



# LEARNING CENTRALITY MEASURES WITH GRAPH NEURAL NETWORKS

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**4.** Experimental Setup and Results

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# **Introduction**

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- Machine Learning subarea:
  - Structures of linear transformations and nonlinear applications.
  - Learning internal representations of data.
  - “Grown” from Artificial Neural Networks.
- Success generally attributed to the heightened parallel processing capacity with GPUs and due to the high data availability.
- Becoming ubiquitous in our daily lives, with manifold applications on diverse areas.



Figure: Recent success which uses deep learning for image processing – Image generation with the StyleGAN model. Source: KARRAS; LAINE; AILA (2018)

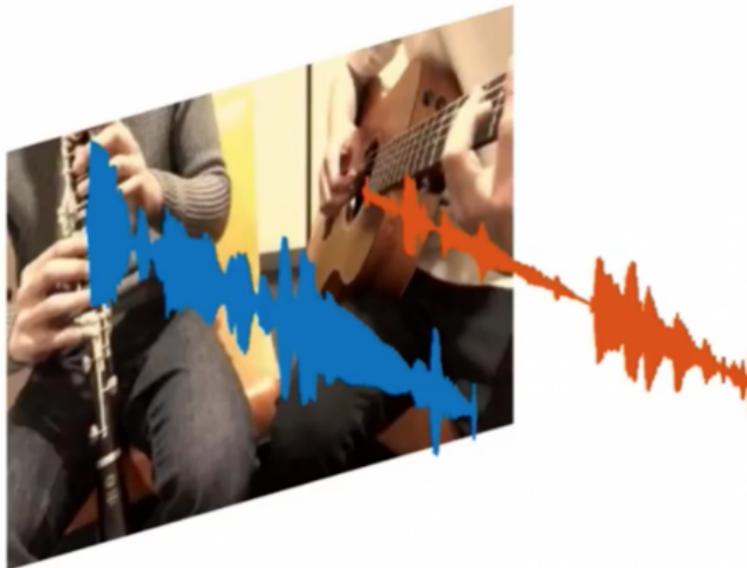


Figure: Recent success which uses deep learning for audio processing – Sound localisation with the PixelPlayer model. Source: ZHAO et al. (2018)

## INTRODUCTION

## RECENT SUCCESSES – TEXT PROCESSING

LEARNING CENTRALITY  
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Figure: Recent success which uses deep learning for text processing – OpenAI's GPT-2 model. Source: OpenAI (RADFORD et al., 2019)

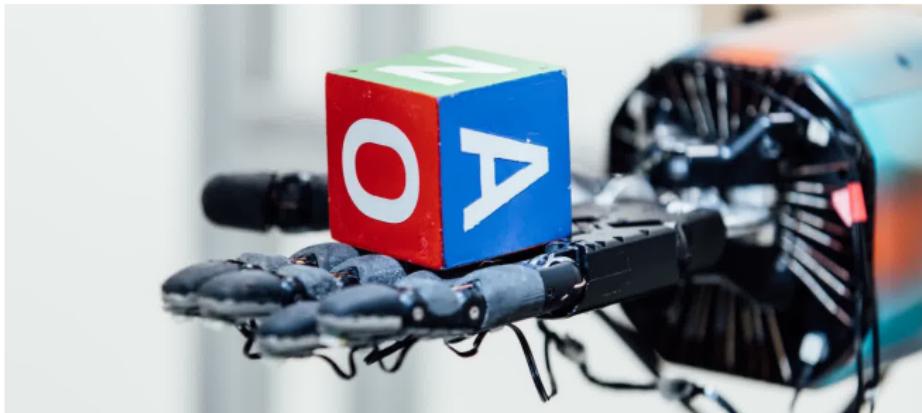


Figure: Recent success which uses deep learning for robotics. Source:  
OpenAI(OPENAI et al., 2018)



Figure: Recent success that uses deep learning for a relational problem – In this case, playing the Chinese boardgame Go. Source: Nature (SILVER et al., 2016)

# RELATIONAL PROBLEMS – NEURAL COMPUTERS

LEARNING CENTRALITY  
MEASURES WITH GRAPH NEURAL  
NETWORKS

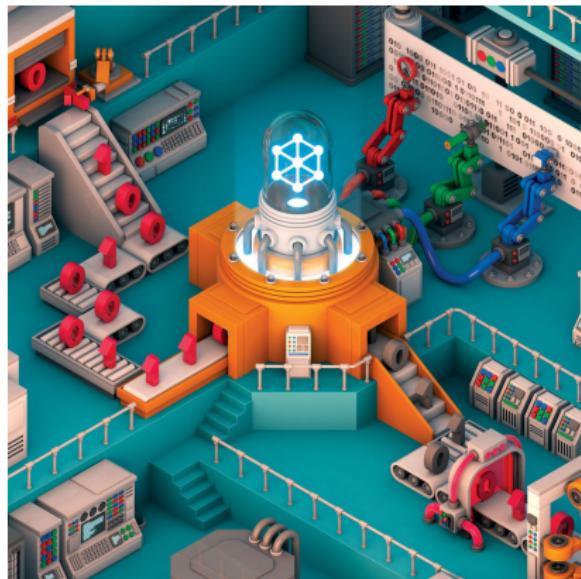


Figure: Recent sucesss that uses deep learning for a relational problem – In this case, the DNC model performs well in question answering and graph processing tasks. Source: Deepmind (GRAVES et al., 2016)

# RELATIONAL PROBLEMS – RELATIONAL VISUAL QUESTION ANSWERING

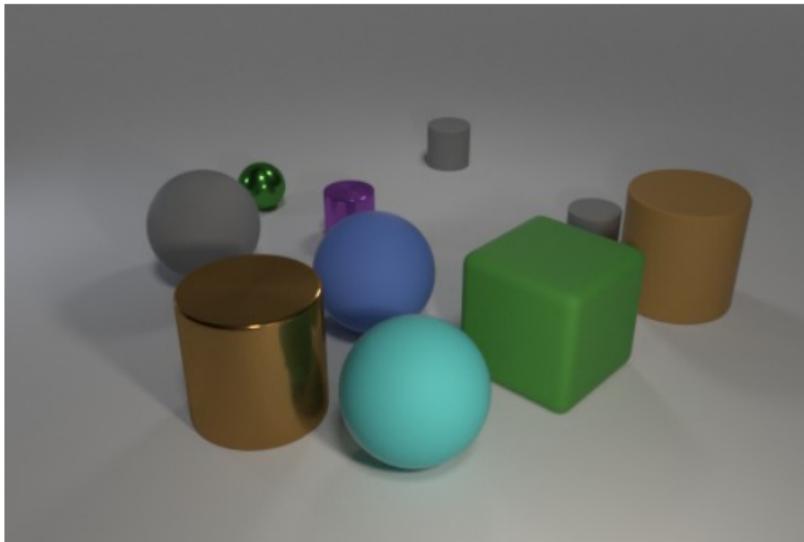


Figure: Recent successes that uses deep learning for a relational problem – In this case, answering relational questions about a synthetic image. Source: SANTORO et al. (2017)

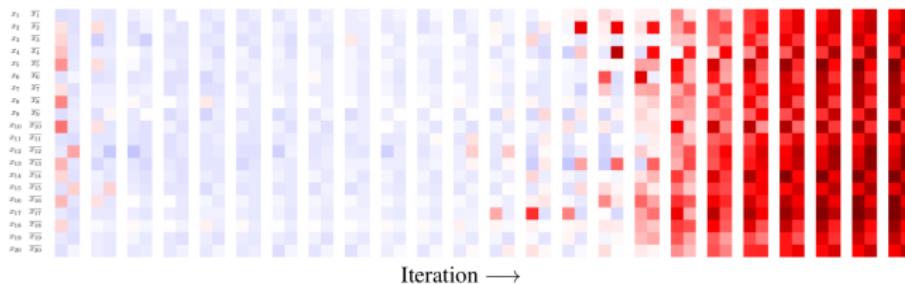


Figure: Recent success that uses deep learning for a relational problem – In this case, solving SAT instances. Source: SELSAM et al. (2018)

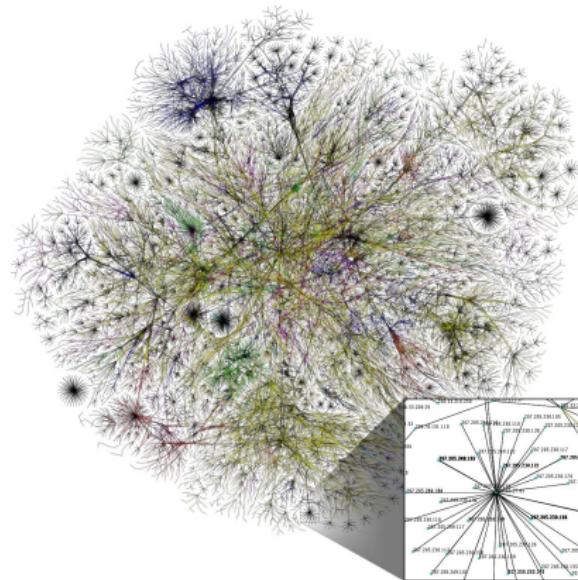


Figure: A partial map of the Internet based in 2005, made by opte.org: The relational structures that support our modern societies have been growing larger and more interconnected by the day. Source: Wikimedia Commons

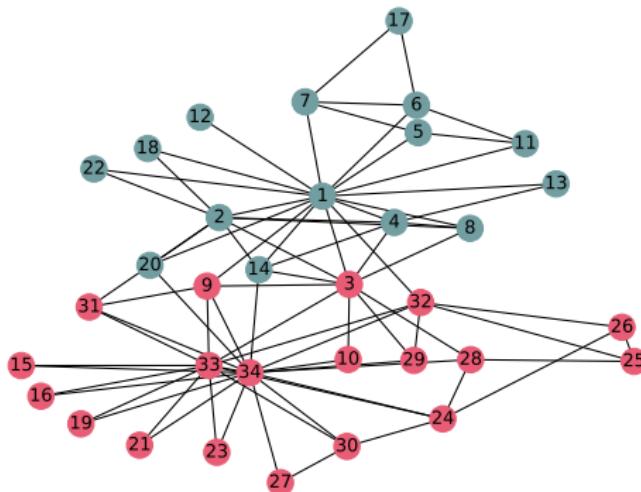


Figure: The connections of the 34 members of Zachary's Karate Club (WAYNE, 1977), a small social network. Here it is easy to see the equivalence between networks and graphs. Source: Author, data from (WAYNE, 1977) plotted using the Networkx Python package (HAGBERG; SWART; CHULT, 2008)

