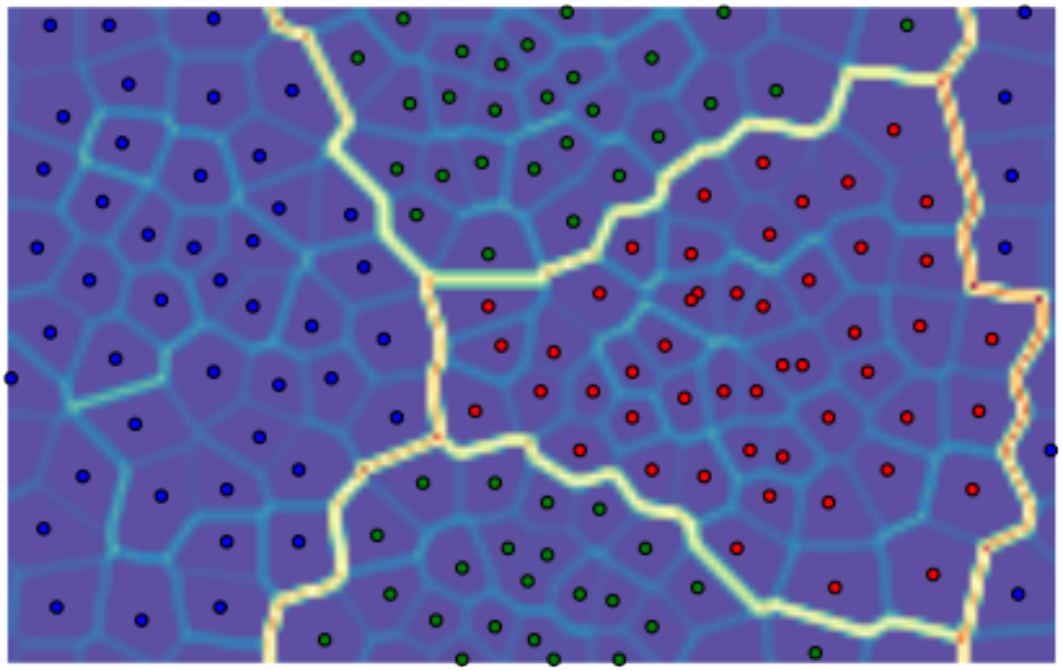



```
<module 'matplotlib.pyplot' from '/usr/lib/python3.5/site-packages/matplotlib/pyplot.
↪py'>
```

## 3.2 Toroid topology, hexagonal grid

We can repeat the above with a toroid topology by specifying the map type as follows:

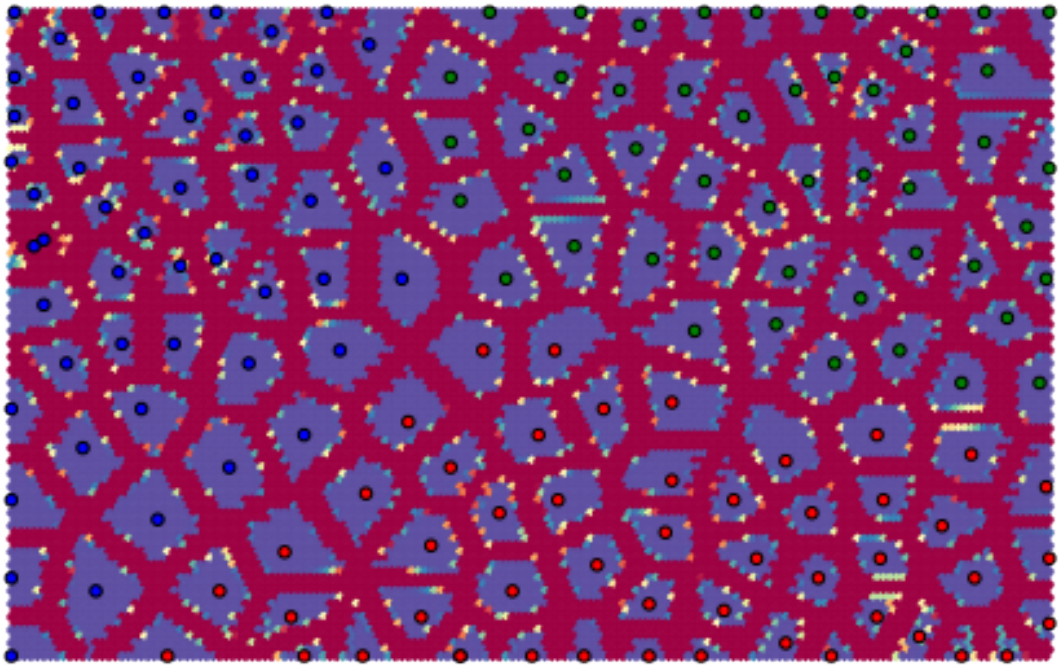
```
som = somoclu.Somoclu(n_columns, n_rows, maptype="toroid",
                      compactsupport=False)
som.train(data)
som.view_umatrix(bestmatches=True, bestmatchcolors=colors)
```



```
<module 'matplotlib.pyplot' from '/usr/lib/python3.5/site-packages/matplotlib/pyplot.
↪py'>
```

