SimpSOM Documentation

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CHAPTER

ONE

INTRODUCTION

SimpSOM is a lightweight implementation of Kohonen Self-Organising Maps (SOM) for Python 2.7, useful for unsupervised learning, clustering and dimensionality reduction.

The package is now available on PyPI, to retrieve it just type pip install SimpSOM or download it from here and install with python setup.py install.

It allows to build and train SOM on your dataset, save/load the trained network weights, and display or print graphs of the network with selected features. The function run_colorsExample() will run a toy model, where a number of colors will be mapped from the 3D RGB space to the 2D network map and clustered according to their similarity in the origin space.

1.1 Dependencies

- Numpy 1.11.0 (older versions may work);
- Matplotlib 1.5.1 (older versions may work);
- Sklearn 0.15 (older versions may work), optional, needed only for clustering with algorithms other than Quality Threshold.

1.2 Example of Usage

Here is a quick example on how to use the library with a raw_data dataset:

```
#Project the datapoints on the new 2D network map.
net.project(raw_data, labels=labels)

#Cluster the datapoints according to the Mean Shift algorithm from sklearn.
net.cluster(raw_data, type='MeanShift')
```

SIMPSOM

2.1 SimpSOM package

2.1.1 Submodules

2.1.2 SimpSOM.densityPeak module

A Rodriguez, A Laio, Clustering by fast search and find of density peaks SCIENCE, 1492, vol 322 (2014)

F. Comitani @2017

class SimpSOM.densityPeak.**collection** (*coorArray*, *typeFunc='gaussian'*, *percent=0.02*) Class for a collection of point objects.

cluster_assign()

Assign a cluster to each point according according to its nearest neighbour with higher density.

core assign()

Assign points as belonging to the core or the halo of a cluster.

decision_graph (show=False, printout=True)

Calculate the decision graph, delta vs rho for the points belonging to the collection and find the cluster centers.

Parameters

- **show** (bool, optional) Choose to display the plot.
- printout (bool, optional) Choose to save the plot to a file.

get_clusterList()

Returns the indeces of the clustered points as a list.

Returns a list of lists containing the points indices belonging to each cluster

Return type clusters (list, int)

refd = None

Make sure rhos are set before setting deltas

set_deltas()

Calculate the distance from higher density points for each point in the dataset.

set_dists()

Calculate the distance matrix for all points.

```
set rhos (typeFunc='step')
```

Calculate the density for each point in the dataset.

Parameters typeFunc (str) – step function type (step, gaussian or logistic)

SimpSOM.densityPeak.densityPeak (sample, show=False, printout=False, percent=0.02)
Run the complete clustering algorithm in one go and returns the clustered indeces as a list.

Parameters

- sample (array) The input dataset
- **show** (bool, optional) Choose to display the decision graph.
- printout (bool, optional) Choose to save the decision graph to a file.

Returns a list of lists containing the points indices belonging to each cluster

Return type clusters (list, int)

```
SimpSOM.densityPeak.dist(p1, p2, metric='euclid')
```

Calculate the distance between two point objects in a N dimensional space according to a given metric.

Parameters

- **p1** (point) First point object for the distance.
- **p2** (point) Second point object for the distance.
- metric (string) Metric to use. For now only euclidean distance is implemented.

Returns The distance between the two points.

Return type float)

```
SimpSOM.densityPeak.gaussian(p1, p2, sigma)
```

Gaussian function of the distance between two points scaled with sigma.

Parameters

- p1 (point) First point object for the distance.
- p2 (point) Second point object for the distance.
- **sigma** (*float*) The scaling factor for the distance.

Returns value of the gaussian function.

Return type (float)

```
class SimpSOM.densityPeak.pt (coordinates)
```

Class for the points to cluster.

```
set_delta(coll)
```

Calculate the distance of the point from higher density points and set the nearest neighbour. [Deprecated]

Parameters coll (collection) – collection containing all the points of the dataset used to calculate the distance.

```
set dist(coll)
```

Calculate the distances from all other points in a collection. [Deprecated]

Parameters coll (collection) – collection containing all the points of the dataset used to calculate the distances.

```
set_rho (coll, typeFunc='step')
```

Calculate the density of the single point for a given dataset. [Deprecated]

Parameters

- **coll** (collection) collection containing all the points of the dataset used to calculate the density.
- **typeFunc** (str) step function type (step, gaussian kernel or logistic).

```
SimpSOM.densityPeak.sigmoid(p1, p2, sigma)
```

Logistic function of the distance between two points scaled with sigma.

Parameters

- p1 (point) First point object for the distance.
- **p2** (point) Second point object for the distance.
- **sigma** (float) The scaling factor for the distance.

Returns value of the logistic function.