## SCALE-FREE PROPERTY OF REAL NETWORKS

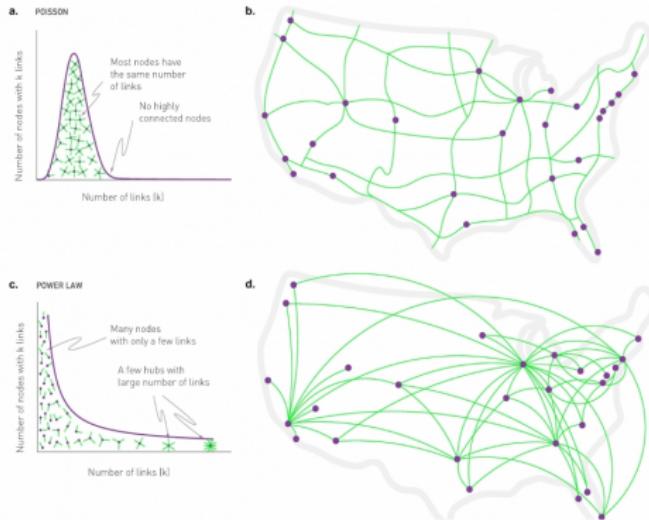


Figure: Two networks consisting of the same vertices, but with different degree distributions, exemplifying the Scale-Free property. Source: BARABÁSI et al. (2016)

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- Many definitions of importance

- Defines how “important” an entity is
- Many definitions of importance
- Uses in (social) network analysis

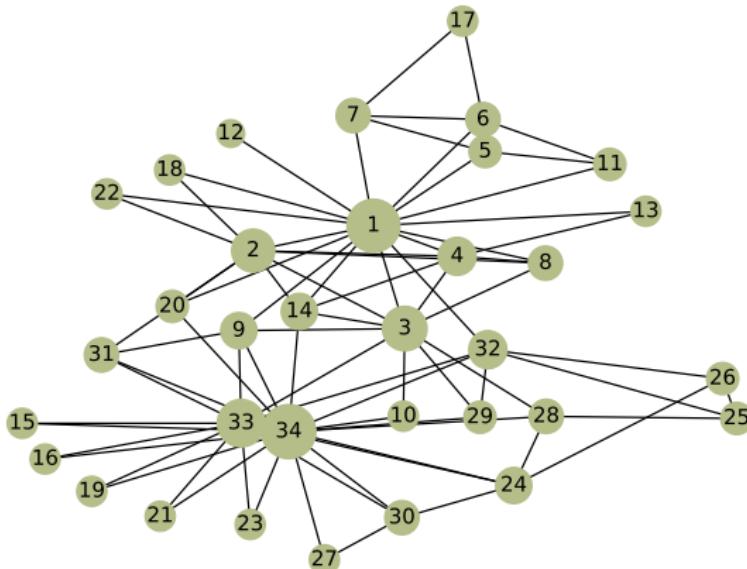


Figure: Zachary's Karate Club with nodes sized by degree. Source: Author, data from (WAYNE, 1977) plotted using the Networkx Python package (HAGBERG; SWART; CHULT, 2008)

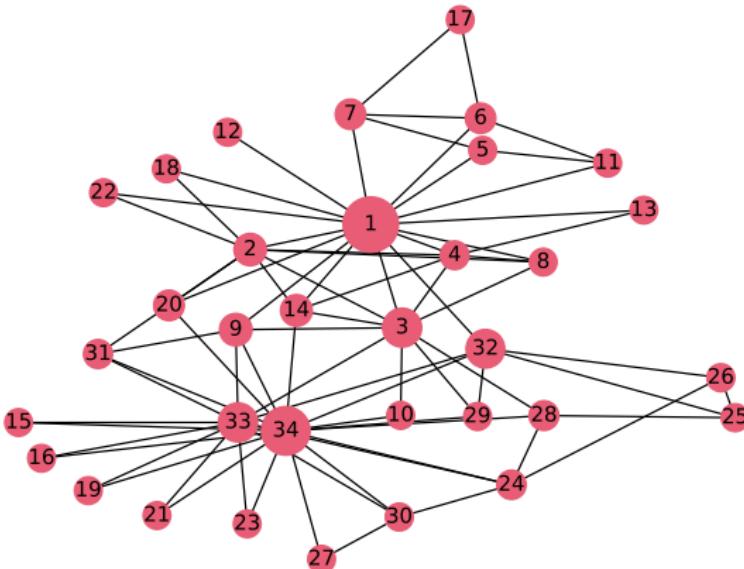


Figure: Zachary's Karate Club with nodes sized by betweenness. Source: Author, data from (WAYNE, 1977) plotted using the Networkx Python package (HAGBERG; SWART; CHULT, 2008)

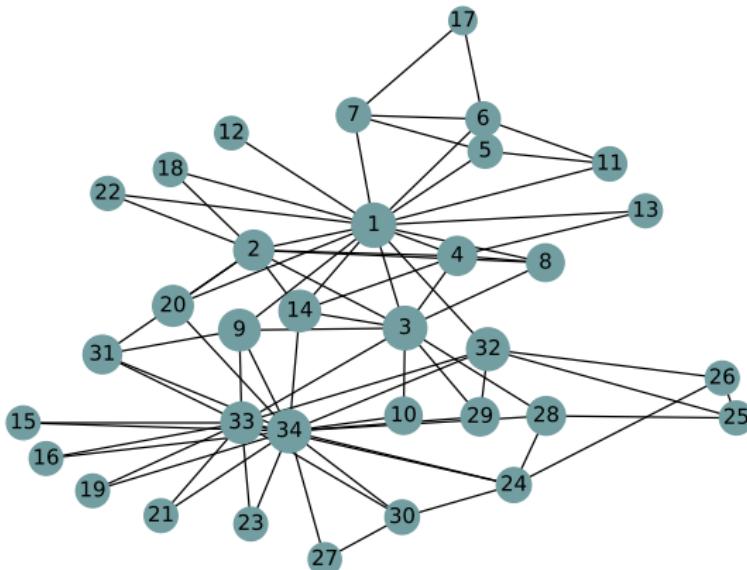


Figure: Zachary's Karate Club with nodes sized by closeness. Source: Author, data from (WAYNE, 1977) plotted using the Networkx Python package (HAGBERG; SWART; CHULT, 2008)

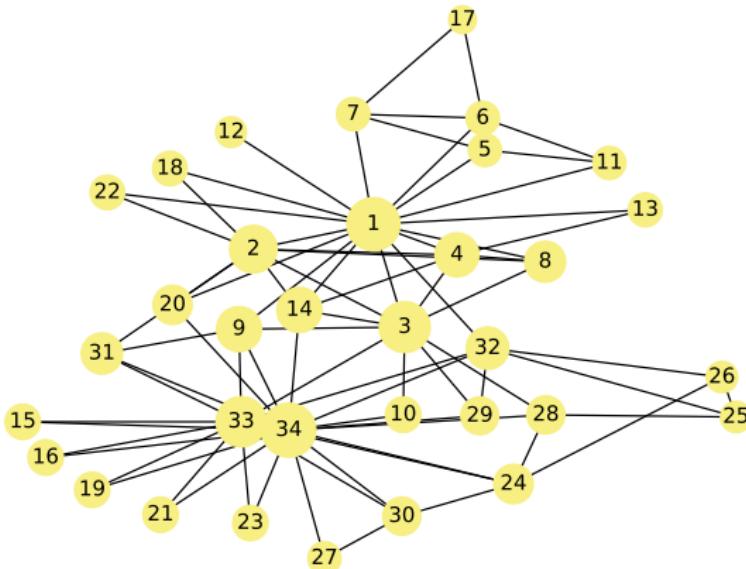


Figure: Zachary's Karate Club with nodes sized by eigenvector. Source: Author, data from (WAYNE, 1977) plotted using the Networkx Python package (HAGBERG; SWART; CHULT, 2008)

# Graph Neural Networks



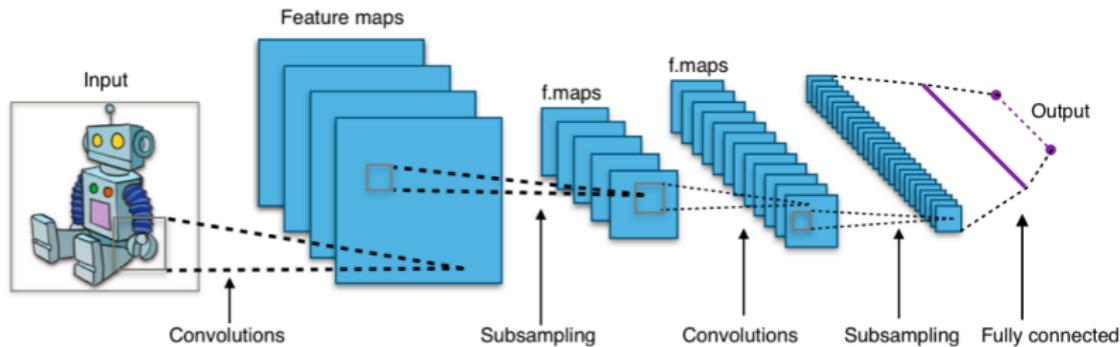


Figure: The typical architecture of a CNN. Source: Wikimedia Commons

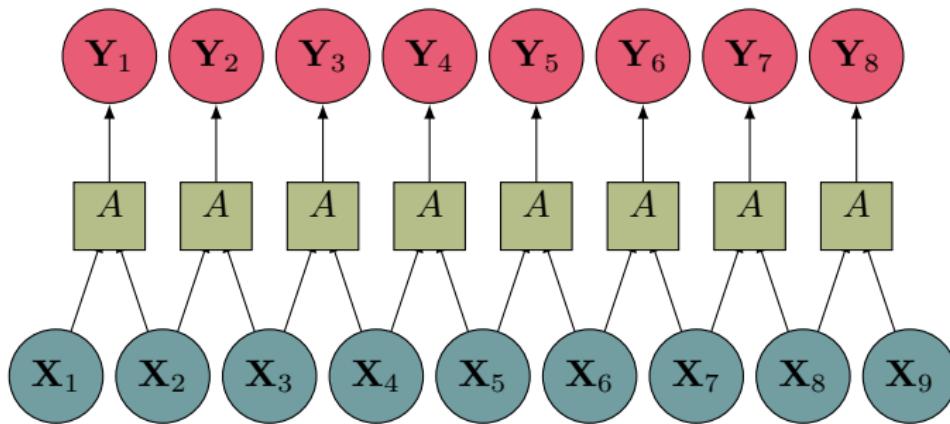


Figure: The application of a 1-dimensional convolutional kernel on a discrete 1-dimensional space. Blue circles are inputs, red circles are outputs and green backgrounds are to represent the whole neural network block. Source: Author, based on (OLAH, 2014)

