Approximating Network Centrality Measures Using Node Embedding and Machine Learning

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Abstract

Analyzing and extracting useful information from real-world complex networks has become a key challenge due to the their large sizes such networks achieve nowadays. For instance, depending on the intended node centrality, it becomes unfeasible to compute it for such large complex networks due to the high computational cost. One way to tackle this problem is by developing fast methods capable of approximating the network centralities. In this paper, we propose an approach capable of efficiently approximating node centralities for large networks using Neural Networks and Node Embedding techniques. We thus call our approach the Network Centrality Approximation using Graph Convolutional Networks (NCA-GCN) model. In contrast to recent related work, the NCA-GCN model requires only the degree centrality of each node in order to predict any other centrality. We show that the NCA-GCN model works well in different node centralities for different network sizes.

1 Introduction

Networks are present in several real-world applications spread among different disciplines, such as biology, mathematics, sociology, and computer science, just to name a few. Therefore, network analysis is a crucial tool for extracting relevant information. However, this analysis may be hindered when performed over large complex networks, given the high computational cost for some network analysis methods. This problem is especially challenging when we consider that nowadays many networks extracted from real-world applications are usually large in scale.

Among the most used approaches for network analysis, node centrality is an essential concept related to the assessment of the relative importance of nodes given some importance criterion. There are several different centrality measures, each with their own definition of a central (i.e., important) node. For example, the most basic node centrality is the degree centrality, which measures the number of connections a node has as a proxy for its relative importance in the network. In this case, a node is considered central when it has many connections. Other examples of common centrality measures are betweenness, closeness, and eigenvector centralities, among others. Centrality measures have already been successfully applied to many real-world problems, as for example: (i) optimization of computer networks [1–4]; (ii) transportation networks [5–8]; (iii) biological networks [9, 10]; (iv) recommendation systems [11, 12]; (v) reinforcement learning [13–16]; and (vi) social networks [17, 18], to name a few domains of application. For more applications, refer to [19–21] for a more in-depth review of real-world examples of network centrality usage.

The size of many complex networks found in real-world applications are large. Depending on the size of a network, the direct calculation of a given network centrality measure may become infeasible due to the required high computational cost. Therefore, many solutions have been proposed for approximating or even calculating the actual centrality value for large networks in a reasonable time, given some constraint or specific target. The first solutions focused on sampling techniques used for static graphs [22–25] or parallel algorithms for specific centrality measures [26]. More recently, researchers have focused on the problem of approximating network centrality for evolving graphs [27, 28]. Another recent approach is to use a Neural Network (NN) to predict node centrality based on lower order node features [19, 29, 30], which is the approach that inspired this work.
In this paper, we focus on the problem of approximating node centrality measures for large complex networks using node embedding and machine learning. To that end, we propose an approach based on Graph Convolutional Networks (GCNs) [31]. Therefore, we call our proposal Network Centrality Approximation using Graph Convolutional Networks (NCA-GCN) model. We train our model over a set of artificial complex networks and then the model can be used to predict the network centrality value of a given node in larger networks. To achieve this, our model only requires the degree centrality of a node in order to predict its value for other centrality measures, whereas other node features are inferred by the GCN model. The main contribution of our approach in relation to other similar works [19, 29, 30] is that we present a more general model that uses little node information and works well for different types of graphs.

The remainder of this paper is organized as follows. In Section 2, we present the basic concepts of node centrality, node embedding, and neural networks, which compose the foundations of this work. We then present some of the related work on node embedding and network centrality approximation in Section 3. In Section 4, we introduce our proposed NCA-GCN model, followed by the description of the experiments and obtained results in Section 5. Finally, we conclude the paper and discuss some future work in Section 6.

2 Centrality Measures

In this section, we briefly describe some important network centrality measures that are widely used and that we consider in this work. In this context, a network is typically represented by a graph $G = (V, E)$, where $V$ is the set of vertices (nodes) and $E$ is the set of edges in the graph. The number of vertices (nodes) in the graph is $n = |V|$. The graph's connectivity is represented by an adjacency matrix $A$, where $a_{ij} \in A$ is the weight of the edge that connects nodes $i$ and $j$. For unweighted graphs, $a_{ij} = 1$ if there exists an edge between nodes $i$ and $j$, and $a_{ij} = 0$ otherwise. For the scope of this work, we consider unweighted undirected graphs.