Notice how the edges of the map connect to the other side. Hexagonal neurons are also implemented:

```
som = somoclu.Somoclu(n_columns, n_rows, gridtype="hexagonal",
                      compactsupport=False)
som.train(data)
som.view_umatrix(bestmatches=True, bestmatchcolors=colors)
```



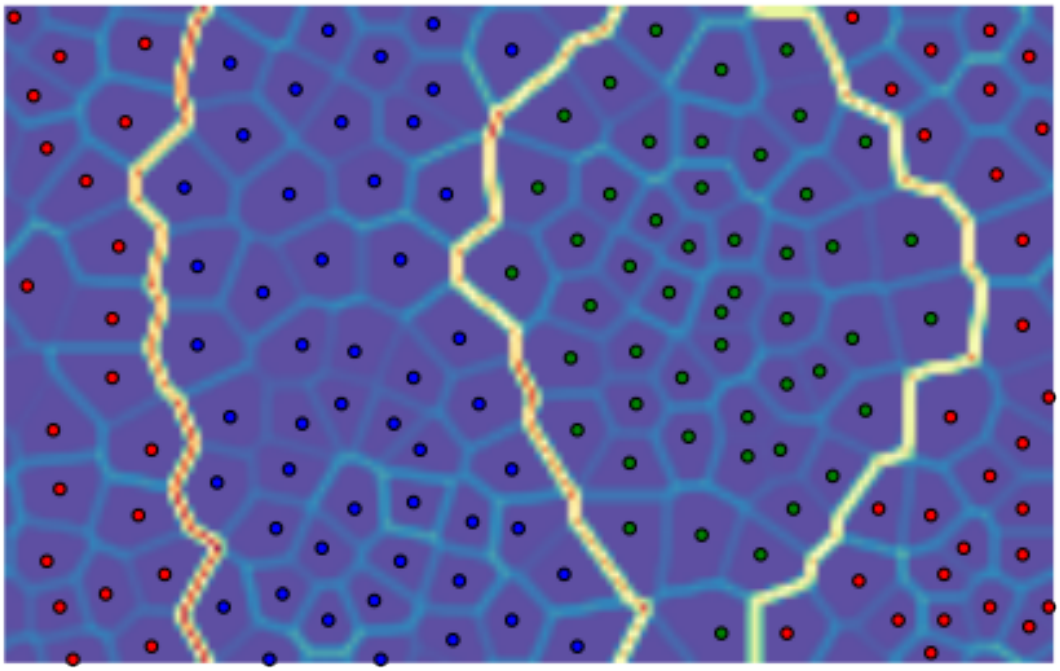
```
<module 'matplotlib.pyplot' from '/usr/lib/python3.5/site-packages/matplotlib/pyplot.
↪py'>
```

The separation of the individual points is more marked with these neurons.

