Experimenting with Machine Learning on Graphs

If your computer has limited amount of memory or just if you want to save time when experimenting, you can work on a subgraph of the airport dataset, for instance only with the most important nodes, or only nodes in a region of the world.

1. Training and Validation set
   (a) Let's start by creating a training set for the Airport dataset. A training set is composed of t edges (taken at random) and t pairs of nodes without edges (taken at random). You can use `random.sample` (https://www.geeksforgeeks.org/python-random-sample-function/) to pick randomly edges (or pairs of nodes). Typically, you can choose $t = L/6$(L is the number of edges in the original graph). Keep randomly chosen edges and non-edges in separated lists. Note that, when the graph is large, creating the list of all pair of nodes without edges is costly. Instead, you can select 2 list of nodes with repetitions of the same size, and then consider that to each position of the lists corresponds a pair of nodes. Don't forget to remove loops, duplicates and actual edges.
   (b) Remove edges of the training set from the graph.(`remove_edges_from`)
2. Computing heuristics
   (a) Using existing functions in `networkx` ,(`adamic_adar_index` , etc., see https://networkx.org/documentation/stable/reference/algorithms/link_prediction.html) compute common heuristics between all (or a sample of) pairs of nodes on the graph.
   (b) Find the 20 node pairs of higher and lower scores, for each heuristic. Are these rankings intuitively a good starting point? (A simple way to sort is to transform the output of heuristics into dictionaries (dict(nx.adamic_adar_index(...))), and then use the same method as in previous experiments (or search for something like *"sort dictionary by value python"* in google.)
3. Using Machine Learning
   (a) We will use the `sklearn.linear_model.LogisticRegression` function to train our model. To train the model, we will use the following method: `clf = LogisticRegression().fit(X, y)` , as in the example of the documentation. We need to prepare X and y. X represents the *input* and can be provided as a list of list: each of the internal list corresponds to the features of one node pair. y is the list of values to predict. For instance, `X=[[1,3,1],[2,20,10]]` , `y=[1,0]` corresponds to a training set with 2 examples, each having 3 features, the first one being an edge and the second one a non-edge. Prepare X (combining all computed heuristics) and y from the training set. (you can create y by using something like `[1]*len(train_edges)+[0]*len(train_non_edges)` . For X, you code can look something like `[[AA[e],CN[e],PA[e]] for e in train_edges+train_non_edges]`
   (b) Train the model. (call `fit(X,y)`)
   (c) Use function `LogisticRegression.predict_proba(Xvalidate)` to get predictions for all pairs of nodes without edges in the original graph.
   (d) Sort the most likely pairs of nodes. Check the results.
4. Going further: Node attributes prediction
   (a) Hide the country information of 20% of airports. We could imagine that this information was missing in the database. Propose a ML based method to assign a country to those airports and check the results.