# graph2class

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def calc\_bc(G, return\_dict):

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Parallel subprocess function to calculate the betweenness centrality.

## **Args**

• G ([networkx graph]): graph

#### Returns

[dictionary]: betweeness centrality dictionary from multiple processes

def calc\_shortest\_pthlen(G, return\_dict):

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Parallel subprocess function to calculate the average shortest path length.

# **Args**

• G ([networkx graph]): graph

#### Returns

[dictionary]: average shortest path length dictionary from multiple processes

# def calc\_graph\_features(G):

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Calculates several graph network features. If not connected, largest subgraph is used. Uses multiprocessing for parallelsim.

## Args

• G ([networkx graph]): graph

#### **Returns**

[dictionary]: features dictionary

def similarity\_measure(x1, x2):

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calculates the similarity between two feature values. similarity = 1 - the relative distance between features (x1 and x2)

## **Args**

- x1 ([float]): feature from graph 1 (must range between 0,1)
- x2 ([float]): feature from graph 2 (must range between 0,1)

## **Returns**

[float]: returns the relative similarity between 2 features

**def calc\_similarity\_score**(G1\_dict, G2\_dict, feature\_list):

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calculates the similarity score of two graphs

# Args

- **G1\_dict ([dict] or [Pandas datafrane]):** graph 1 features dictionary or dataframe. must be able to use a key to access values
- **G2\_dict ([dict] or [Pandas datafrane]):** graph 2 features dictionary or dataframe. must be able to use a key to access values
- features\_list ([list]): list of graph features to compare. must be keys in graph features dictionary (above)

#### Returns

[float]: similarity score (0,1) where 1 is an identical graph.

def process\_graphs(graph\_fnames):

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take a list of graph files, calculate their features, and return as a dataframe

## Args

• graph\_fnames ([list]): list of graph filenames to process

#### **Returns**

[pandas dataframe]: dataframe containing graph features for each graph in filename list

def classify\_graphs(class\_file\_list, sample\_file\_list, feature\_list):

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Classifies a similarity score from a list of Class and Sample graphs

## **Args**

- **class\_file\_list ([list]):** list of control/reference graph files (classes)
- sample\_file\_list ([list]): list of non-control/non-reference graph files (samples)
- **feature\_list ([list]):** list of which features to use for similarity score. must be a valid key to the graph features dictionary/dataframe (above)

#### Returns

[pandas dataframe]: each colummn is a class and each row is the similarity score of the sampled graph

def process\_similarity\_df(class\_similarity\_df):

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Generates y\_true and y\_pred based on the similarity score dataframe.

y\_true is a list where each index is a class and each value is the class value. E.g., class 1 is y\_true[1] = 1, class 2 is y\_true[2]=2, etc.

y\_pred is a list where each index is a sample and each value is the maximum similarity score for that sample.

Note: This assumes the correct classification is along the diagonal of the similarity matrix/dataframe.

ref: https://scikit-

 $learn.org/stable/modules/generated/sklearn.metrics.classification\_report.html \# sklearn.metrics.classification\_report. \\$ 

# Args

• class\_similarity\_df ([pandas dataframe]): each column is a class graph and each row is a sample graph. A\_ij is the similarity score between graphs i and j. The exception is one column 'name' which contains the names of the sampled graphs for each row.

# **Returns**

([tuple of lists]): y\_true, y\_pred