



LEARNING CENTRALITY MEASURES WITH GRAPH NEURAL NETWORKS

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1. Introduction
2. Graph Neural Networks
3. Related Work
4. Experimental Setup and Results
5. Conclusions

Introduction

- Machine Learning subarea:

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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)

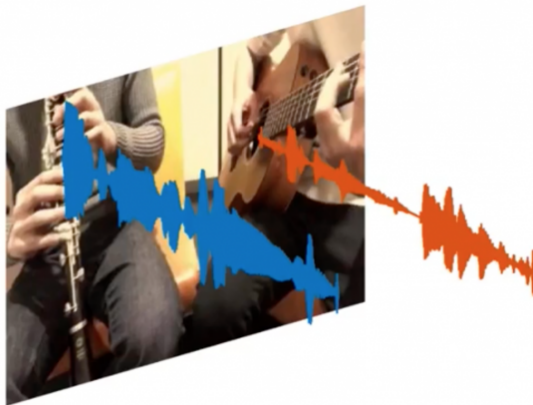


Figure: Recent success which uses deep learning for audio processing – Sound localisation with the PixelPlayer model. Source: ZHAO et al. (2018)

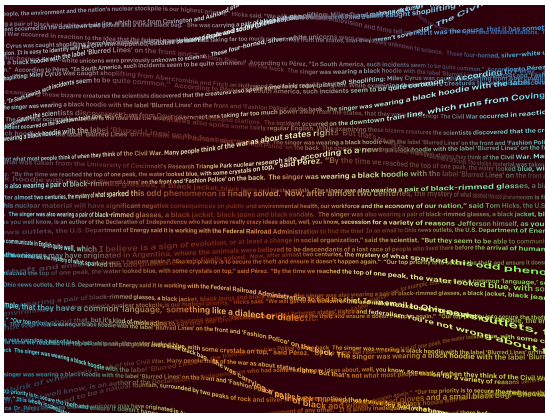


Figure: Recent success which uses deep learning for text processing – OpenAI's GPT-2 model. Source: OpenAI (RADFORD et al., 2019)

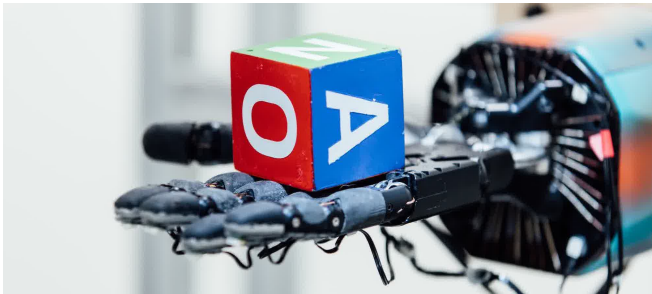


Figure: Recent success which uses deep learning for robotics. Source: OpenAI (OPENAI et al., 2018)



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)

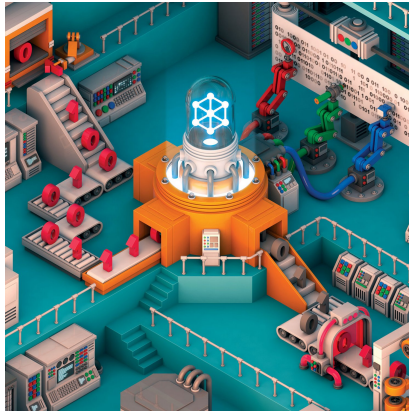


Figure: Recent success that uses deep learning for a relational problem – In this case, the DNC model performs well in question answering and graph processing tasks. Source: Deepmind (GRAVES et al., 2016)

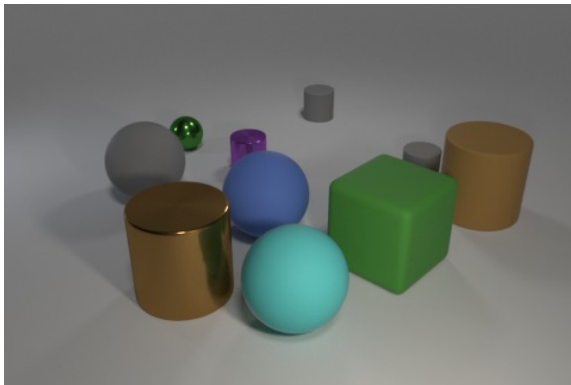


Figure: Recent successes that uses deep learning for a relational problem – In this case, answering relational questions about a synthetic image. Source: SANTORO et al. (2017)

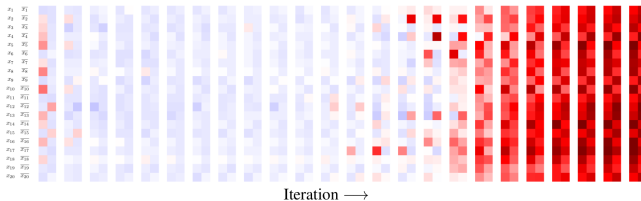


Figure: Recent success that uses deep learning for a relational problem – In this case, solving SAT instances. Source: SELSAM et al. (2018)