There are several ways to define the relative importance of a given node in a graph. This is done using centrality measures: A score given to each node that measures its relative importance in a given context; thus leading to a node ranking.

2.1 Degree Centrality

The degree $d_i$ of node $i$ is given by $d_i = \sum_{j \in V} a_{ij}$. The degree centrality allows the identification of highly connected nodes. Each node then contributes equally to the degree centrality of each of its neighbors. This represents the most simple centrality measure, but sometimes this centrality is insufficient to explain certain node properties, leading to the definition of more meaningful centrality measures.

2.2 Eigenvector Centrality

In contrast to the degree centrality, in the eigenvector centrality, central nodes contribute more to the centrality of their neighbor nodes. The eigenvector centrality of a node is thus proportional to the sum of the eigenvector centralities of its neighbor nodes. Therefore, central nodes are usually connected to other central nodes or are connected to a relatively large number of low centrality nodes. The most central nodes typically have both. The eigenvector centrality $x_i$ of node $i$ is formally defined as:

$$x_i = \frac{1}{\lambda} \sum_{j \in V} a_{ij}x_j,$$

where $\lambda$ is an eigenvalue of the adjacency matrix $A$ associated with the eigenvector $x$. Therefore, the eigenvector centrality of each node in a graph can be calculated by solving the eigenvector problem

$$Ax = \lambda x.$$
2.3 Closeness Centrality

The closeness centrality of a node is given by the mean distance from this node to all other nodes in the graph. The formal definition of closeness centrality for node $i$ is the inverse of the mean minimum distance from that node to all other $n - 1$ nodes in the network, given by

$$c_i = \frac{n - 1}{\sum_{j \neq i \in V} \delta(i, j)},$$

(3)

where $\delta(i, j)$ is the distance between nodes $i$ and $j$. A high closeness centrality means that the node is on average closer to all other nodes in the network.

2.4 Harmonic Centrality

Harmonic centrality \cite{32} represents a variation of the closeness centrality. Instead of calculating the inverse of the overall sum of minimum distances from one node $i$ to all other nodes, harmonic centrality computes the sum of the inverse minimum distances, i.e.

$$h_i = \sum_{j \neq i \in V} \frac{1}{\delta(i, j)},$$

(4)

Note that this allows infinity distances (for unconnected graphs), which is not allowed for closeness centrality.

2.5 Betweenness Centrality

In some scenarios, it is desirable to identify nodes by which many shortest paths pass through. This is achieved by betweenness centrality. In other words, the betweenness centrality of node $i$ measures the relation of the number of shortest paths (between any two nodes) that passes through a specific node $i$ and the total number of shortest paths connecting all node pairs. The betweenness centrality of node $i$ is then formally given by:

$$b_i = \sum_{s \neq i \neq t \in V} \frac{\sigma_{st}(i)}{\sigma_{st}},$$

(5)

where $\sigma_{st}(i)$ is the number of shortest paths between nodes $s$ and $t$ that passes through $i$ and $\sigma_{st}$ is the total number of shortest paths between $s$ and $t$.

3 Related Work

In this section, we briefly review some of the recent advances in node centrality prediction and node embedding, which are the techniques that lay the foundation for this work.

3.1 Node and Graph Embedding

Node and graph embedding allows methods to encode certain node characteristics and topological information into low dimension vectors. There are several different embedding methods, which can be separated into different classes \cite{33}: (i) methods based on factorization; (ii) methods based on random walks; and (iii) methods based on deep learning. For this work, we focus on methods based on deep learning. The interested reader may refer to one of the many recent surveys on node and graph embedding \cite{33,34,35,36} for a more in-depth analysis of this area.

Wang et al. \cite{37} presents the Structural Deep Network Embedding (SDNE), a semi-supervised model that builds node embeddings that minimize the First and Second-Order proximity measures. The former refers to the proximity between two nodes based on the weight of the edge connecting them. The latter defines the similarity between two nodes based on their neighborhood, where two nodes are similar when their neighborhood are similar. Therefore, SDNE uses two modules in order to build node embeddings that obey these two proximity measures: an unsupervised and a supervised model. The unsupervised model is comprised of two autoencoders that receive a vector $x_i, x_j \in \mathbb{R}^n$ for nodes $i$ and $j$, where $n$ is the number of vertices. The vector $x_i$ is actually the row $i$ of the graph’s adjacency matrix. These autoencoders learn how to map the neighborhood of each node into a latent state representation within
their hidden layers that consider information of each node’s neighborhood. The supervised model, in its turn, uses the latent representation of the autoencoders and minimizes the distance between the latent representation of nodes that are connected in the graph. This allows the model to learn a node embedding that minimizes the first and second-order proximity at the same time.