## 3.3 Initialization with principal component analysis and clustering the results

We can pass an initial codebook of our choice, but we can also ask Somoclu to initialize the codebook with vectors from the subspace spanned by the first two eigenvalues of the correlation matrix. To do this, we need to pass an optional argument to the constructor:

```
som = somoclu.Somoclu(n_columns, n_rows, maptype="toroid",
                      compactsupport=False, initialization="pca")
som.train(data)
som.view_umatrix(bestmatches=True, bestmatchcolors=colors)
```

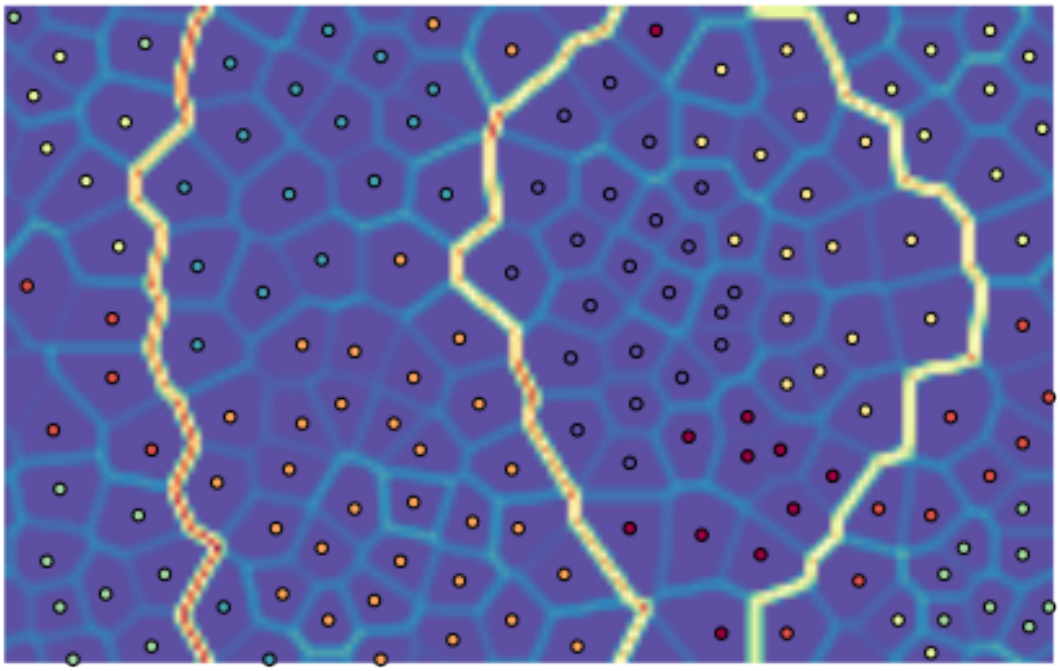


```
<module 'matplotlib.pyplot' from '/usr/lib/python3.5/site-packages/matplotlib/pyplot.
↪py'>
```

While one would expect entirely deterministic results on repeated runs with the initialization based on PCA, this is not the case. The order in which the data instances arrive matters: since Somoclu uses multiple cores, there is no control over the order of each batch, hence the maps will show small variation even with a PCA initalization.

We can also postprocess the codebook with an arbitrary clustering algorithm that is included in scikit-learn. The default algorithm is K-means with eight clusters. After clustering, the labels for each node are available in the SOM object in the `clusters` class variable. If we do not pass colors to the matrix viewing functions and clustering is already done, the plotting routines automatically color the best matching units according to the clustering structure.