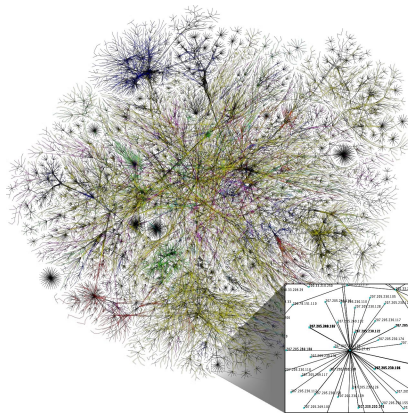


Figure: A partial map of the Internet based in 2005, made by opte.org: The relational structures that support our modern societies have been growing larger and more interconnected by the day. Source: Wikimedia Commons

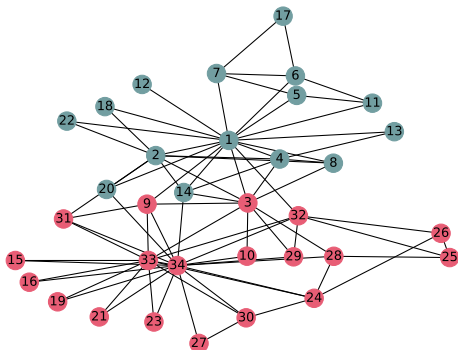


Figure: The connections of the 34 members of Zachary's Karate Club (WAYNE, 1977), a small social network. Here it is easy to see the equivalence between networks and graphs. Source: Author, data from (WAYNE, 1977) plotted using the Networkx Python package (HAGBERG; SWART; CHULT, 2008)

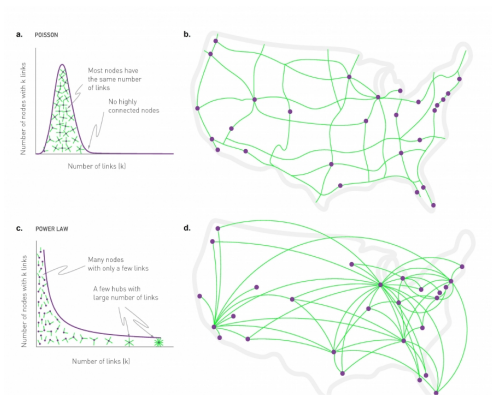


Figure: Two networks consisting of the same vertices, but with different degree distributions, exemplifying the Scale-Free property. Source: BARABÁSI et al. (2016)

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- Many definitions of importance
- Uses in (social) network analysis

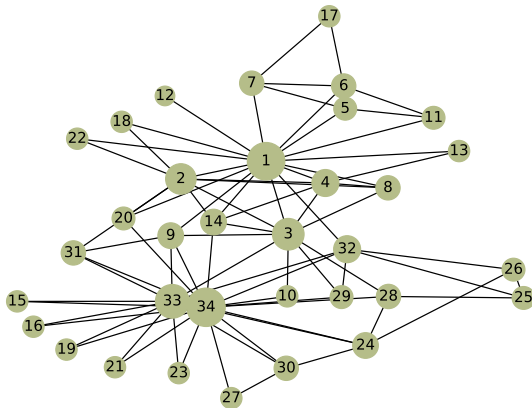


Figure: Zachary's Karate Club with nodes sized by degree. Source: Author, data from (WAYNE, 1977) plotted using the Networkx Python package (HAGBERG; SWART; CHULT, 2008)

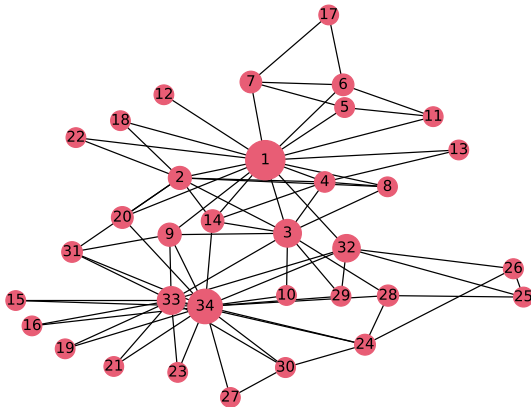


Figure: Zachary's Karate Club with nodes sized by betweenness. Source: Author, data from (WAYNE, 1977) plotted using the Networkx Python package (HAGBERG; SWART; CHULT, 2008)

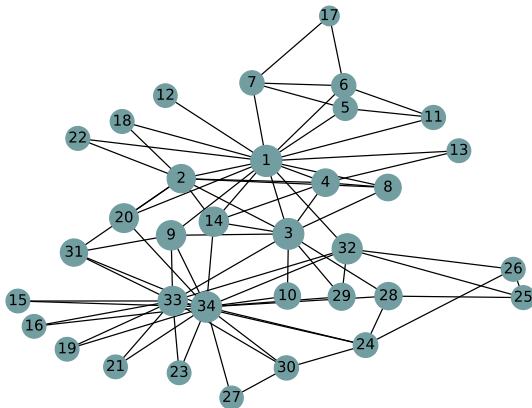


Figure: Zachary's Karate Club with nodes sized by closeness. Source: Author, data from (WAYNE, 1977) plotted using the Networkx Python package (HAGBERG; SWART; CHULT, 2008)