Graph Convolutional Networks (GCN) [31] represent another node embedding method that uses the data and its underlying graph structure to build powerful latent representations of a node. This architecture receives a matrix \( X \in \mathbb{R}^{N \times C} \) of \( C \) features for each of the \( N \) nodes as an input and outputs a matrix \( Z \in \mathbb{R}^{N \times F} \) of \( F \) higher-order features for each of the \( N \) nodes, which can be the label of each node, for example (\( F \) being the number of possible labels). Each layer \( l \) of the neural network computes an intermediate matrix \( H \) given by:

\[
H^{(l+1)} = \sigma \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right),
\]

where \( \sigma \) is an activation function, \( \tilde{A} = A + I \) is the adjacency matrix plus the identity matrix \( I \), \( \tilde{D}_{ii} = \sum_j \tilde{A}_{ij} \), and \( W^{(l)} \) is the parameter matrix of layer \( l \). Here, \( H^0 \) is given by the input matrix \( X \) and the output matrix \( Z \) corresponds to the matrix \( H \) of the last layer. This formulation is especially interesting because it is isomorphic graph invariant, i.e., the result is the same regardless of the order of the nodes (which yields different adjacency and diagonal matrices).

Structure2Vec [35] is a recent graph embedding approach where each node is codified by considering a given information of the node and the embedding of all of its neighborhood. It is a recursive approach that updates each node embedding through a given number of iterations. After \( T \) iterations, the node embedding \( \mu_i^T \) of node \( i \) in iteration \( T \) considers the topological information of all nodes in its \( T \)-hop neighborhood. If we run the method for \( D \) iterations, where \( D \) is the diameter of the graph, then the node embedding considers the topological information of the entire graph. Since the diameter of real-world networks is usually small compared with the network size, then the number of iterations required to embed the whole graph is also small. Formally, the embedding \( \mu_i \) of a node \( i \) at iteration \( t \) is defined as:

\[
\mu_i^{t+1} = F \left( x_i, \sum_{n \in \mathcal{N}(i)} \mu_n^t \right),
\]

where \( F \) is any nonlinear function, \( \mathcal{N}(i) \) is the set of neighbors of node \( i \), and \( x_i \) is any relevant node information that should be embedded. The node embeddings are then summed in order to generate a graph embedding, which is used for graph classification problems.

Hanjun et al. [39] adopt a similar approach, also based on the Structure2Vec embedding, but instead of using it for classification problems, the authors adapt the method to work with reinforcement learning in order to solve combinatorial graph problems.

### 3.2 Network Centrality Prediction

There has been several attempts to create reliable methods capable of efficiently predicting node centrality measures in complex networks. A notable method for approximating centrality measures is presented in [22] and [23], where betweenness and closeness centralities are approximated using a sampling technique, respectively. These methods calculate the single source shortest path (SSSP) for a given sample of nodes, which is then used to define their exact centrality value. These SSSPs are also used to approximate the centrality value of other non-sampled nodes that belong to the SSSP. Brandes et al. [24] complements these approaches by testing different sampling methods, where it shows that the best way to select the node sample is through random selection. Cohen et al. [23] improves over the sampling technique for closeness centrality by also using a technique called pivoting, which essentially approximates the closeness centrality of a node \( v \) by the value of the closest node \( x \) that belongs to the sample set, called pivot. Other existing sampling methods for approximating the betweenness centrality improved upon the previous ideas by adding an error guarantee value [10] and adapting sampling techniques for evolving graphs [27]. However, as stated by Grando et al. [19], sampling techniques are still computationally expensive, given that even calculating the exact betweenness or closeness centrality values for only a small portion of the nodes is still costly.