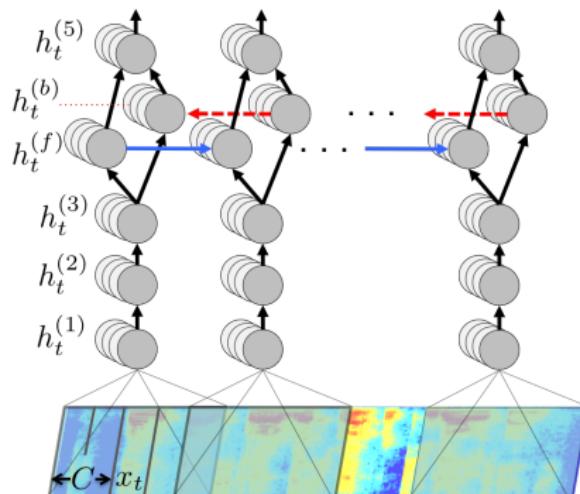


Figure: Deep Speech RNN architecture. Source: HANNUN et al. (2014)

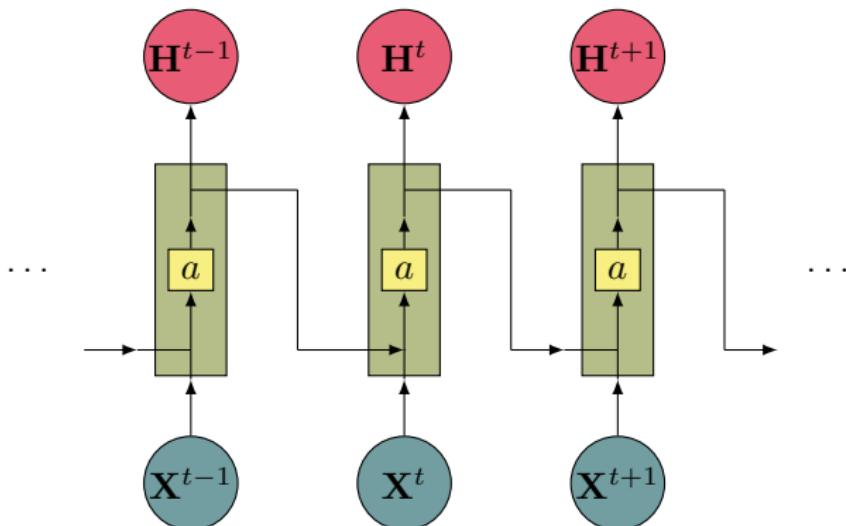


Figure: An unrolled recursive neural network. Yellow squares are neural network layers, blue circles are inputs, red circles are outputs and green backgrounds are to represent the whole neural network block. Source: Author, based on (OLAH, 2015)

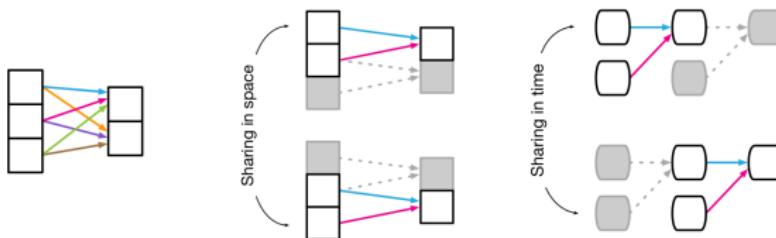


Figure: There is weight reuse across convolutional (middle) and recurrent (right) layers, but not in fully connected (left) layers. Source: BATTAGLIA et al. (2018)

- RNNs work on sequences

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- CNNs work on discrete spaces

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- CNNs work on discrete spaces
- What about graphs?

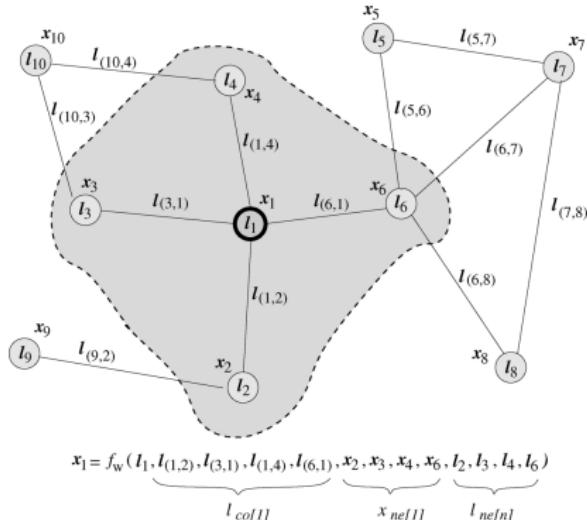


Figure: The representation of the Graph Neural Network Model, with the vertex being updated using the information on its neighbourhood Source: SCARSELLI et al. (2009)

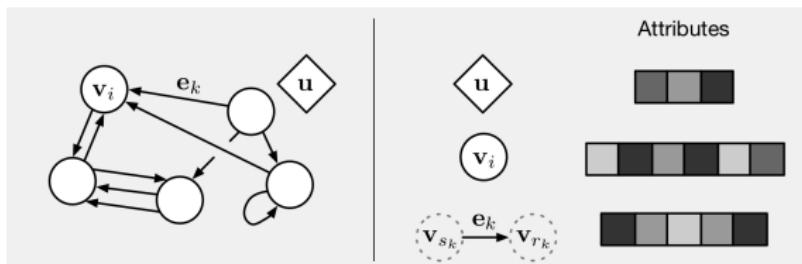


Figure: The representation of the Graph Network Model. Source: BATTAGLIA et al. (2018)

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- Reformalisation of the GNN model to generalise the concept of a vertex to a vertex's type.

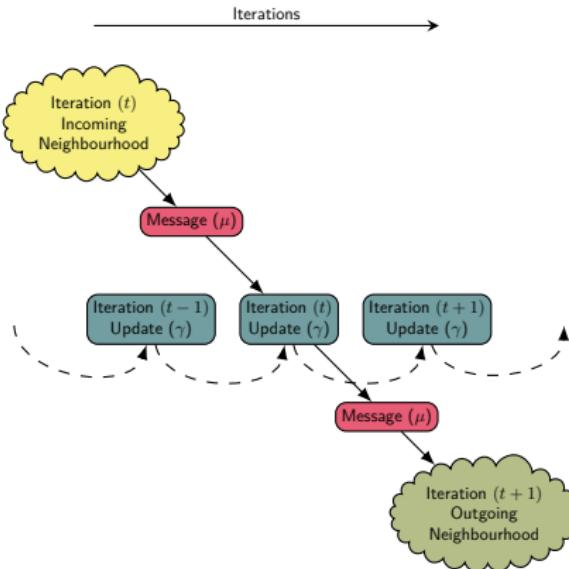


Figure: Pictorial representation of a Typed Graph Network from the perspective of a vertex  $v$ . Source: Author