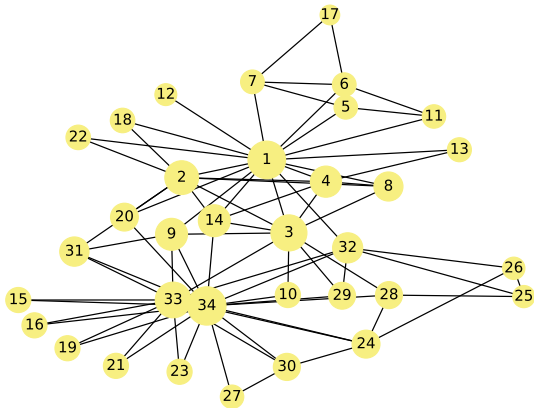


Figure: Zachary's Karate Club with nodes sized by eigenvector. Source: Author, data from (WAYNE, 1977) plotted using the Networkx Python package (HAGBERG; SWART; CHULT, 2008)

Graph Neural Networks

2

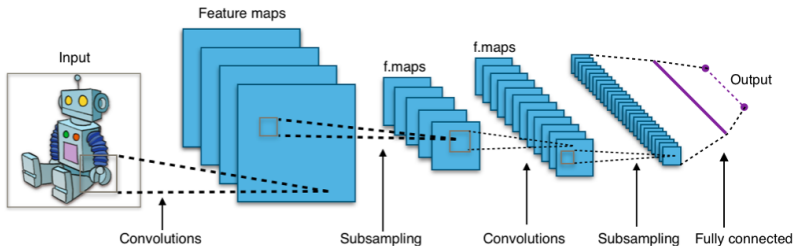


Figure: The typical architecture of a CNN. Source: Wikimedia Commons

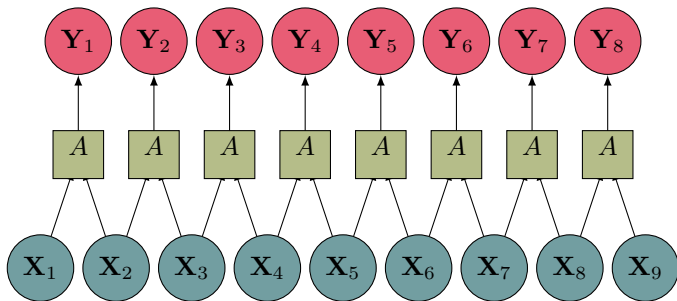


Figure: The application of a 1-dimensional convolutional kernel on a discrete 1-dimensional space. Blue circles are inputs, red circles are outputs and green backgrounds are to represent the whole neural network block. Source: Author, based on (OLAH, 2014)

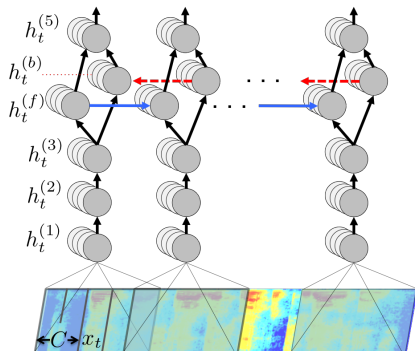


Figure: Deep Speech RNN architecture. Source: HANNUN et al. (2014)

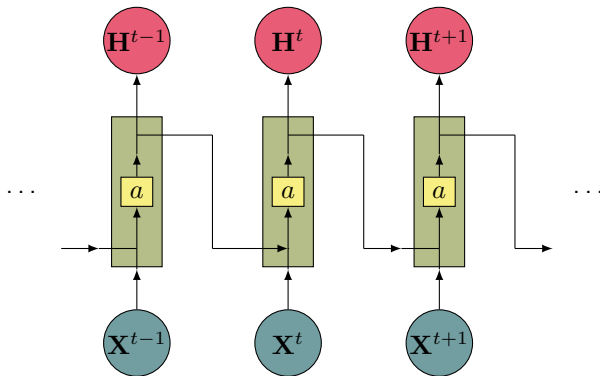


Figure: An unrolled recursive neural network. Yellow squares are neural network layers, blue circles are inputs, red circles are outputs and green backgrounds are to represent the whole neural network block. Source: Author, based on (OLAH, 2015)

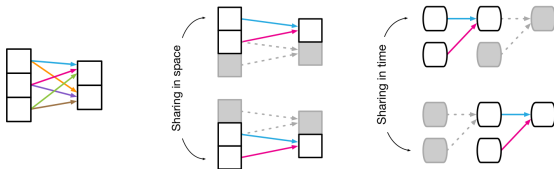


Figure: There is weight reuse across convolutional (middle) and recurrent (right) layers, but not in fully connected (left) layers. Source: BATTAGLIA et al. (2018)

2

GRAPH NEURAL NETWORKS

RELATIONAL INDUCTIVE BIAS

LEARNING CENTRALITY
MEASURES WITH GRAPH NEURAL
NETWORKS

- RNNs work on sequences

2

- RNNs work on sequences
- CNNs work on discrete spaces

2

- RNNs work on sequences
- CNNs work on discrete spaces
- What about graphs?