More recently, Grando et al. [29] present a more general approach that approximates 8 different node centralities by using a neural network (NN). The NN model predicts one centrality value by receiving as inputs for each node the 7 remaining centrality values. The main novelty of this approach is that
Figure 1: Neural network architecture used for the proposed Network Centrality Approximation using Graph Convolutional Networks (NCA-GCN) model. The inputs are represented in yellow, hidden layers are in blue, constants are represented in green, and the output is represented in red. For each batch, we require the feature matrix containing the features of all nodes, the node id vector containing the id of all nodes in the batch, and the \( \tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)} \) matrix, which is treated as a constant. The output is a single value for each node in the batch, representing the normalized rank of the desired centrality.

it is very fast to predict a node centrality after the NN is properly trained. The drawback is that this model requires the computation of 7 node centralities in order to predict the 8th centrality value for each node. The authors then expanded upon their initial idea [19, 30] by creating a NN model that receives only 2 centrality values as an input for each node in order to predict any other centrality: (i) degree and (ii) eigenvector centralities. This marks a great improvement over the initial idea, given that the degree and eigenvector centralities both have a low computational cost and can be used to predict the values of centralities with a high computational cost, such as betweenness and closeness. The NN is trained using a set of artificial complex networks with different sizes (varying from 100 to 1000 nodes), and the exact centrality measures for each node. After the model is trained, it generalizes well for other networks, even larger ones.

We present here a parallel model for predicting node centralities that requires less information for each node and that achieves similar results to the work presented by Grando et al. [19]. In Section 4.2, we present the details of our model and how it differentiates from the current state-of-the-art.

4 The Proposed NCA-GCN Model

We present here the Network Centrality Approximation using Graph Convolutional Networks (NCA-GCN) model, capable of approximating any node centrality using only the degree centrality as an input. The approach outlined in this paper is inspired by two distinct approaches: (i) the NN node centrality prediction model recently introduced by Grando et al. [19]; and (ii) the Graph Convolutional Network (GCN) node embedding method [31]. The proposed idea is to codify each node into an embedding vector that is calculated using only the degree centrality of a given node. We then pass these inputs to a NN model, which outputs an approximation of the desired centrality, which can be any centrality other than the degree (since it is already used as input). In the remainder of this section, we discuss our proposal in more details.

4.1 Node Embedding and Neural Network model

Each node is codified using the GCN node embedding technique. The feature matrix \( X \) (Eq. 6) used here is comprised solely of the rank of the degree centrality of the nodes in the graph. The nodes are embedded through a recursive process, as depicted in Eq. 6 where the number of layers determines the number of iterations. We parameterize the node embedding process of Eq. 7 as follows:

\[
H^{(l+1)} = \text{relu} \left( \tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)} \right),
\]

(8)

where \( \text{relu}(.) \) is the rectified non-linearity function and the remaining variables are the same as in Eq. 6.

We used 2 layers, where \( W^1 \in \mathbb{R}^{C \times F}, W^2 \in \mathbb{R}^{F \times F}, C \) being the number of initial used features and \( F \) being the embedding size. As already mentioned, we use only a single feature: the normalized degree rank of a node, thus, \( C = 1 \). After computing the output matrix \( Z \), we select only the embeddings of the nodes being analyzed in the current batch. The selected nodes are given by:

5
where $O \in \mathbb{R}^{b \times N}$ is the one-hot encoding of the id of the nodes in the batch and $b$ represents the size of the batch. The centrality prediction outputted by the NN is then given by:

$$c = \text{relu}(\text{relu}(\mu W^3)W^4)W^5,$$

where $W^3 \in \mathbb{R}^{F \times k}$, $W^4 \in \mathbb{R}^{k \times k}$ and $W^5 \in \mathbb{R}^{k}$, $k = \frac{F}{2}$ being the number of neurons that we set in the fully connected layers. As we can see from Eq. 8 and 10, the GCN method requires the complete adjacency matrix $A$ and the one-hot encoding of the nodes in the current batch. To achieve a fast training time for the architecture, we use sparse tensor representations. The overall architecture of our model is presented in Figure 1.

The input of our proposed model is the normalized rank value of the degree centrality of a given node and the output is the normalized value of the rank of the desired higher order centrality, both within the range $[0, 1]$. Therefore, the only information required by our model is the degree centrality of each node, which is a very low cost and simple centrality to be obtained. We experimented using the normalized value of the exact degree centrality as an input, but the results were not as good as using the normalized value of the degree rank, even when we intended to predict the normalized value of the exact centrality as output.