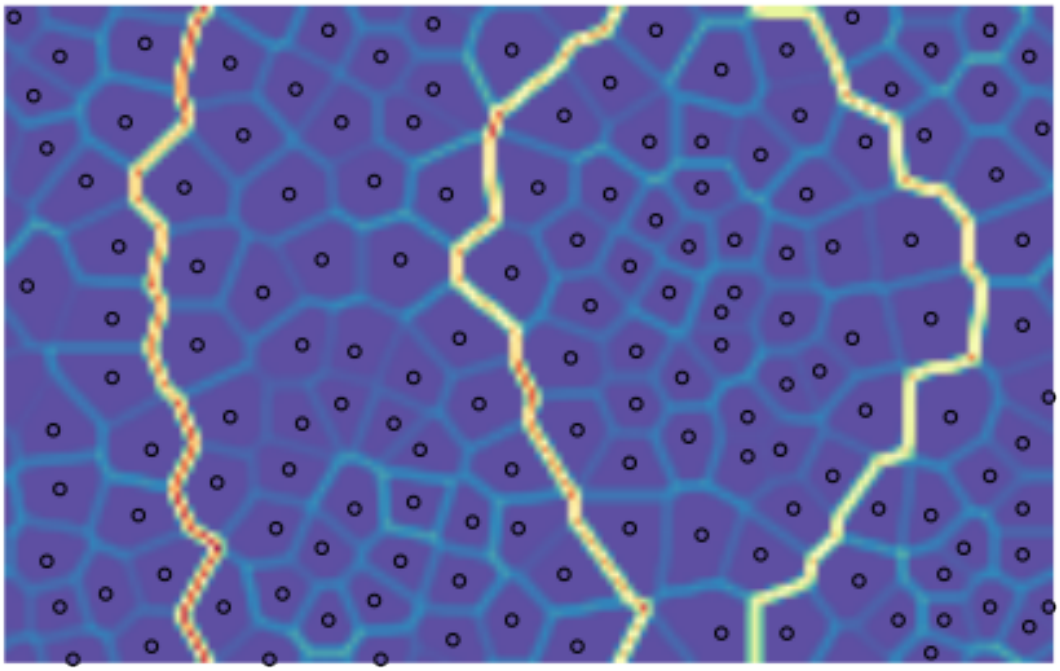
```
som.cluster()
som.view_umatrix(bestmatches=True)
```



```
<module 'matplotlib.pyplot' from '/usr/lib/python3.5/site-packages/matplotlib/pyplot.
↪py'>
```

We can, of course, choose another clustering algorithm, but topological clustering methods will make little sense with their default parameterization. DBSCAN, for instance, will assign the same class to all nodes:

```
from sklearn.cluster import DBSCAN
algorithm = DBSCAN()
som.cluster(algorithm=algorithm)
som.view_umatrix(bestmatches=True)
```



```
<module 'matplotlib.pyplot' from '/usr/lib/python3.5/site-packages/matplotlib/pyplot.
↪py'>
```

## 3.4 Evolving maps

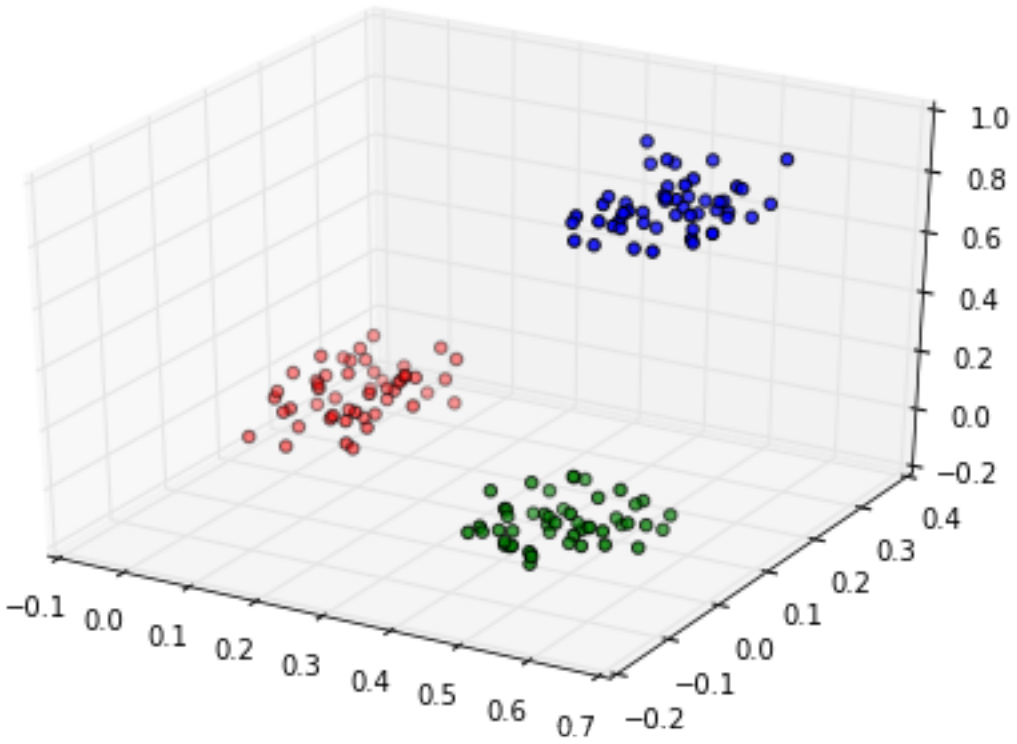
One of the great advantages of self-organizing maps is that they are incremental, they can be updated with new data. This is especially interesting if the data points retain their old label, that is, the properties of the vectors change in the high-dimensional space. Let us train again a toroid rectangular emergent map on the same data:

```
som = somoclu.Somoclu(n_columns, n_rows, maptype="toroid")
som.train(data)
```