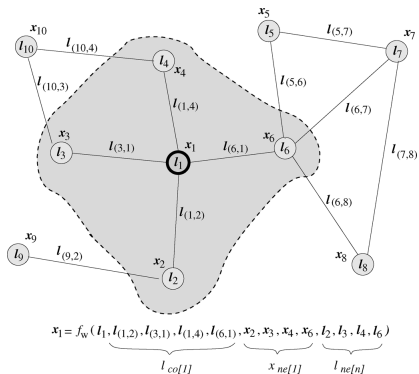


Figure: The representation of the Graph Neural Network Model, with the vertex being updated using the information on its neighbourhood Source: SCARSELLI et al. (2009)

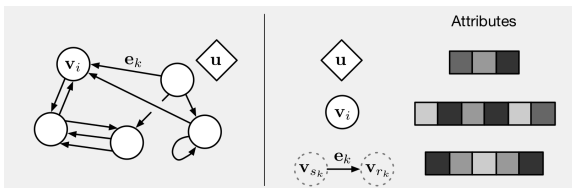


Figure: The representation of the Graph Network Model. Source: BATTAGLIA et al. (2018)

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

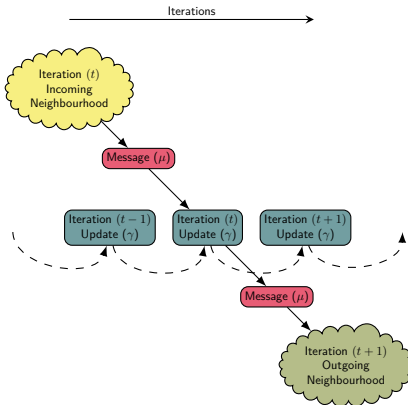


Figure: Pictorial representation of a Typed Graph Network from the perspective of a vertex v . Source: Author