Return type (float)

```
SimpSOM.densityPeak.step(p1, p2, cutoff)
```

Step function activated when the distance of two points is less than the cutoff.

Parameters

- p1 (point) First point object for the distance.
- **p2** (point) Second point object for the distance.
- **cutoff** (*float*) The cutoff to define the proximity of the points.

Returns 1 if the points are closer than the cutoff, 0 otherwise.

Return type (int)

```
SimpSOM.densityPeak.test()
```

Run the complete clustering algorithm on a test case and print the clustered points graph.

2.1.3 Module contents

SimpSOM (Simple Self-Organizing Maps) v1.2.0 F. Comitani @2017

A lightweight python library for Kohonen Self-Organising Maps (SOM).

```
SimpSOM.run_colorsExample()
```

Example of usage of SimpSOM: a number of vectors of length three (corresponding to the RGB values of a color) are used to briefly train a small network. Different example graphs are then printed from the trained network.

class SimpSOM.somNet (netHeight, netWidth, data, loadFile=None)

Kohonen SOM Network class.

Clusters the data in a given array according to the SOM trained map. The clusters can also be plotted.

Parameters

• array (np.array) - An array containing datapoints to be clustered.

- **type** (*str*, *optional*) The type of clustering to be applied, so far only quality threshold (qthresh) algorithm is directly implemented, other algorithms require sklearn.
- **cutoff** (*float*, *optional*) Cutoff for the quality threshold algorithm. This also doubles as maximum distance of two points to be considered in the same cluster with DBSCAN.
- **percent** (*float*, *optional*) The percentile that defines the reference distance in density peak clustering (dpeak).
- quant (float, optional) Quantile used to calculate the bandwidth of the mean shift algorithm.
- **savefile** (bool, optional) Choose to save the resulting clusters in a text file.
- **filetype** (*string*, *optional*) Format of the file where the clusters will be saved (csv or dat)
- **show** (bool, optional) Choose to display the plot.
- **printout** (bool, optional) Choose to save the plot to a file.

Returns A nested list containing the clusters with indexes of the input array points.

Return type (list of int)

data = None

Load the weights from file or generate them randomly.

diff graph (show=False, printout=True)

Plot a 2D map with nodes and weights difference among neighbouring nodes.

Parameters

- **show** (bool, optional) Choose to display the plot.
- **printout** (bool, optional) Choose to save the plot to a file.

find bmu (vec)

Find the best matching unit (BMU) for a given vector.

Parameters vec (np.array) – The vector to match.

Returns The best matching unit node.

Return type bmu (somNode)

nodes graph (colnum=0, show=False, printout=True)

Plot a 2D map with nodes and weights values

Parameters

- **colnum** (*int*) The index of the weight that will be shown as colormap.
- **show** (bool, optional) Choose to display the plot.
- printout (bool, optional) Choose to save the plot to a file.

project (array, colnum=0, labels=[], show=False, printout=True)

Project the datapoints of a given array to the 2D space of the SOM by calculating the bmus. If requested plot a 2D map with as implemented in nodes_graph and adds circles to the bmu of each datapoint in a given array.

Parameters

- **array** (np.array) An array containing datapoints to be mapped.
- **colnum** (*int*) The index of the weight that will be shown as colormap.
- **show** (bool, optional) Choose to display the plot.
- printout (bool, optional) Choose to save the plot to a file.

Returns bmu x,y position for each input array datapoint.

Return type (list)

save (fileName='somNet_trained')

Saves the nodes weights to a file.

Parameters fileName (str, optional) - Name of file where the weights will be saved.

train (epochs=5000, startLearnRate=0.01)

Train the SOM.

Parameters

- **epochs** (*int*) Number of training iterations.
- **startLearnRate** (*float*) Initial learning rate.

update_lrate(iter)

Update the learning rate.

Parameters iter (int) – Iteration number.

update sigma(iter)

Update the gaussian sigma.

Parameters iter (int) – Iteration number.

class SimpSOM.**somNode** (x, y, numWeights, weiArray=[])

Single Kohonen SOM Node class.

get_distance (vec)

Calculate the distance between the weights vector of the node and a given vector.

Parameters vec (np.array) – The vector from which the distance is calculated.

Returns The distance between the two weight vectors.

Return type (float)

get nodeDistance(node)

Calculate the distance within the network between the node and another node.

Parameters node (somNode) – The node from which the distance is calculated.

Returns The distance between the two nodes.

Return type (float)

update_weights (inputVec, sigma, lrate, bmu)

Update the node Weights.

Parameters

- **inputVec** (np.array) A weights vector whose distance drives the direction of the update.
- **sigma** (float) The updated gaussian sigma.
- **lrate** (*float*) The updated learning rate.

• bmu (somNode) - The best matching unit.

CHAPTER

THREE

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PYTHON MODULE INDEX

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