The source code for the model presented here is publicly available at GitHub.\footnote{https://github.com/MatheusMRFM/NCA-GCN}

4.2 Training the Neural Network

The training procedure adopted is similar to the methodology used by Grando et al. \cite{19}: We train the NN over a set of 1000 artificial complex networks, with the network size ranging from 100 to 1000 nodes. All networks were created using the scale-free generation model \cite{41}.

The NN model defined in Equation 10 and outlined in Figure 1 has the following dimensions for the inputs and hidden layers:

- **Input 1**: the normalized degree rank is a simple float;
- **Hidden layers** $W^1, W^2, W^3, W^4$: fully connected layers with an output size of 512 (embed size or number of higher order features $F$) for $W^1$ and $W^2$, and 256 for $W^3$ and $W^4$;
- **Hidden layer** $W^5$: fully connected layer with an output size of 256 ($F/2$).

The error function used for our NN model is the mean squared error between the predicted centrality and the expected value. We also used an L2 regularization function to avoid over-fitting. Therefore, the adopted loss function is:

$$\mathcal{L}_{\text{TOTAL}} = \mathcal{L}_{\text{MSE}} + \lambda \mathcal{L}_{\text{REGUL}},$$

where $\mathcal{L}_{\text{MSE}}$ is the loss function for the Mean Squared Error, $\mathcal{L}_{\text{REGUL}}$ is the L2 regularization loss, and $\lambda$ is a variable that controls the weight given to the regularization term. We set $\lambda = 0.001$ through the preliminary experiments. We used the Adam algorithm as the optimization function, the gradients were truncated in the range $[-1, 1]$, and the batch size was set to 128. We trained our model using $T$ worker threads and only one global instance of the NN, where each thread worked with a different graph. All threads populated the current batch in parallel. This guaranteed that each batch contained data collected from different graphs. We used $T = 7$ threads in our experiments.

It is important to note that the model is trained specifically for each kind of centrality. Therefore, for instance, when the model is trained using the betweenness centrality, it will not be able to accurately predict other centralities.

4.3 Baseline Model

We reproduced the model created by Grando et al. \cite{19, 30} in order to compare their results with ours. This model will from now on be called the baseline model, and we chose it because it is one of the few architectures that serve a similar purpose to the work presented here. In the remainder of this section,
we detail our implementation of the baseline model. The source code for this model is also available at GitHub.

We follow the neural network architecture described in the original paper [30]: The inputs are the normalized ranks of degree and eigenvector centralities in the range [-1, 1], the output is the normalized rank of the desired node centrality, also in the range [-1, 1] (note that this differs from our approach, where the input and output are in the range of [0, 1]), and four fully connected hidden layers with 20 neurons each, where each hidden layer is followed by the hyperbolic tangent activation function. We used the same loss function that we used for our model, depicted in Equation 11, where we used the same $\lambda = 0.001$ (the original paper did not use a regularization term). We used the Adam optimizer as the optimization function, differently than the Levenberg-Marquardt optimizer used in the original paper. The gradients were also clipped in the range of [-1, 1] similarly to our approach, but this process is not specified in the original paper. We also used only one global instance of the NN and $T = 7$ threads that updated the NN in parallel.

5 Performance Evaluation

As detailed in Section 4.2, we train the proposed NCA-GCN model by iterating over all nodes in a set of training graphs. Each node fed to the model is considered a step. Figure 2 presents the mean squared error (MSE) for the baseline and the NCA-GCN models in relation to the number of steps for the training stage while trying to approximate the normalized rank for different node centralities. Since the input and output values for the baseline and NCA-GCN models are in the range of [-1, 1] and [0, 1], respectively, the MSE for each method is in a different scale. Hence, we cannot compare these measures directly.