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1: procedure TGN( $\mathcal{G} = (\mathcal{V} = \bigcup_{i=1}^N \mathcal{V}_i, \mathcal{E} = \bigcup_{k=1}^K \mathcal{E}_k), \mathcal{I} = \bigcup_{i=1}^N \mathbf{V}_i^{(0)}$ )
2:   for  $t = 1 \dots t_{max}$  do
3:     for  $i = 1 \dots N$  do
4:       Let  $K_i \leftarrow \{k \mid \forall k, \pi_k = (s, i)\}$ 
5:       for all  $v_b \in \mathcal{V}_i$  do
6:         for all  $k \in K_i$  do
7:            $\bar{\mu}_{k,b}^{(t)} \leftarrow \{\mu_k(\mathbf{V}_{s(a)}^{(t-1)}) \mid \forall v_a \in \mathcal{V}_s, (v_a, v_b) \in \mathcal{E}_k\}$ 
8:            $\bar{\alpha}_{k,v_t}^{(t)} \leftarrow \alpha_k(\bar{\mu}_{k,b}^{(t)})$ 
9:         end for
10:         $\bar{\rho}_{i,b}^{(t)} = \rho_i(\{\bar{\alpha}_{k,b}^{(t)} \mid \forall k \in K_i\})$ 
11:         $\mathbf{V}_i^{(t)} \leftarrow \gamma_i(\mathbf{V}_i^{(t)}, \bar{\rho}_{i,b}^{(t)})$ 
12:      end for
13:    end for
14:  end for
15:  return  $\{\mathbf{V}_i^{(t_{max})} \mid i = 1 \dots N\}$ 
16: end procedure

```

$$K_i = \{k \mid \forall i, \pi_k = (s, i)\} \quad (1)$$

$$\bar{\mu}_{k,b}^{(t)} = \{\mu_k(\mathbf{V}_{\mathbf{s}(a)}^{(t-1)}) \mid \forall v_a \in \mathcal{V}_s, (v_a, v_b) \in \mathcal{E}_k\} \quad (2)$$

$$\bar{\alpha}_{k,b}^{(t)} = \alpha_k(\bar{\mu}_k^{(t)}) \mid 1 \leq k \leq K \quad (3)$$

$$\bar{\rho}_{i,b}^{(t)} = \rho_i(\bar{\alpha}_{k,b}^{(t)}) \quad \forall 1 \leq i \leq N, v_b \in \mathcal{V}_i \quad (4)$$

$$\mathbf{V}_{\mathbf{i}(b)}^{(t)} = \gamma(\mathbf{V}_{\mathbf{i}(b)}^{(t-1)}, \bar{\rho}_i^{(t)}) \quad (5)$$

## **Related Work**

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- GRANDO; LAMB (2015) and GRANDO; LAMB (2016) uses neural networks to estimate centrality measures

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- Uses a priori knowledge of other centralities to approximate a different one.
- GRANDO; LAMB (2018) also produces a ranking of the centrality measures, but again do so using the degree and eigenvector centralities as input.

- KUMAR; MEHROTRA; MOHAN (2015) uses local and global features:

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  - vertex degree
  - sum of the degrees on vertex's neighbourhood

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- Does not focus on other centrality measures
- Does not consider the multitask transfer between centralities.

## **Experimental Setup and Results**

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- 1 Can a neural network infer a vertex's centrality value only from the network structure?

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- 3 Can the representation from such a network benefit from the correlations between centrality measures and hold information about multiple centrality measures?
- 4 Will the algorithm learned by this neural network be scalable and be able to run for more iterations?
- 5 Will the algorithm learned by this neural network behave correctly for graphs larger than the ones it was trained?

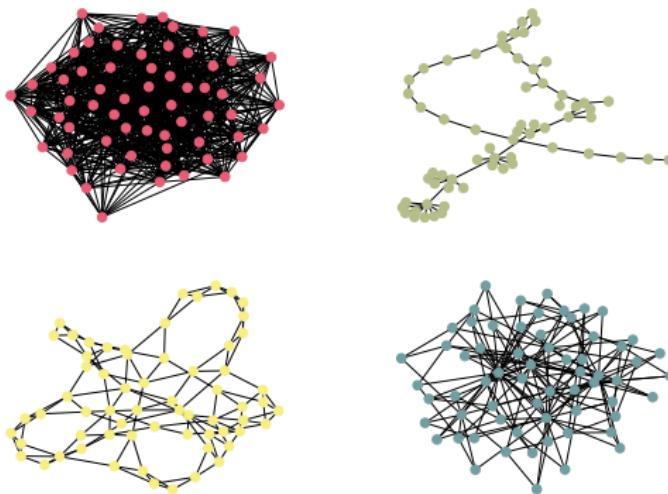


Figure: Examples of training instances with  $n = 64$  vertices for each graph distribution, clockwise from the top left: Erdős-Rényi in red, Random power law tree in green, Holme-Kim in blue and Watts-Strogatz in yellow. Source: Author

Dataset	Size Range	Instances per Graph Type
Train	32-128	4096
Test	32-128	4096
Large	128-256	64
Different Sizes	32-128	256
	32-256	$256 \cdot 15^{\dagger}$
Real	1174-4036	1*

Table: Dataset names and sizes. Source: Author.

Graph Distribution	Parameters	Dataset
Erdős-Rényi	$p = 0.25$	Train, Test, Large, Sizes
Random power law tree	$\gamma = 3$	Train, Test, Large, Sizes
Watts-Strogatz	$k = 4, p = 0.25$	Train, Test, Large, Sizes
Holme-Kim	$m = 4, p = 0.1$	Train, Test, Large, Sizes
Circular Shell	$p_{inter} = 0.25, p_{intra} = 0.1$	Different
Barabási-Albert	$m \in \mathcal{U}(2, 5)$	Different

Table: Training instances generation parameters. Source: Author.

Name	Source	Vertices	Edges	Maximum	Degree Average	Minimum
<b>power-eris1176</b>	NR	1174	9861	100	16.8	2
<b>econ-mahindas</b>	NR	1258	7619	206	12.1	2
<b>socfb-haverford76</b>	NR	1446	59590	374	82.4	1
<b>ego-Facebook</b>	SN	4036	88243	1044	43.7	1
<b>bio-SC-GT</b>	NR	1708	33982	549	39.8	1
<b>ca-GrQc</b>	SN	4158	13428	81	6.46	1

Table: Statistics for the real instances and their source, where NR stands for (ROSSI; AHMED, 2015) and SN for (LESKOVEC; KREVL, 2014) Source: Author with data from (ROSSI; AHMED, 2015; LESKOVEC; KREVL, 2014).