Next, let us assume that the green cluster moves to the left, the other points remaining invariant:

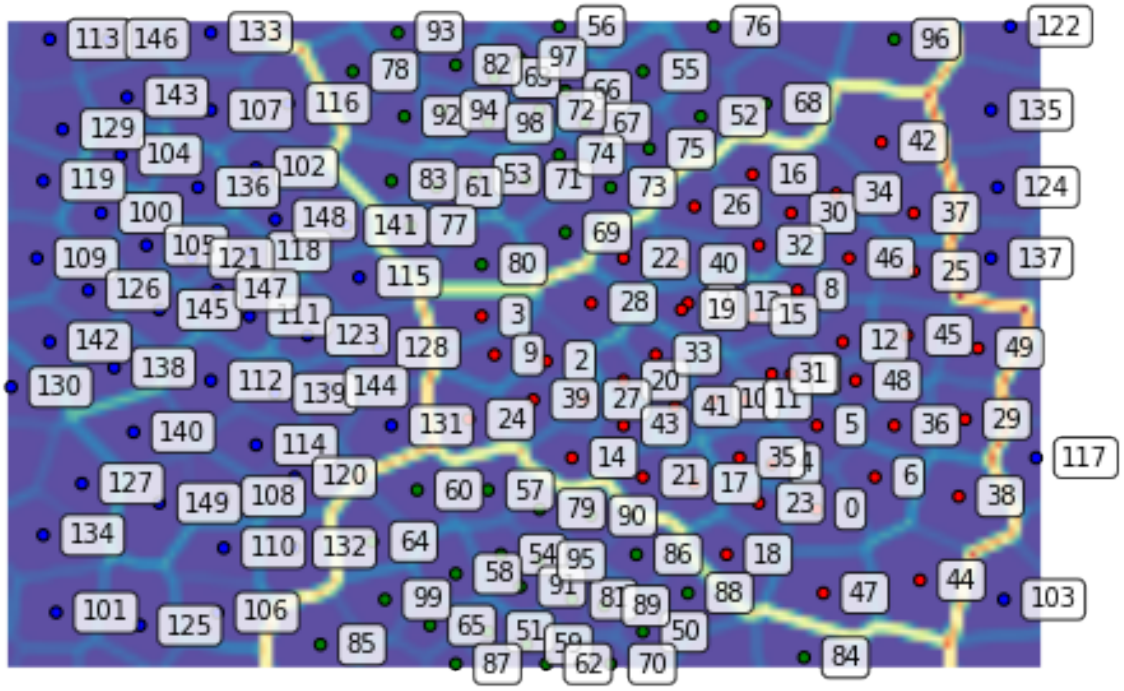
```
c2_shifted = c2 - 0.2
updated_data = np.float32(np.concatenate((c1, c2_shifted, c3)))
fig = plt.figure()
ax = Axes3D(fig)
ax.scatter(updated_data[:, 0], updated_data[:, 1], updated_data[:, 2], c=colors)
```