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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:         $\mathbf{V}_{i(b)}^{(t)} \leftarrow \gamma_i(\mathbf{V}_i^{(t)}, \bar{\rho}_{i,b}^{(t)})$ 
12:      end for
13:    end for
14:  end for
15:  return  $\{\mathbf{V}_i^{(t_{max})} \mid i = 1 \dots N\}$ 
16: end procedure

```

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

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

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

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

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

Related Work

- 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.

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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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 - number of vertices in a network
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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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- 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?

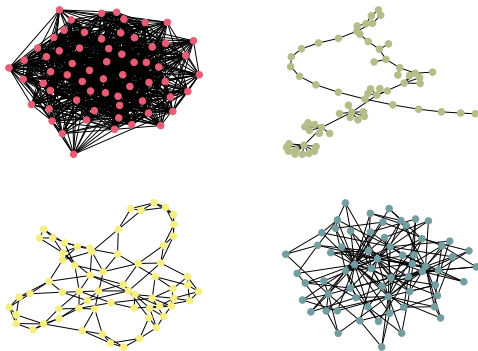


Figure: Examples of training instances with $n = 64$ vertices for each graph distribution, clockwise from the top left: Erdős-Rényi in red, Random power law tree in green, Holme-Kim in blue and Watts-Strogatz in yellow. Source: Author

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

Table: Dataset names and sizes. Source: Author.

PARAMETERS FOR GRAPH GENERATION

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
power-eris1176	NR	1174	9861	100	16.8	2
econ-mahindas	NR	1258	7619	206	12.1	2
socfb-haverford76	NR	1446	59590	374	82.4	1
ego-Facebook	SN	4036	88243	1044	43.7	1
bio-SC-GT	NR	1708	33982	549	39.8	1
ca-GrQc	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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 - C for the pure centrality value
 - 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%	89.6%
	Closeness(R)	77.8%	16.3%	15.3%
	Degree(R)	55.5%	38.9%	43.6%
	Eigenvector(A)	0.0438	0.0251	0.0230
"large"	Betweenness(R)	91.7%	419%	94.2%
	Closeness(R)	274%	85.9%	75.0%
	Degree(R)	58.9%	210%	50.6%
	Eigenvector(A)	0.0569	0.0518	0.0734
<u>"large"</u> <u>"train"</u>	Betweenness	0.989	3.52	1.05