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- When not multitasking, each centrality will have a separate model
- When multitasking, each centrality will share the same TGN block, but will learn different output functions for each centrality

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  - CN1 for the normalised centrality value
  - CN2 for normalised centrality, with normalisation on the model's output

		C	CN1	CN2
“train”	Betweenness(R)	92.7%	119%	<b>89.6%</b>
	Closeness(R)	77.8%	16.3%	<b>15.3%</b>
	Degree(R)	55.5%	<b>38.9%</b>	43.6%
	Eigenvector(A)	0.0438	0.0251	<b>0.0230</b>
“large”	Betweenness(R)	<b>91.7%</b>	419%	94.2%
	Closeness(R)	274%	85.9%	<b>75.0%</b>
	Degree(R)	58.9%	210%	<b>50.6%</b>
	Eigenvector(A)	0.0569	<b>0.0518</b>	0.0734
<u>“large”</u> <u>“train”</u>	Betweenness	<b>0.989</b>	3.52	1.05
	Closeness	<b>3.52</b>	5.26	4.90
	Degree	<b>1.06</b>	5.40	1.16
	Eigenvector	<b>1.3</b>	2.06	3.19

Table: Errors (Relative/Absolute) of the multitask learning performance for the proposed models on a sample of the “train” dataset and on the full “large”. The best values are in **bold**. Source: Author

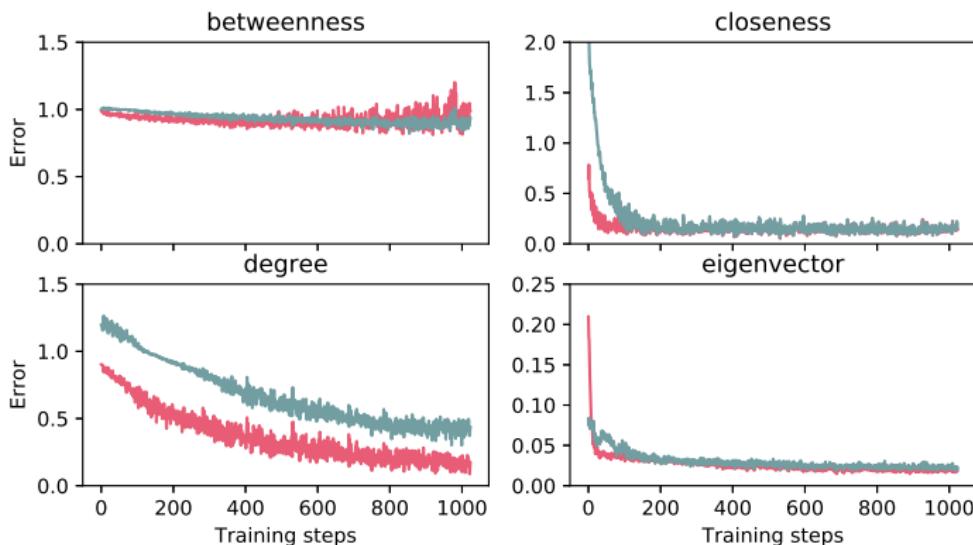


Figure: Training Performance for the CN2 model, **with multitasking** and **without multitasking**. Source: Author

	Error Type	Centrality	"test"
Relative (%)	Betweenness	95.96	<b>/89.54</b>
	Closeness	13.49	<b>/13.38</b>
	Degree	<b>16.75</b>	/43.39
	Average	<b>42.07</b>	/48.77
Absolute	Eigenvector	<b>0.01946</b>	/0.02286
	Betweenness	<b>0.01462</b>	/0.01464
	Closeness	0.004785	<b>/0.003710</b>
	Degree	<b>0.03465</b>	/0.03705
	Eigenvector	0.01694	<b>/0.008880</b>
MSE	Average	0.01775	<b>/0.01607</b>

Table: Loss (MSE) and performance metrics (Relative/Absolute error) for the CN2 model on the "test" dataset (without/with multitasking). The best values are in **bold**. Source: Author

	Error Type	Centrality	“large”
Relative (%)	Betweenness		<b>91.03</b> /94.17
	Closeness		79.00/ <b>74.76</b>
	Degree		<b>27.88</b> /50.06
	Average		<b>65.97</b> /72.99
Absolute	Eigenvector		0.08311/ <b>0.07214</b>
	Betweenness		<b>0.01462</b> /0.01464
	Closeness		0.004785/ <b>0.003710</b>
	Degree		<b>0.03465</b> /0.03705
	Eigenvector		0.01694/ <b>0.008880</b>
MSE	Average		<b>0.01775</b> / <b>0.01607</b>

Table: Loss (MSE) and performance metrics (Relative/Absolute error) for the CN2 model on the “large” dataset (without/with multitasking). The best values are in **bold**. Source: Author

	Error Type	Centrality	“different”
Relative (%)	Betweenness	99.94	<b>/83.88</b>
	Closeness	<b>19.13</b>	/21.35
	Degree	<b>25.84</b>	/45.32
	Average	<b>48.30</b>	/50.18
Absolute	Eigenvector	<b>0.04854</b>	/0.05282
	Betweenness	<b>0.001376</b>	/0.001445
	Closeness	<b>0.008956</b>	/0.01079
	Degree	<b>0.01026</b>	/0.01758
	Eigenvector	<b>0.003974</b>	/0.004940
MSE	Average	<b>0.006142</b>	/0.008689

Table: Loss (MSE) and performance metrics (Relative/Absolute error) for the CN2 model on the “different” dataset (without/with multitasking). The best values are in **bold**. Source: Author

- Results were unsatisfactory.

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- However, CN2 model performed better in minimising the Mean Squared Error
- Maybe further pre-processing could improve performance
- However, the task here is significantly harder
- (GRANDO; LAMB, 2016; GRANDO; GRANVILLE; LAMB, 2018; GRANDO; LAMB, 2018) focused on ranking the centrality measures.

- Turning to producing rankings for each centrality measure.

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- Considered a comparison matrix as a form of producing a ranking

$$\begin{pmatrix} P(v_1 >_c v_1) & P(v_2 >_c v_1) & P(v_3 >_c v_1) \\ P(v_1 >_c v_2) & P(v_2 >_c v_2) & P(v_3 >_c v_2) \\ P(v_1 >_c v_3) & P(v_2 >_c v_3) & P(v_3 >_c v_3) \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

Figure: Example of a fuzzy comparison matrix. Source: Altered from (AVELAR et al., 2018)

- Also allows one to consider two possible setups

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RC Which is trained as the CN2 model, but with the performance based on the comparisons

- Also allows one to consider two possible setups
  - RC Which is trained as the CN2 model, but with the performance based on the comparisons