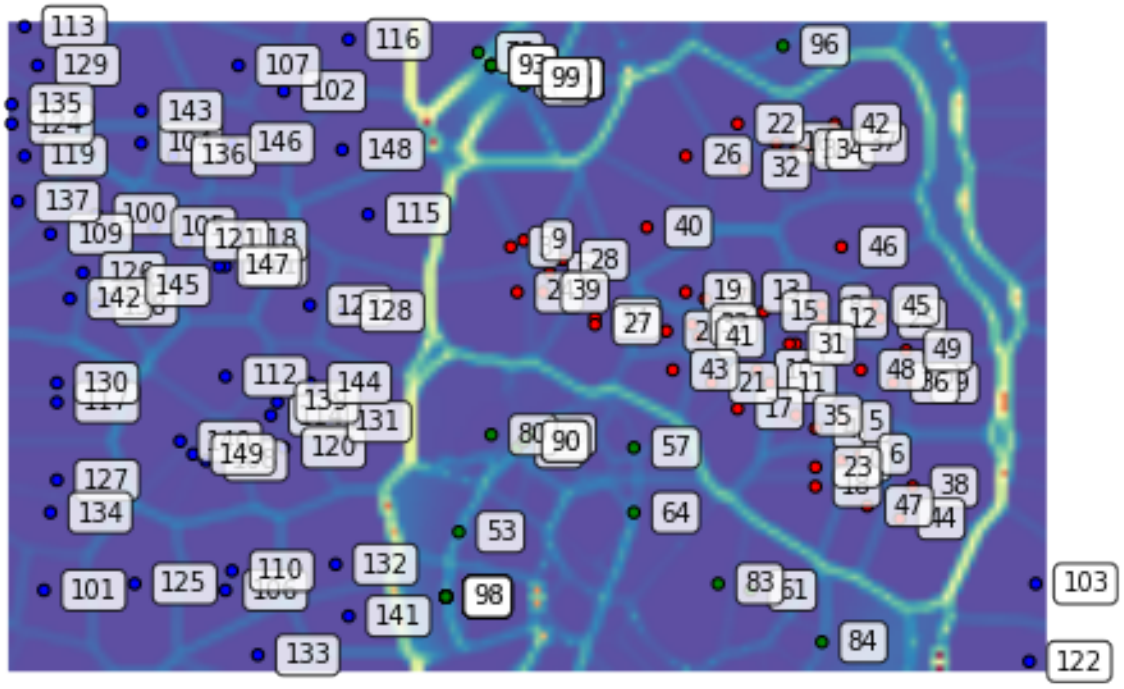
```
<mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x7fc9cf752470>
```




We can update the map to reflect this shift. We plot the map before and after continuing the training:

```
som.view_umatrix(bestmatches=True, bestmatchcolors=colors, labels=labels)
som.update_data(updated_data)
som.train(epochs=2, radius0=20, scale0=0.02)
som.view_umatrix(bestmatches=True, bestmatchcolors=colors, labels=labels)
```





```
<module 'matplotlib.pyplot' from '/usr/lib/python3.5/site-packages/matplotlib/pyplot.
↪py'>
```

As a result of the shift, the blue points do not move around much. On the other hand, the relationship of the red and green clusters is being redefined as their coordinates inched closer in the original space.

# CHAPTER 4

# Function Reference

**class Somoclu**(*n_columns*, *n_rows*, *initialcodebook=None*, *kerneltype=0*, *maptype='planar'*, *gridtype='rectangular'*, *compactsupport=False*, *neighborhood='gaussian'*, *std_coeff=0.5*, *initialization=None*)

Class for training and visualizing a self-organizing map.