	Closeness	3.52	5.26	4.90
	Degree	1.06	5.40	1.16
	Eigenvector	1.3	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

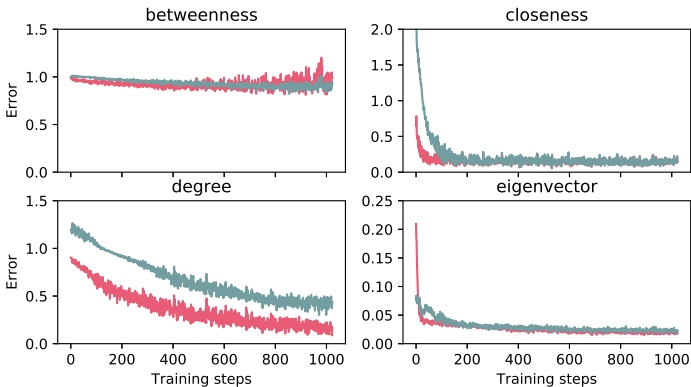


Figure: Training Performance for the CN2 model, **with multitasking** and **without multitasking**. Source: Author

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

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	91.03 /94.17
	Closeness	79.00/ 74.76
	Degree	27.88 /50.06
	Average	65.97 /72.99
Absolute	Eigenvector	0.08311/ 0.07214
	Betweenness	0.01462 /0.01464
	Closeness	0.004785/ 0.003710
	Degree	0.03465 /0.03705
	Eigenvector	0.01694/ 0.008880
MSE	Average	0.01775/ 0.01607

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/ 83.88
	Closeness	19.13 /21.35
	Degree	25.84 /45.32
	Average	48.30 /50.18
Absolute	Eigenvector	0.04854 /0.05282
	Betweenness	0.001376 /0.001445
	Closeness	0.008956 /0.01079
	Degree	0.01026 /0.01758
	Eigenvector	0.003974 /0.004940
MSE	Average	0.006142 /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

4

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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.

4

- 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)

4

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 - 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”

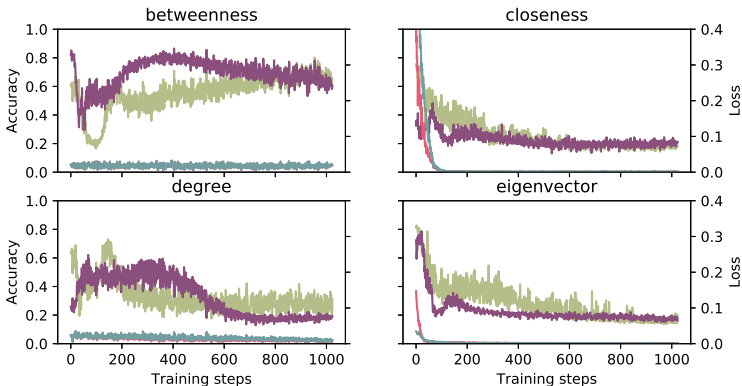


Figure: Loss plotted in red and blue and accuracy in green and purple for training without and with multitasking, respectively. Source: Author

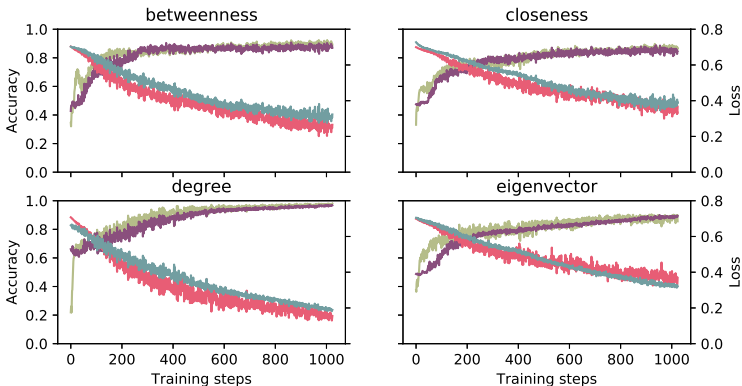


Figure: Loss plotted in red and blue and accuracy in green and purple for training without and with multitasking, respectively. Source: Author

Model	Centrality	P (%)	R (%)	TN (%)	Acc (%)
RN	Betweenness	90.26 /87.18	88.52 /87.24	90.99 /88.89	89.83 /87.94
	Closeness	88.39 /86.88	84.54 /81.96	89.75 /88.72	87.30 /85.52
	Degree	99.27 /98.31	94.94 /92.41	99.44 /98.98	97.64 /96.38
	Eigenvector	86.24/ 89.80	90.18 /88.26	82.32/ 90.41	86.28/ 89.40
	Average	91.04 /90.54	89.55 /87.47	90.62/ 91.75	90.26 /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/ 85.12	87.39 /75.87	69.44/ 88.10	78.35/ 81.83
	Closeness	63.32/ 69.95	61.19 /58.36	89.04 /88.94	75.60 /74.12
	Degree	77.16 /76.82	73.44 /70.85	99.82 /98.80	87.42 /85.85