  - RN Which is a model that computes the comparisons “natively”

## RESULTS FOR THE APPROXIMATION METHOD

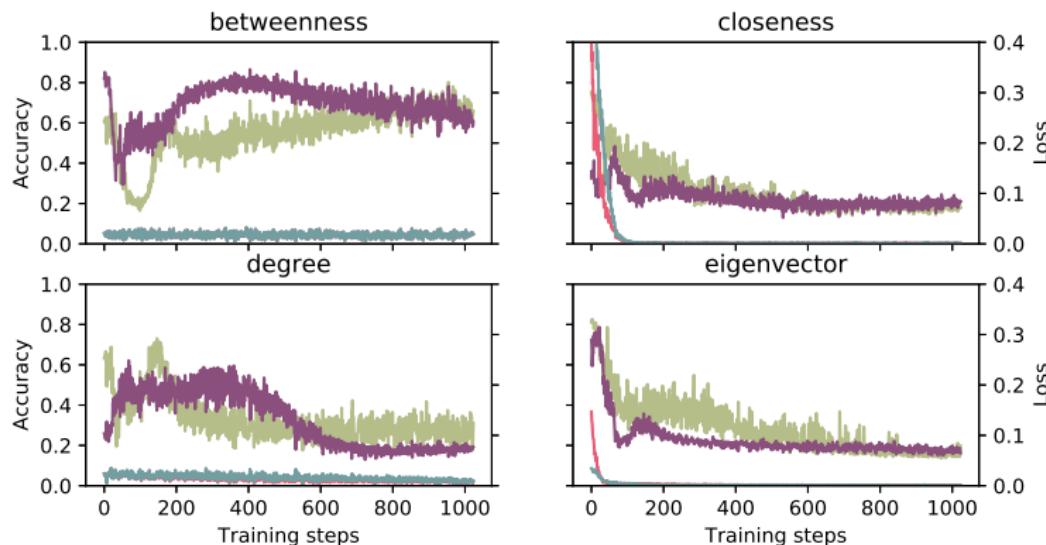


Figure: Loss plotted in red and blue and accuracy in green and purple for training without and with multitasking, respectively. Source: Author

## RESULTS FOR THE NATIVE METHOD

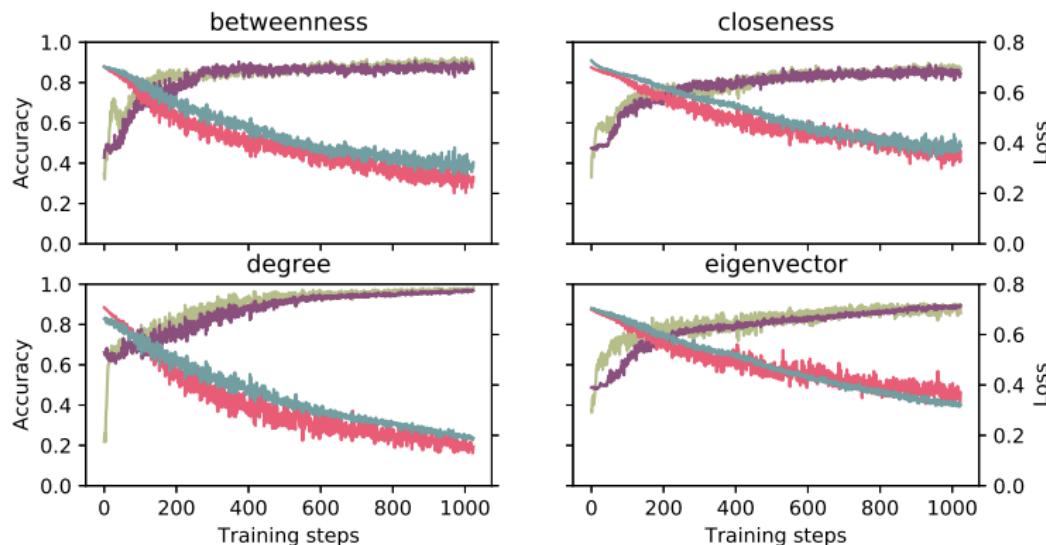


Figure: Loss plotted in red and blue and accuracy in green and purple for training without and with multitasking, respectively. Source: Author

Model	Centrality	P (%)	R (%)	TN (%)	Acc (%)
RN	Betweenness	<b>90.26</b> /87.18	<b>88.52</b> /87.24	<b>90.99</b> /88.89	<b>89.83</b> /87.94
	Closeness	<b>88.39</b> /86.88	<b>84.54</b> /81.96	<b>89.75</b> /88.72	<b>87.30</b> /85.52
	Degree	<b>99.27</b> /98.31	<b>94.94</b> /92.41	<b>99.44</b> /98.98	<b>97.64</b> /96.38
	Eigenvector	86.24/ <b>89.80</b>	<b>90.18</b> /88.26	82.32/ <b>90.41</b>	86.28/ <b>89.40</b>
	Average	<b>91.04</b> /90.54	<b>89.55</b> /87.47	90.62/ <b>91.75</b>	<b>90.26</b> /89.91
RC	Betweenness	64.04/58.60	64.58/59.25	71.01/65.54	68.73/63.29
	Closeness	13.36/15.84	13.56/16.06	19.77/22.01	16.89/19.25
	Degree	13.23/03.87	14.23/05.30	33.77/24.60	27.16/17.78
	Eigenvector	17.07/14.09	17.07/14.09	21.43/18.58	19.38/16.46
	Average	26.93/23.10	27.36/23.67	36.50/32.68	33.04/29.20

Table: Performance metrics (Precision, Recall, True Negative rate, Accuracy) for both models on the “test” dataset (without/with multitasking). The best values are in **bold**. Source: Author

Model	Centrality	P (%)	R (%)	TN (%)	Acc (%)
RN	Betweenness	78.67/ <b>85.12</b>	<b>87.39</b> /75.87	69.44/ <b>88.10</b>	78.35/ <b>81.83</b>
	Closeness	63.32/ <b>69.95</b>	<b>61.19</b> /58.36	<b>89.04</b> /88.94	<b>75.60</b> /74.12
	Degree	<b>77.16</b> /76.82	<b>73.44</b> /70.85	<b>99.82</b> /98.80	<b>87.42</b> /85.85
	Eigenvector	70.96/ <b>77.56</b>	67.66/ <b>87.16</b>	<b>89.76</b> /65.91	<b>78.79</b> /76.54
	Average	72.53/ <b>77.36</b>	72.42/ <b>73.06</b>	<b>87.01</b> /85.44	<b>80.04</b> /79.59
RC	Betweenness	64.89/59.87	65.14/60.59	71.45/66.01	69.18/64.09
	Closeness	13.60/15.65	13.61/15.66	16.42/18.35	15.06/17.05
	Degree	24.51/26.58	25.38/28.95	43.82/45.09	37.93/39.90
	Eigenvector	14.78/15.54	14.76/15.53	16.63/17.46	15.72/16.52
	Average	29.87/29.41	29.72/30.18	37.08/36.73	34.48/34.39

Table: Performance metrics (Precision, Recall, True Negative rate, Accuracy) for both models on the “large” dataset (without/with multitasking). The best values are in **bold**. Source: Author

Centrality	P (%)	R (%)	TN (%)	Acc (%)
Betweenness	<b>81.21</b> /77.92	<b>77.47</b> /77.01	<b>81.82</b> /78.45	<b>79.71</b> /77.75
Closeness	<b>81.66</b> /79.57	75.25/ <b>77.47</b>	<b>84.22</b> /81.45	<b>79.88</b> /79.52
Degree	86.38/ <b>87.44</b>	72.46/ <b>74.88</b>	89.04/ <b>90.98</b>	82.08/ <b>83.97</b>
Eigenvector	<b>84.95</b> /79.59	<b>87.95</b> /80.54	<b>83.80</b> /79.95	<b>85.84</b> /80.24
Average	<b>83.55</b> /81.13	<b>78.28</b> /77.48	<b>84.72</b> /82.71	<b>81.88</b> /80.37

Table: Performance metrics (Precision, Recall, True Negative rate, Accuracy) for the RN model on the “different” dataset (without/with multitasking). The best values are in **bold**. Source: Author

Centrality	Accuracy (%)						
	PowEris	EconMah	SocHav	SC-GT	GrQc	EGO	Average
Betweenness	64/ <b>66</b>	77/ <b>81</b>	84/ <b>85</b>	<b>84</b> /83	<b>81</b> /75	<b>77</b> /75	<b>78</b> /66
Closeness	<b>71</b> /65	81/ <b>83</b>	60/ <b>74</b>	<b>77</b> / <b>80</b>	62/ <b>68</b>	<b>64</b> /58	<b>69</b> /61
Degree	<b>78</b> / <b>82</b>	<b>86</b> /83	67/ <b>73</b>	<b>80</b> / <b>80</b>	<b>82</b> / <b>84</b>	<b>74</b> /72	<b>78</b> /68
Eigenvector	<b>67</b> /63	<b>73</b> /73	<b>87</b> /69	<b>86</b> /79	62/ <b>64</b>	<b>66</b> /57	<b>74</b> /58
Average	<b>70</b> /69	79/ <b>80</b>	74/ <b>75</b>	<b>82</b> /81	72/ <b>73</b>	<b>70</b> /65	<b>75</b> /74

Table: Accuracy for the RN model on the “real” dataset (without/with multitasking). The best values are in **bold**. Source: Author

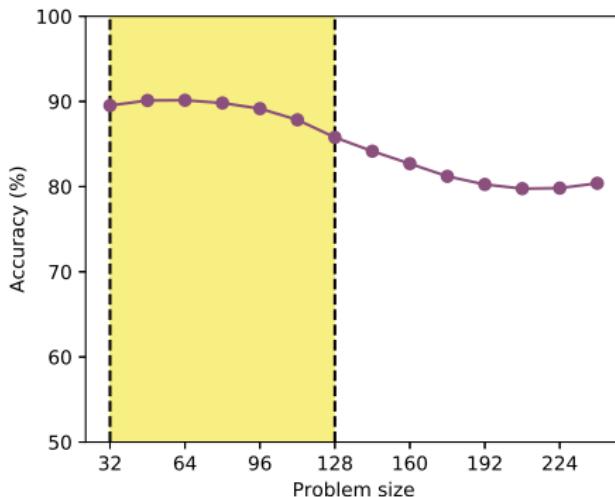


Figure: Overall accuracy multitasking RN model by number of vertices Source:  
Author

## RESULTS – VARYING SIZES NON-MULTITASKING I

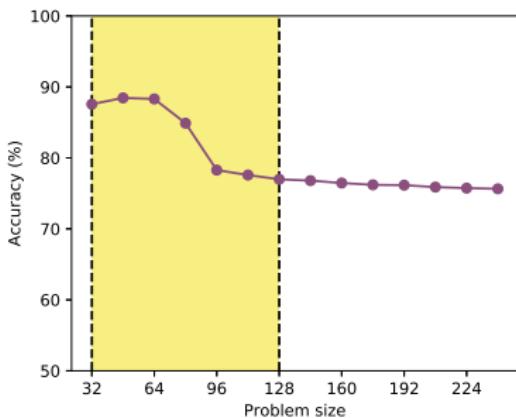
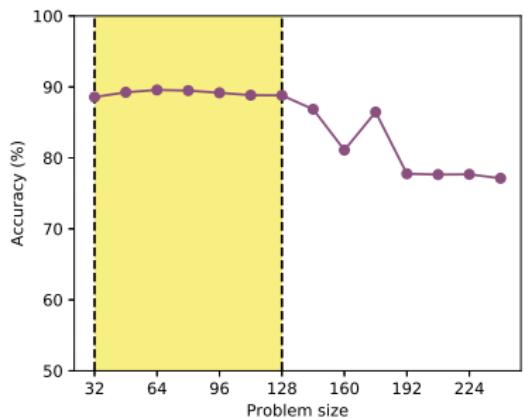


Figure: Overall accuracy non-multitasking RN model by number of vertices.  
Betweenness (left) and closeness. Source: Author

## RESULTS – VARYING SIZES NON-MULTITASKING II

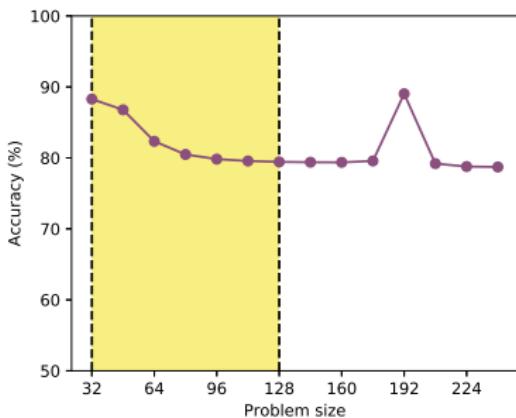