As stated in Grando et al. [19], the MSE is not a reliable metric to evaluate how well a model that predicts the centrality rank of a node is performing. This is due to the fact that we are interested in a model that predicts the correct rank ordering of a given centrality measure for all nodes, not the resulting absolute rank value. Therefore, we follow the methodology adopted by Grando et al. [19] and use the Kendall $\tau$-b rank correlation coefficient to determine the quality of the NCA-GCN rank prediction for network centralities. The Kendall $\tau$-b coefficient varies in the range of [-1, 1] and it measures the correlation between two ranking lists. A value of -1 indicates that the two lists are fully reversed (that is, if index X is ranked first in one list, it is ranked last in the other, and so on for the other rank positions). A value of 0 means that there are no correlation, whereas a value of 1 indicates that both lists fully agree with the ranks of every node. Therefore, to measure the performance of a prediction model, we first build two rank lists: (i) a list in which the value in index $i$ indicates the true normalized rank of node $i$, and (ii) a similar list that stores the predicted normalized rank. We then measure the Kendall $\tau$-b coefficient between these two lists, where a value near 1 indicates a good performance, since the prediction model managed to rank most of the nodes correctly.

We tested the NCA-GCN model with four different node centralities: (i) betweenness, (ii) closeness,
5.1 Experimental Results with Real-World Networks

We evaluate the NCA-GCN model with the real-world networks. These networks were extracted from the Stanford Large Network Dataset Collection [43]. The networks used and their respective properties are listed in Table 1.

| Abbreviation       | Nodes | Edges    |
|--------------------|-------|----------|
| email-Eu-core      | 1,005 | 25,571   |
| facebook_combined  | 4,039 | 88,234   |
| Deezer_RO          | 41,773| 125,826  |
| Deezer_HR          | 54,573| 498,202  |
| Deezer_HU          | 47,538| 222,887  |
| p2p-Gnutella30      | 36,682| 88,328   |
| p2p-Gnutella31      | 62,586| 147,892  |
| soc-Slashdot0811    | 77,360| 905,468  |

As previously mentioned, for each network analyzed, we measure the Kendall $\tau$-b coefficient between the true rank of each node and the predicted ranks. Hence, each network is associated with a Kendall $\tau$-b coefficient indicating how well the rank for a given centrality measure is predicted.

Figure 3 shows that the NCA-GCN model is capable of achieving a good performance in predicting different network centralities for real-world networks by only analyzing the degree of each node in these networks. This shows that our approach can effectively approximate complex node centralities by only considering a simple feature, such as the node degree. Note that the NCA-GCN model achieves a similar performance as the baseline model without using any higher order feature, such as the eigenvector centrality. We note that for the betweenness centrality, the NCA-GCN model performed better when compared with the results for closeness and harmonic centralities. For these two latter centralities, the NCA-GCN model did not achieve the same results as the baseline model, although the coefficients achieved were considerably close. There are also two more interesting aspects that we can observe in Figure 3: (i) the results for betweenness and eigenvector centralities are very similar; and (ii) the same can be said about the closeness and harmonic centralities. While the former is not very clear as to why this happens, the latter can be explained by the similarities in how closeness and harmonic centralities are computed.

Since the NCA-GCN results for the closeness and harmonic centralities were not as good as those for the baseline model, we experimented using for the NCA-GCN model the same input as for the baseline model, i.e., the normalized degree rank and the normalized eigenvector rank. Thus, we executed an experiment where we used two features instead of one ($C = 2$) for the closeness and harmonic centralities. The results are depicted in Figure 4 where we can see that by using the degree and the eigenvector centralities as input, the NCA-GCN model performs better for both these centralities, achieving virtually the same results as the baseline model. We also tested this approach for the betweenness centrality, but the results were kept the same. Given that we achieve a better result for the closeness and harmonic centralities by using two features, we kept this approach for the remaining experiments. For the betweenness and eigenvector centralities, we maintained $C = 1$, that is, we use only the degree as input.

5.2 Experimental Results with Synthetic Networks

Our second experiment consists in using our NCA-GCN model to predict the normalized centrality rank of all nodes of synthetically generated networks. To that end, we created 4 test network sets, each one built using different generation models: (i) random networks [44]; (ii) small-world [45]; (iii) scale-free [41]; and (iv) a mixture of all three types of networks. Each set contains 100 artificial graphs.
5.2 Experimental Results with Synthetic Networks

Figure 3: Comparison of the mean Kendall Rank Coefficient for the real-world networks described in Table 1 for the baseline and the NCA-GCN models for each considered centrality. These results depict the mean value for 5 executions. Note that we do not compare the results for the Eigenvector centrality because the baseline method can not predict this centrality, given that it is used as the input for this method.