	Eigenvector	70.96/ 77.56	67.66/ 87.16	89.76 /65.91	78.79 /76.54
	Average	72.53/ 77.36	72.42/ 73.06	87.01 /85.44	80.04 /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	81.21 /77.92	77.47 /77.01	81.82 /78.45	79.71 /77.75
Closeness	81.66 /79.57	75.25/ 77.47	84.22 /81.45	79.88 /79.52
Degree	86.38/ 87.44	72.46/ 74.88	89.04/ 90.98	82.08/ 83.97
Eigenvector	84.95 /79.59	87.95 /80.54	83.80 /79.95	85.84 /80.24
Average	83.55 /81.13	78.28 /77.48	84.72 /82.71	81.88 /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 (%)						Average
	PowEris	EconMah	SocHav	SC-GT	GrQc	EGO	
Betweenness	64/ 66	77/ 81	84/ 85	84 /83	81 /75	77 /75	78 /66
Closeness	71 /65	81/ 83	60/ 74	77/ 80	62/ 68	64 /58	69 /61
Degree	78/ 82	86 /83	67/ 73	80/ 80	82/ 84	74 /72	78 /68
Eigenvector	67 /63	73 /73	87 /69	86 /79	62/ 64	66 /57	74 /58
Average	70 /69	79/ 80	74/ 75	82 /81	72/ 73	70 /65	75 /74

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

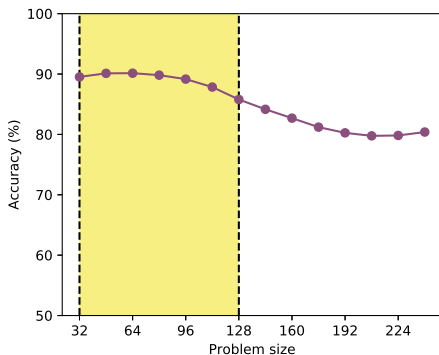


Figure: Overall accuracy multitasking RN model by number of vertices Source: Author

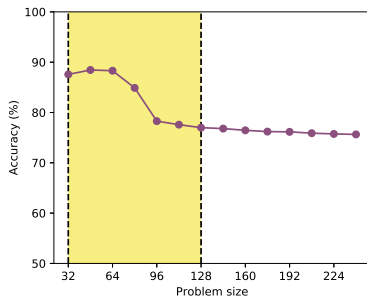
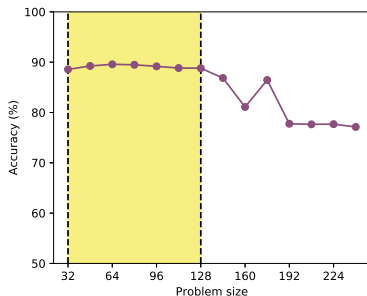


Figure: Overall accuracy non-multitasking RN model by number of vertices. Betweenness (left) and closeness. Source: Author

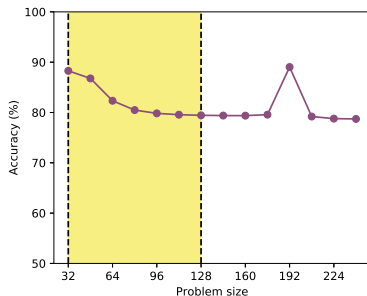
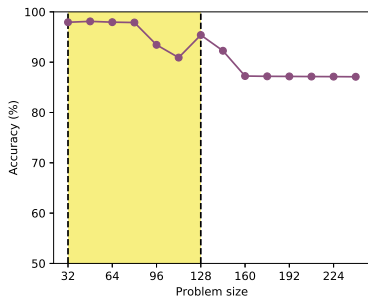


Figure: Overall accuracy non-multitasking RN model by number of vertices. Degree (left) and eigenvector. Source: Author

4

EXPERIMENTAL SETUP AND RESULTS

INTERPRETING THE INTERNAL REPRESENTATION

LEARNING CENTRALITY MEASURES WITH GRAPH NEURAL NETWORKS

- Used Principal Component Analysis (PCA) on the Embeddings

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- It was expected that the PCA had a good visual fit with the centrality in question
- Many different behaviours were observed, both good and bad

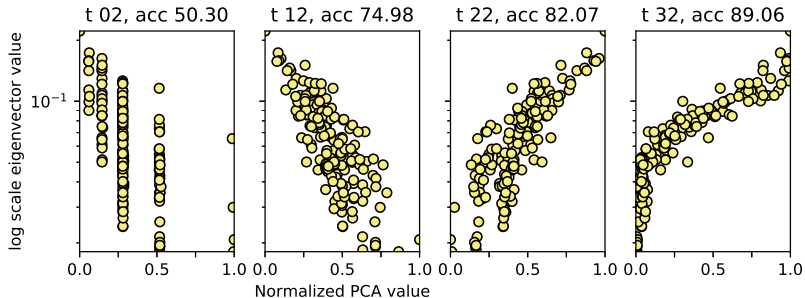


Figure: 1D PCA of a non-multitasking model for the eigenvector centrality of an Watts-Strogatz Small World graph on the “large” dataset. Source: Author

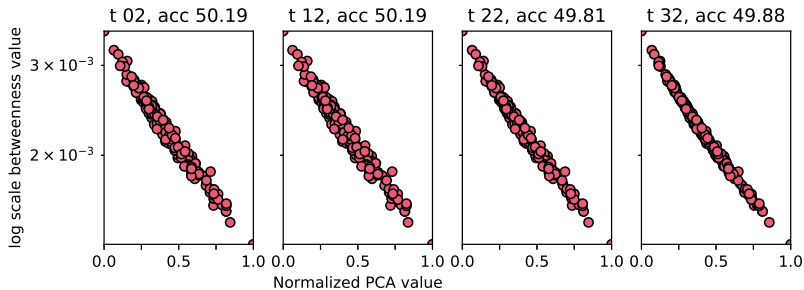


Figure: 1D PCA of a non-multitasking model for the betweenness centrality of an Erdős-Renyi graph on the “large” dataset. Source: Author

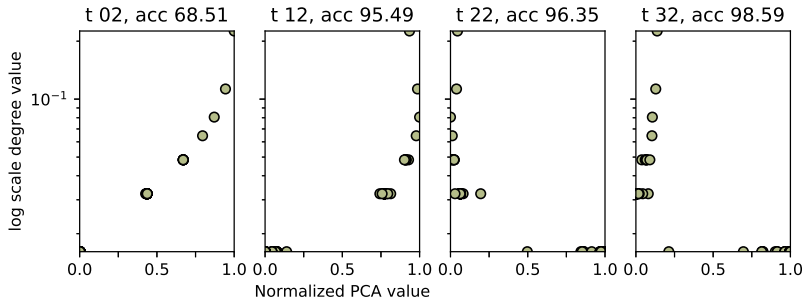