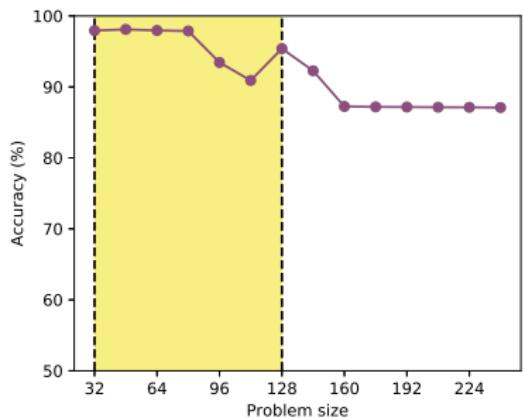


Figure: Overall accuracy non-multitasking RN model by number of vertices.  
Degree (left) and eigenvector. Source: Author

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- Many different behaviours were observed, both good and bad

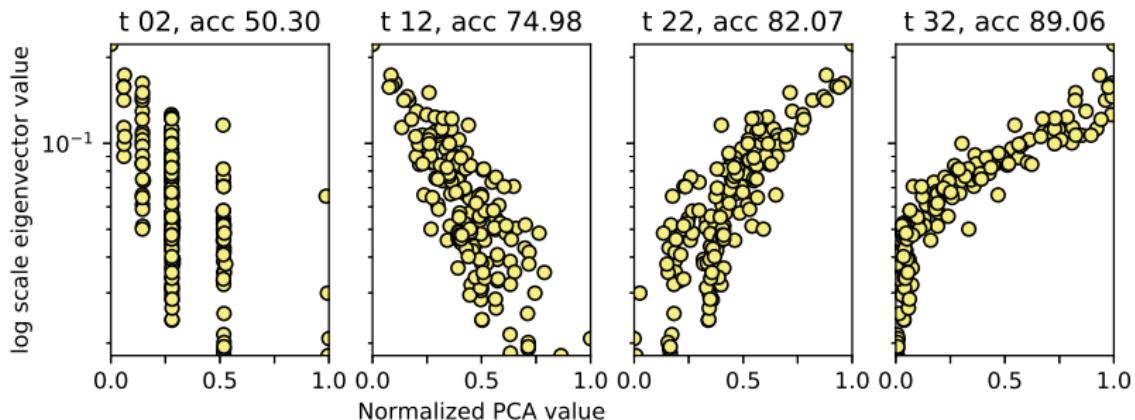


Figure: 1D PCA of a non-multitasking model for the eigenvector centrality of an Watts-Strogatz Small World graph on the “large” dataset. Source: Author

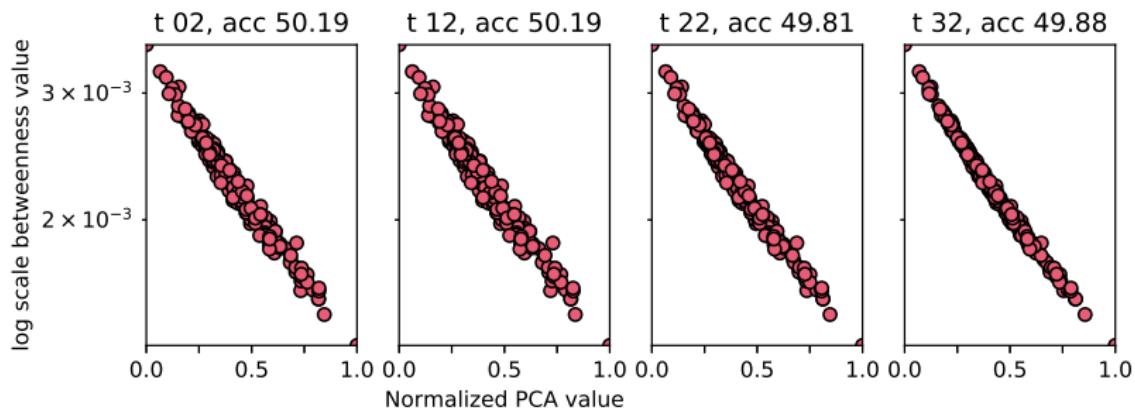


Figure: 1D PCA of a non-multitasking model for the betweenness centrality of an Erdős-Renyi graph on the “large” dataset. Source: Author

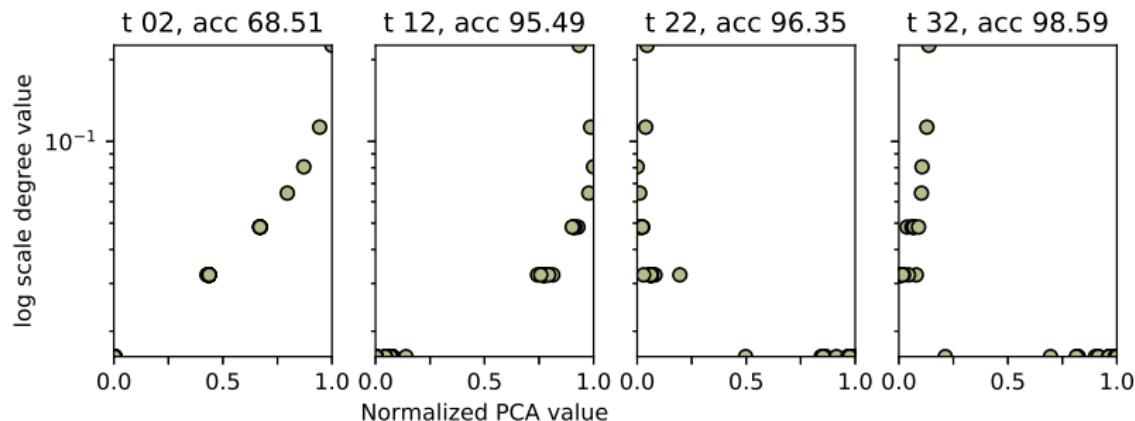


Figure: 1D PCA of a multitasking model for the degree centrality of a Powerlaw-Tree graph on the “small” dataset. Source: Author

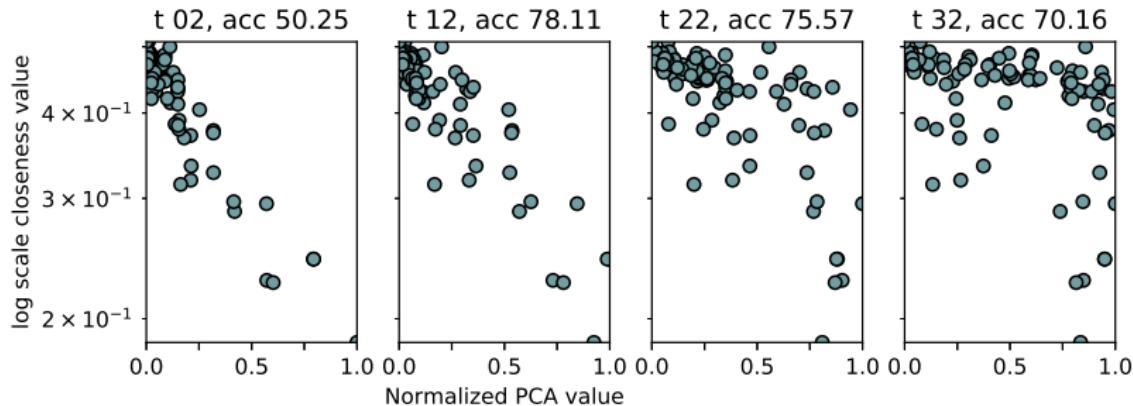


Figure: 1D PCA of a multitasking model for the closeness centrality of a Shell graph on the “different” dataset. Source: Author

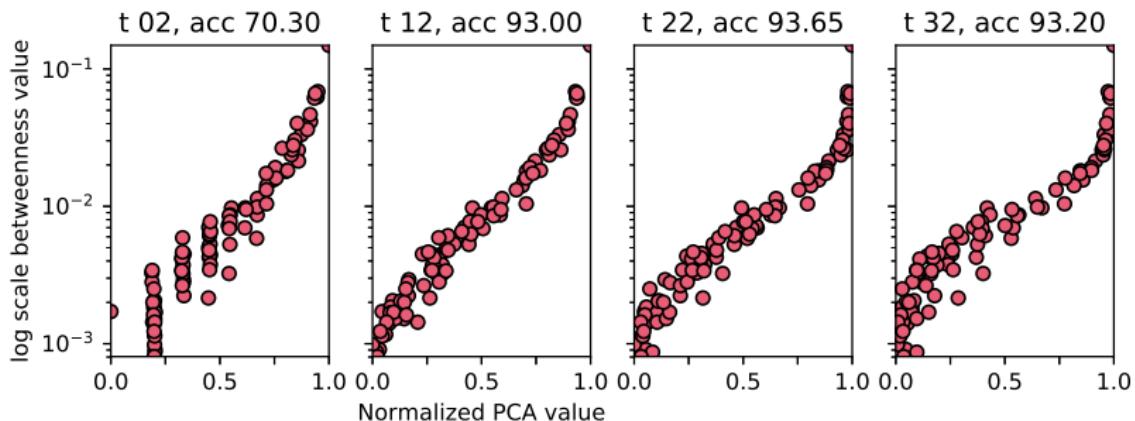


Figure: 1D PCA of a non-multitasking model for the betweenness centrality of an Barabási-Albert graph on the “different”. Source: Author

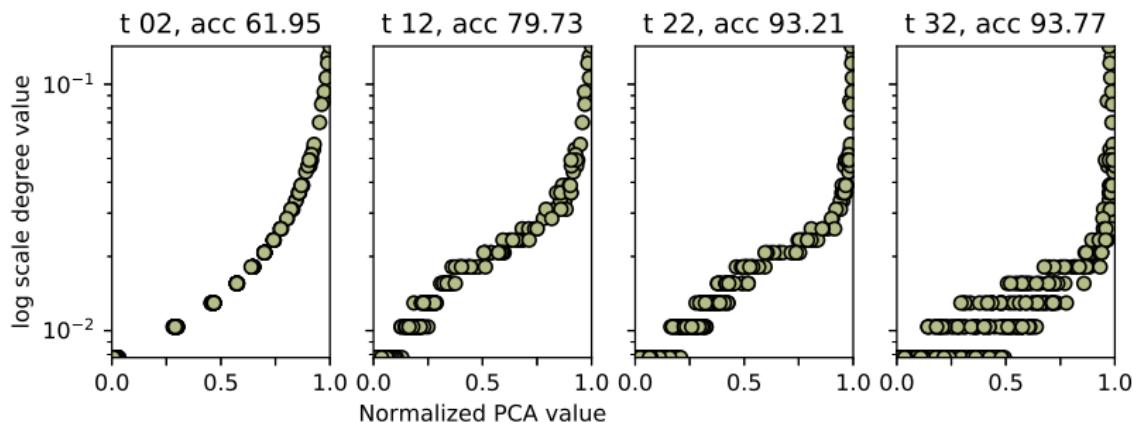


Figure: 1D PCA of a non-multitasking model for the degree centrality of a Holme-Kim graph on the “large”. Source: Author

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- In the end, the model generally had worse performance than when ran for the usual 32 iterations
- One possibility for this might be the lack of an adversarial training strategy, as done by SELSAM et al. (2018)

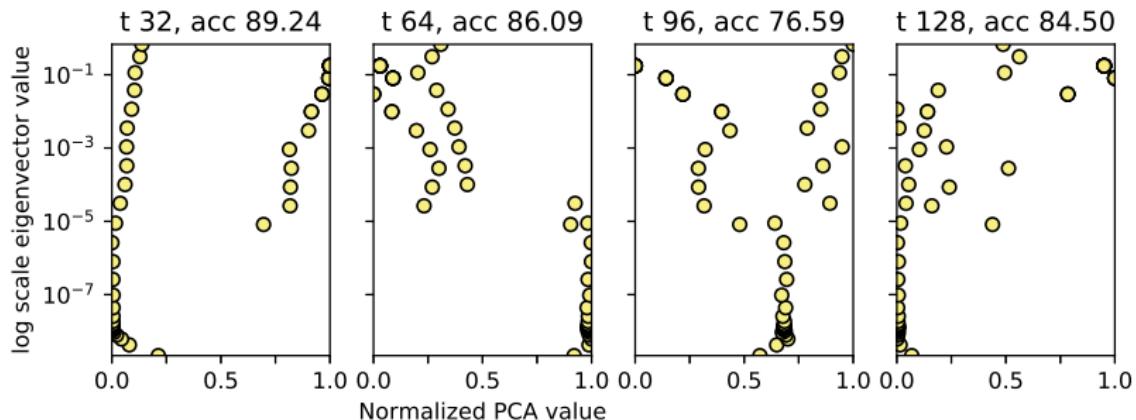


Figure: 1D PCA of a multitasking model for the eigenvector centrality of a Powerlaw Tree graph on the “small”. Source: Author

## UNSTABLE PCA WITH MORE ITERATIONS

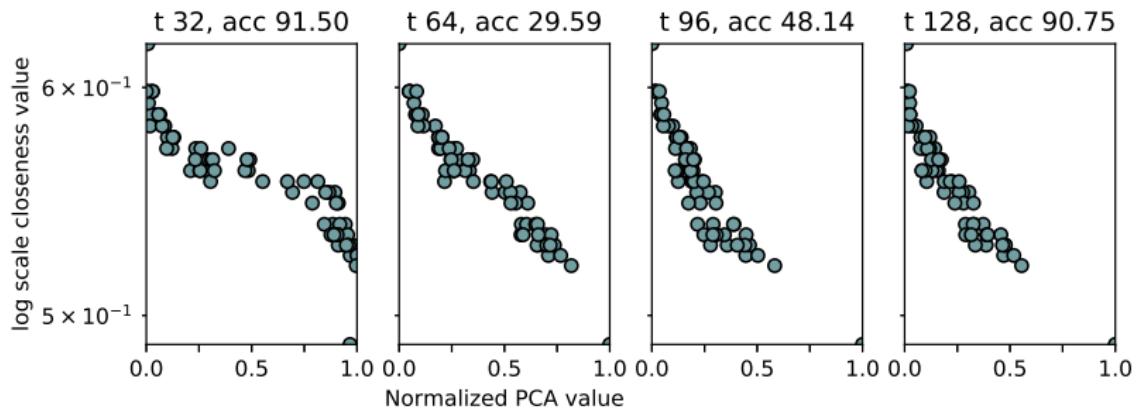


Figure: 1D PCA of a multitasking model for the closeness centrality of an Erdős-Renyi graph on the “small”. Source: Author

## **Conclusions**

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# 5

CONCLUSIONS

CONTRIBUTIONS

LEARNING CENTRALITY  
MEASURES WITH GRAPH NEURAL  
NETWORKS

- Analysis of the performance of a GNN model for 4 different centralities.

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  - Model is lighter if many centralities are learned jointly than if ran separately

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  - Such decay was expected
  - May be due to global information and numerical problems

# 5

CONCLUSIONS

FUTURE WORK

LEARNING CENTRALITY  
MEASURES WITH GRAPH NEURAL  
NETWORKS

- More centrality measures.

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- Deeper analysis of internal embeddings.

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- Experimenting with Transfer Learning instead of Multitask Learning

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- >.

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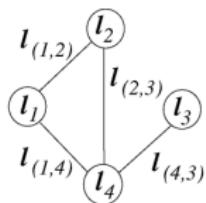


Figure: Source: SCARSELLI et al. (2009)

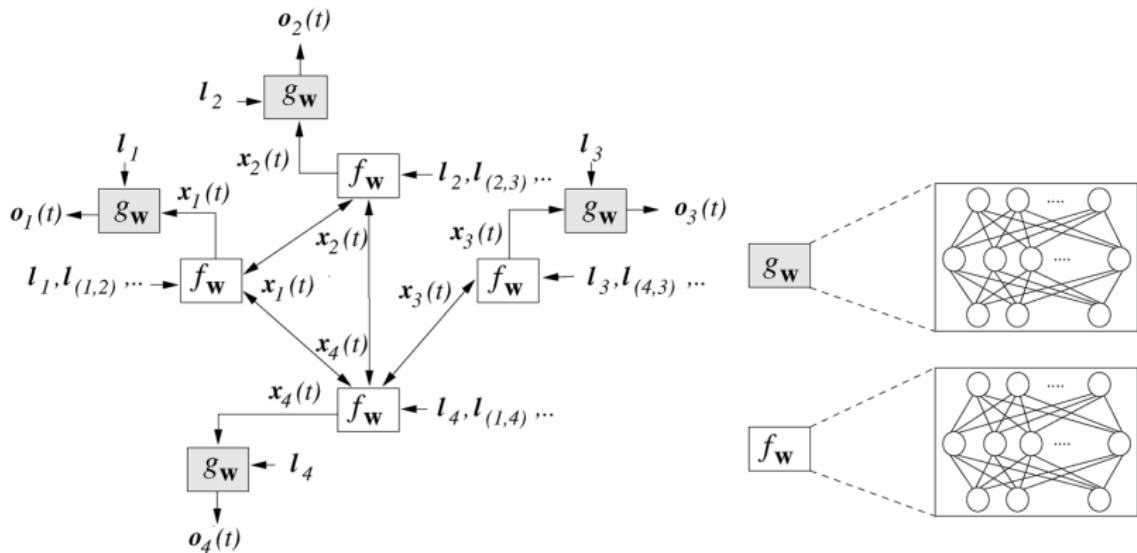


Figure: Source: SCARSELLI et al. (2009)

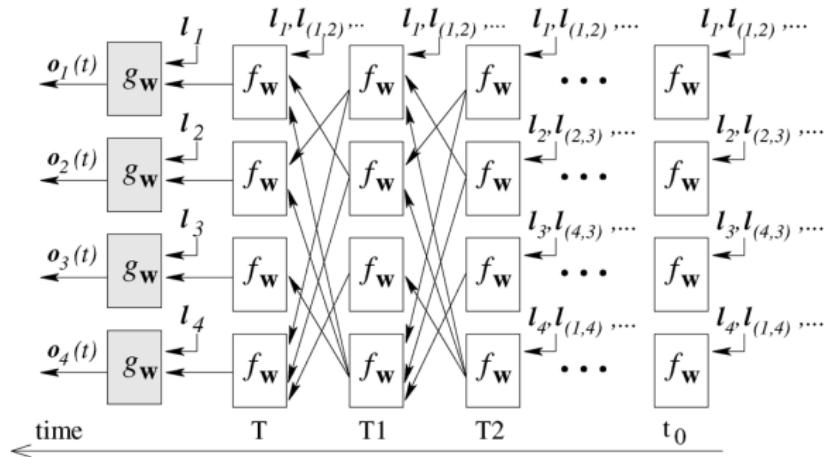


Figure: Source: SCARSELLI et al. (2009)

# FITTING THE DIMENSIONALITY OF THE MODEL – APPROXIMATING

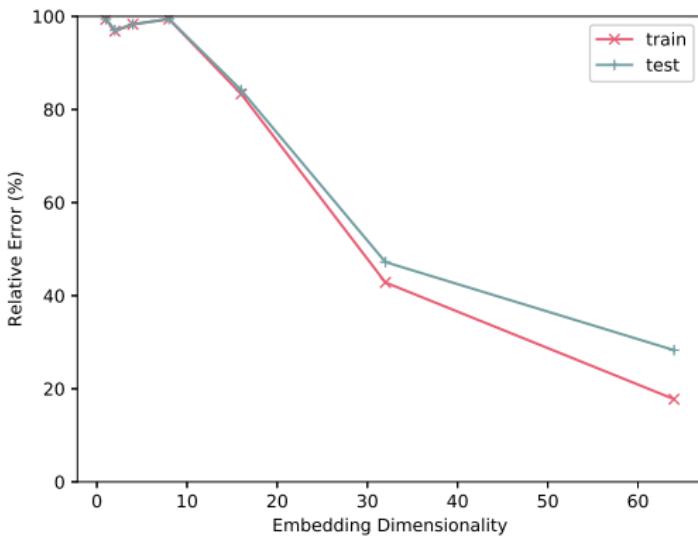


Figure: Relative Error (degree centrality) on the “train” (in red) and “large” datasets (in blue) by embedding dimensionality  $d$  for the CN2 model. Source: Author

# APPROXIMATING – PROBLEM SIZE INFLUENCE ON MULTITASK MODEL

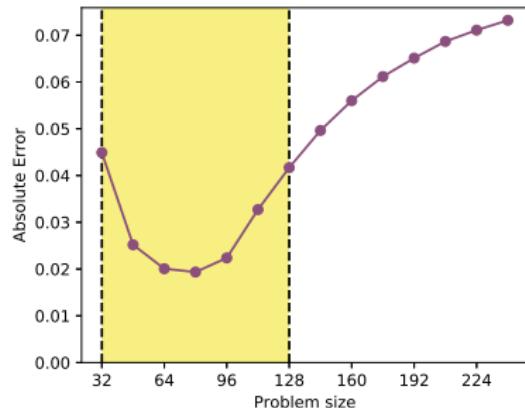
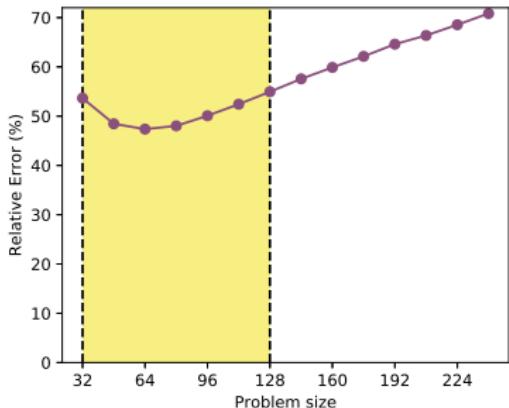


Figure: The overall relative (left) and absolute (right) error for the CN2 multitask model  
Source: Author

# APPROXIMATING – PROBLEM SIZE INFLUENCE ON NON-MULTITASK MODEL I

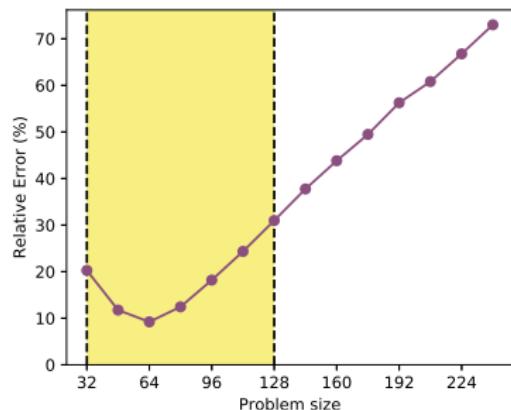
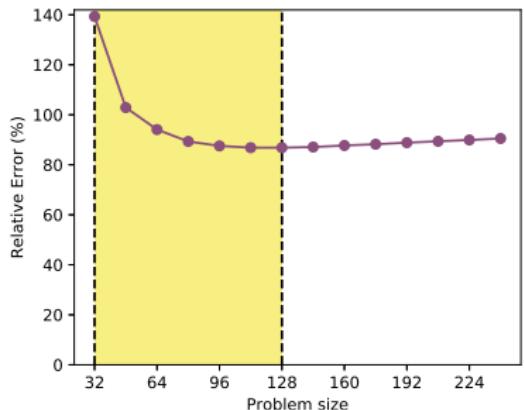


Figure: Overall relative error for the non-multitasking RN model by number of vertices. Betweenness (left) and closeness. Source: Author

# APPROXIMATING – PROBLEM SIZE INFLUENCE ON NON-MULTITASK MODEL I

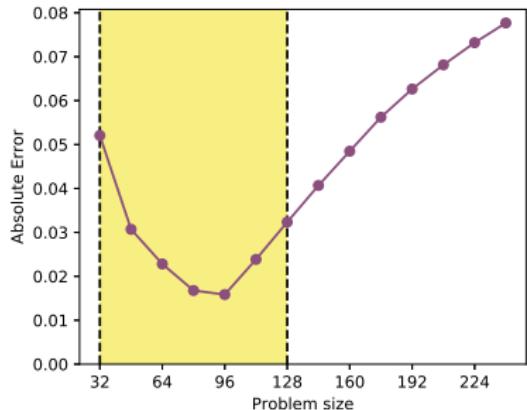
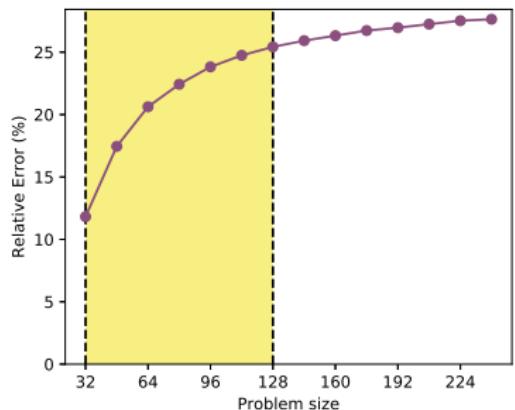


Figure: Overall relative (left) and absolute (right) error for the non-multitasking RN model by number of vertices. Degree (left) and Eigenvector. Source: Author