Figure 5 shows the mean Kendall $\tau_b$ coefficient for the networks of each of the test network sets and for the four previously mentioned centralities. These results were obtained by executing each experiment five times and then taking the mean. The standard deviation is also presented as the error bars, just like the previous experiments. For the betweenness, closeness, and harmonic centralities, we compared the NCA-GCN with the baseline model. For the eigenvector centrality this comparison was not possible, since the baseline model uses this centrality as its input. From these results, we can see that the betweenness and eigenvector centralities performed very well for the artificial scale-free networks, which makes sense, since the training set used for all experiments were comprised entirely of artificial scale-free networks. However, the NCA-GCN for these two centralities did not perform as well for the other test sets, namely the random, small-world, and mixture of networks, although it still managed to score good results. The same phenomenon can be seen for the closeness and harmonic centralities for the NCA-GCN and for all three centralities for the baseline model, although in a smaller scale. Finally, we can see that for the closeness and harmonic centralities, the NCA-GCN performed very similar to the baseline model, while the betweenness centrality did not perform as well as the baseline for the random, small-world, and mix test sets. It is important to note that the results for the closeness and harmonic centralities used two features: degree and eigenvector centralities, as previously mentioned.

As we have shown in the results, our model performed very similarly to the baseline approach used in [19]. However, our approach is more general, in the sense that it is capable of achieving the same results using even less node information, given that other node properties are infered by the graph structure given by the GCN. We also argue that our approach is also more easily adaptable to other tasks that require an intrinsic knowledge of the graph structure and that can benefit of knowing node centrality properties,
Figure 4: Comparison of the mean Kendall Rank Coefficient for the real-world networks while considering the baseline and the NCA-GCN models. In this experiment, however, the NCA-GCN model predicts the closeness and harmonic ranks using two features instead of one ($F = 2$): the normalized degree rank and the normalized eigenvector rank, similar to the input of the baseline model. These results depict the mean value for 5 executions.

As a final remark, the NCA-GCN model is very fast for both training and testing stages, even when running it for large real-world networks. Although it uses the adjacency matrix as an input to the model, this matrix is usually very sparse, which simplifies the computation time when we use sparse matrix representations. In our case, we use Tensorflow's sparse matrix structure, which made the execution of the model very fast. Therefore, running the NCA-GCN model in order to predict the node’s betweenness centrality, for example, requires only a few seconds even for a large network, while calculating the true value can be very expensive, as stated by Grando et al. [19].

### 6 Conclusions and Future Work

We presented the Network Centrality Approximation using Graph Convolutional Networks (NCA-GCN) model, which is a model capable of approximating node centralities of large real-world graphs using only node degrees as an input. More so, the model is trained using only small artificial scale-free graphs, which shows that the proposed approach is robust.

The NCA-GCN model was compared with the current state-of-the-art model for predicting node centrality based on machine learning, achieving a similar performance. In contrast, the main difference between the two models resides in the input of each predictive model: The baseline model uses the degree and the eigenvector centrality of each node in order to predict the target centrality, whereas the proposed NCA-GCN model uses only the degree information. This shows that the NCA-GCN model uses a powerful internal node representation (i.e., given by the GCN model), which can be useful in other network analysis tasks, such as discovering other node-specific features. Therefore, in this paper, we show that the NCA-GCN approach allows the use of the method previously proposed by Grando et al. [19] with simpler features because it infers through the GCN the remaining features given as input.

As future work, we intend to expand the NCA-GCN model to predict other node centrality measures as well as to perform predictions on other node-specific features. We aim to adapt the NCA-GCN to predict a node’s time centrality [16] in relation to its diffusive capabilities in the network by adding the task of embedding nodes in Time Varying Graphs (TVGs) [17] into the model presented here.

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Figure 5: Mean Kendall coefficient for the test network set after training for 1,000,000 steps for the baseline and NCA-GCN models. Each result is the mean value for 5 executions. We separated the results based on 4 different test network sets: small-world set (SW), scale-free set (SF), random graphs set (RND), and a mixed set containing all previous 3 graph types (MIX). The results of the NCA-GCN model for the closeness and harmonic centralities used the degree and eigenvector centralities as input ($F = 2$).

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