**Attributes:** codebook The codebook of the self-organizing map. bmus The BMUs corresponding to the data points.

**Parameters**

- **n_columns** (*int.*) – The number of columns in the map.
- **n_rows** (*int.*) – The number of rows in the map.
- **initialcodebook** (*2D numpy.array of float32.*) – Optional parameter to start the training with a given codebook.
- **kerneltype** (*int.*) – Optional parameter to specify which kernel to use:
  - 0: dense CPU kernel (default)
  - 1: dense GPU kernel (if compiled with it)
- **maptype** (*str.*) – Optional parameter to specify the map topology:
  - "planar": Planar map (default)
  - "toroid": Toroid map
- **gridtype** (*str.*) – Optional parameter to specify the grid form of the nodes:
  - "rectangular": rectangular neurons (default)
  - "hexagonal": hexagonal neurons
- **compactsupport** (*bool.*) – Optional parameter to cut off map updates beyond the training radius with the Gaussian neighborhood. Default: True.
- **neighborhood** (*str.*) – Optional parameter to specify the neighborhood:

  - ”gaussian”: Gaussian neighborhood (default)
  - ”bubble”: bubble neighborhood function
- **std_coeff** (*float.*) – Optional parameter to set the coefficient in the Gaussian neighborhood function exp(-||x-y||^2/(2*(coeff*radius)^2)) Default: 0.5
- **initialization** (*str.*) – Optional parameter to specify the initalization:
  - ”random”: random weights in the codebook
  - ”pca”: codebook is initialized from the first subspace spanned by the first two eigenvectors of the correlation matrix
- **verbose** (*int.*) – Optional parameter to specify verbosity (0, 1, or 2).

**cluster**(*algorithm=None*)

Cluster the codebook. The clusters of the data instances can be assigned based on the BMUs. The method populates the class variable Somoclu.clusters. If viewing methods are called after clustering, but without colors for best matching units, colors will be automatically assigned based on cluster membership.

**Parameters** **algorithm** – Optional parameter to specify a scikit-learn clustering algorithm. The default is K-means with eight clusters.

**get_surface_state**(*data=None)*)

Return the dot product of the codebook and the data.

**Parameters** **data** (*2D numpy.array of float32.*) – Optional parameter to specify data, otherwise the data used previously to train the SOM is used.

**Returns** The the dot product of the codebook and the data.

**Return type** 2D numpy.array

**get_bmus**(*activation_map*)

Return Best Matching Unit indexes of the activation map.

**Parameters** **activation_map** (*2D numpy.array*) – Activation map computed with self.get_surface_state()

**Returns** The bmus indexes corresponding to this activation map (same as self.bmus for the training samples).

**Return type** 2D numpy.array

**load_bmus**(*filename*)

Load the best matching units from a file to the Somoclu object.

**Parameters** **filename** (*str.*) – The name of the file.

**load_codebook**(*filename*)

Load the codebook from a file to the Somoclu object.

**Parameters** **filename** (*str.*) – The name of the file.

**load_umatrix**(*filename*)

Load the umatrix from a file to the Somoclu object.

**Parameters** **filename** (*str.*) – The name of the file.

**train**(*data=None*, *epochs=10*, *radius0=0*, *radiusN=1*, *radiuscooling='linear'*, *scale0=0.1*, *scaleN=0.01*, *scalecooling='linear'*)

Train the map on the current data in the Somoclu object.

**Parameters**

- **data** (*2D numpy.array of float32.*) – Training data..
- **epochs** (*int.*) – The number of epochs to train the map for.
- **radius0** (*float.*) – The initial radius on the map where the update happens around a best matching unit. Default value of 0 will trigger a value of min(n_columns, n_rows)/2.
- **radiusN** (*float.*) – The radius on the map where the update happens around a best matching unit in the final epoch. Default: 1.
- **radiuscooling** – The cooling strategy between radius0 and radiusN:
  - "linear": Linear interpolation (default)
  - "exponential": Exponential decay
- **scale0** (*float.*) – The initial learning scale. Default value: 0.1.
- **scaleN** (*float.*) – The learning scale in the final epoch. Default: 0.01.
- **scalecooling** (*str.*) – The cooling strategy between scale0 and scaleN:
  - "linear": Linear interpolation (default)
  - "exponential": Exponential decay