```
1: procedure GNN-CENTRALITY( $\mathcal{G} = (\mathcal{V}, \mathcal{E}), \mathcal{C}$ )
2:    $\mathbf{M}[i, j] \leftarrow 1$  if  $(v_i, v_j) \in \mathcal{E}$  else 0
3:    $\mathbf{V}^1[i, :] \leftarrow V_{init} \mid \forall v_i \in \mathcal{V}$ 
4:   for  $t = 1 \dots t_{max}$  do
5:      $\mathbf{V}^{t+1}, \mathbf{V}_h^{t+1} \leftarrow V_u(\mathbf{V}^t, \mathbf{M} \times \text{src}_{\text{msg}}(\mathbf{V}^t), \mathbf{M}^T \times \text{tgt}_{\text{msg}}(\mathbf{V}^t))$ 
6:   end for
7:   for  $c \in \mathcal{C}$  do
8:      $\mathbf{M}_{\gtrapprox_c}[i, j] \leftarrow \text{cmp}_c(\mathbf{V}^{t_{max}}[i, :], \mathbf{V}^{t_{max}}[j, :]) \mid \forall v_i, v_j \in \mathcal{V}$ 
9:      $\mathbf{M}_{>c} \leftarrow M_{\gtrapprox_c} > \frac{1}{2}$ 
10:  end for
11: end procedure
```

# FITTING THE DIMENSIONALITY OF THE MODEL – COMPARING

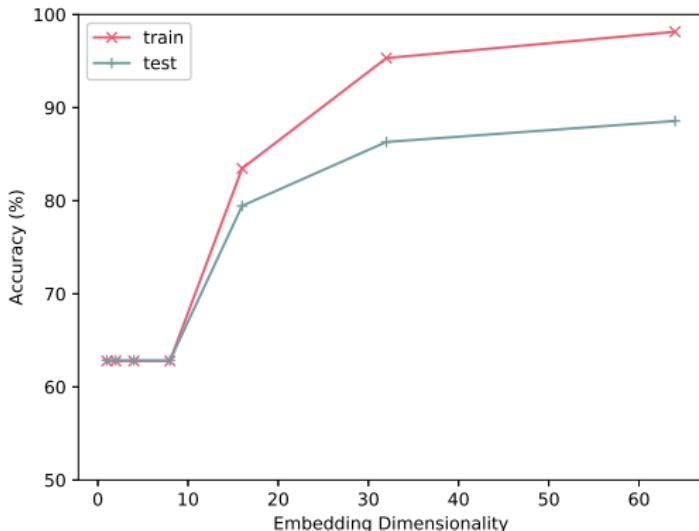


Figure: Accuracy (degree centrality) on the “train” (in red) and “large” datasets (in blue) by embedding dimensionality  $d$  for the RN model. Source: Author