**view_activation_map**(*data_vector=None*, *data_index=None*, *activation_map=None*, *figsize=None*, *colormap=cm.Spectral_r*, *colorbar=False*, *bestmatches=False*, *bestmatchcolors=None*, *labels=None*, *zoom=None*, *filename=None*)

Plot the activation map of a given data instance or a new data vector

**Parameters**

- **data_vector** (*numpy.array*) – Optional parameter for a new vector
- **data_index** (*int.*) – Optional parameter for the index of the data instance
- **activation_map** (*numpy.array*) – Optional parameter to pass the an activation map
- **figsize** (*(int, int)*) – Optional parameter to specify the size of the figure.
- **colormap** (*matplotlib.colors.Colormap*) – Optional parameter to specify the color map to be used.
- **colorbar** (*bool.*) – Optional parameter to include a colormap as legend.
- **bestmatches** (*bool.*) – Optional parameter to plot best matching units.
- **bestmatchcolors** (*list of int.*) – Optional parameter to specify the color of each best matching unit.
- **labels** (*list of str.*) – Optional parameter to specify the label of each point.
- **zoom** (*((int, int), (int, int))*) – Optional parameter to zoom into a region on the map. The first two coordinates of the tuple are the row limits, the second tuple contains the column limits.
- **filename** (*str.*) – If specified, the plot will not be shown but saved to this file.

**view_component_planes**(*dimensions=None*, *figsize=None*, *colormap=cm.Spectral_r*, *colorbar=False*, *bestmatches=False*, *bestmatchcolors=None*, *labels=None*, *zoom=None*, *filename=None*)

Observe the component planes in the codebook of the SOM.

**Parameters**

- **dimensions** – Optional parameter to specify along which dimension or dimensions should the plotting happen. By default, each dimension is plotted in a sequence of plots.
- **figsize** (*(int, int)*) – Optional parameter to specify the size of the figure.
- **colormap** (*matplotlib.colors.Colormap*) – Optional parameter to specify the color map to be used.
- **colorbar** (*bool.*) – Optional parameter to include a colormap as legend.
- **bestmatches** (*bool.*) – Optional parameter to plot best matching units.
- **bestmatchcolors** (*list of int.*) – Optional parameter to specify the color of each best matching unit.
- **labels** (*list of str.*) – Optional parameter to specify the label of each point.
- **zoom** (*((int, int), (int, int))*) – Optional parameter to zoom into a region on the map. The first two coordinates of the tuple are the row limits, the second tuple contains the column limits.
- **filename** (*str.*) – If specified, the plot will not be shown but saved to this file.

**view_similarity_matrix**(*data=None*, *labels=None*, *figsize=None*, *filename=None*)

Plot the similarity map according to the activation map

**Parameters**

- **data** (*numpy.array*) – Optional parameter for data points to calculate the similarity with
- **figsize** (*(int, int)*) – Optional parameter to specify the size of the figure.
- **labels** (*list of str.*) – Optional parameter to specify the label of each point.
- **filename** (*str.*) – If specified, the plot will not be shown but saved to this file.

**view_umatrix**(*figsize=None*, *colormap=<Mock name=cm.Spectral_r*, *colorbar=False*, *bestmatches=False*, *bestmatchcolors=None*, *labels=None*, *zoom=None*, *filename=None*)

Plot the U-matrix of the trained map.

**Parameters**

- **figsize** (*(int, int)*) – Optional parameter to specify the size of the figure.
- **colormap** (*matplotlib.colors.Colormap*) – Optional parameter to specify the color map to be used.
- **colorbar** (*bool.*) – Optional parameter to include a colormap as legend.
- **bestmatches** (*bool.*) – Optional parameter to plot best matching units.
- **bestmatchcolors** (*list of int.*) – Optional parameter to specify the color of each best matching unit.
- **labels** (*list of str.*) – Optional parameter to specify the label of each point.
- **zoom** (*((int, int), (int, int))*) – Optional parameter to zoom into a region on the map. The first two coordinates of the tuple are the row limits, the second tuple contains the column limits.
- **filename** (*str.*) – If specified, the plot will not be shown but saved to this file.

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