Figure: 1D PCA of a multitasking model for the degree centrality of a Powerlaw-Tree graph on the “small” dataset. Source: Author

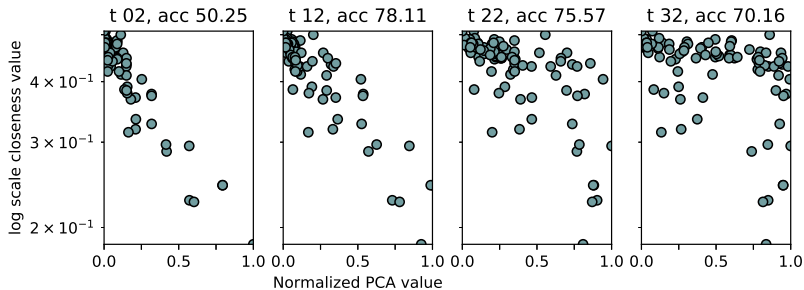


Figure: 1D PCA of a multitasking model for the closeness centrality of a Shell graph on the “different” dataset. Source: Author

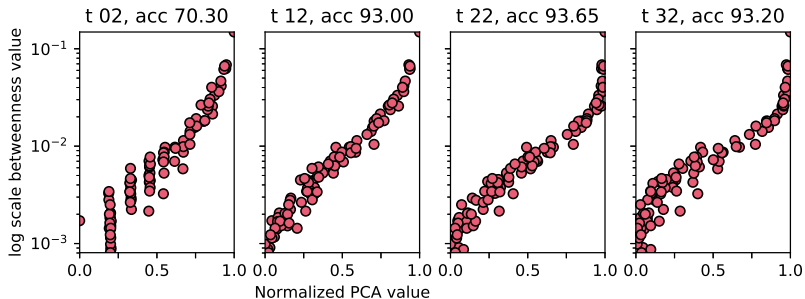


Figure: 1D PCA of a non-multitasking model for the betweenness centrality of an Barabási-Albert graph on the “different”. Source: Author

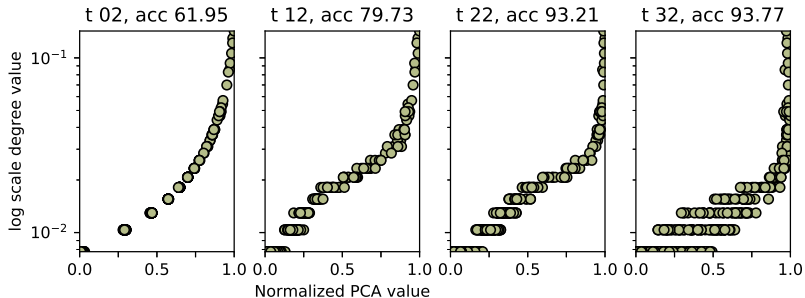


Figure: 1D PCA of a non-multitasking model for the degree centrality of a Holme-Kim graph on the “large”. Source: Author

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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)

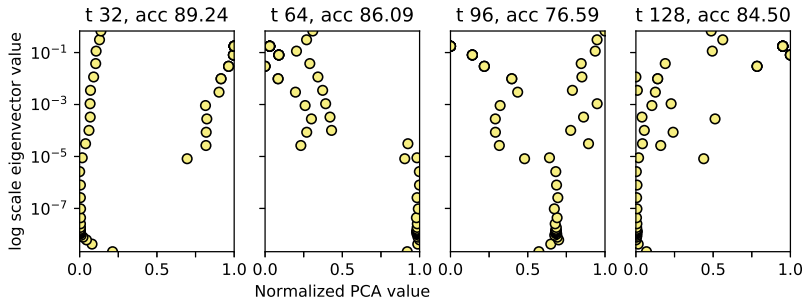


Figure: 1D PCA of a multitasking model for the eigenvector centrality of a Powerlaw Tree graph on the “small”. Source: Author

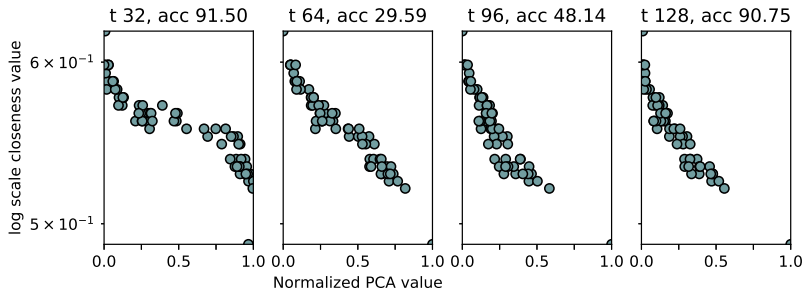


Figure: 1D PCA of a multitasking model for the closeness centrality of an Erdős-Renyi graph on the “small”. Source: Author

Conclusions

- 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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 - May be due to global information and numerical problems

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- More centrality measures.
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- Experimenting with Transfer Learning instead of Multitask Learning


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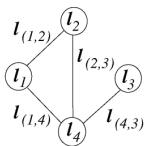


Figure: Source: SCARSELLI et al. (2009)

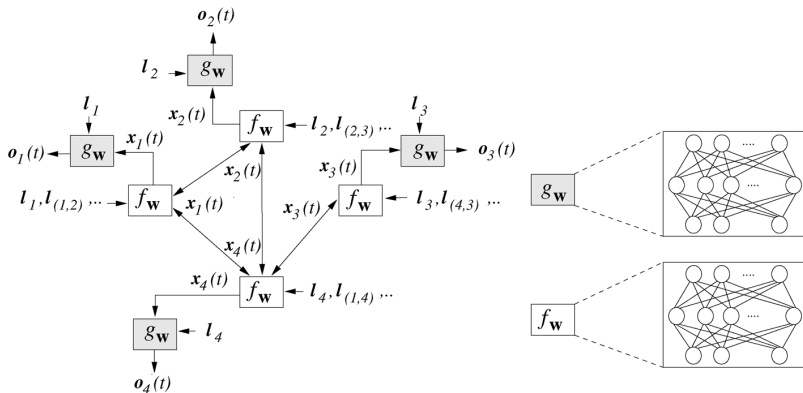


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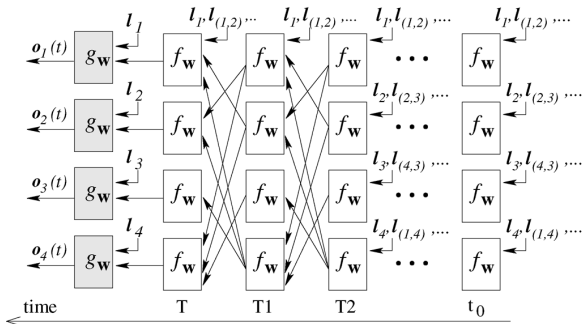


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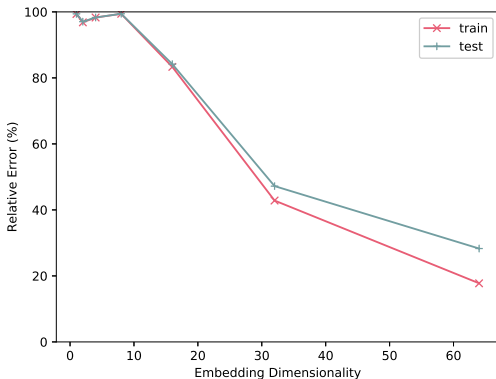


Figure: Relative Error (degree centrality) on the “train” (in red) and “large” datasets (in blue) by embedding dimensionality d for the CN2 model. Source: Author

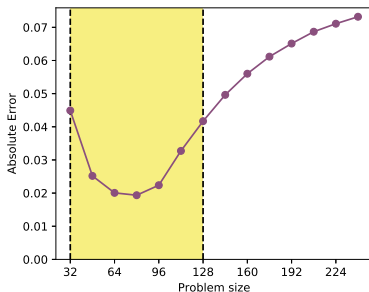
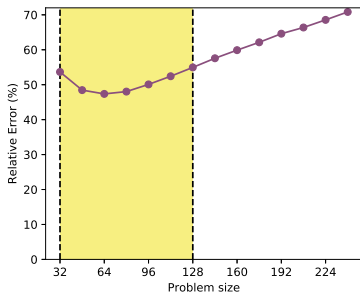
APPROXIMATING – PROBLEM SIZE INFLUENCE
ON MULTITASK MODEL

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

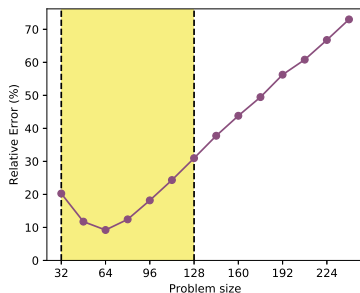
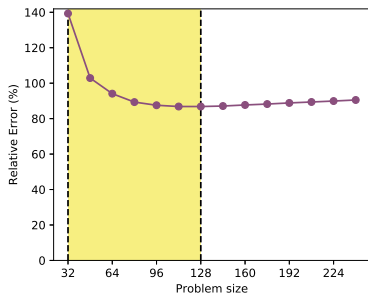
APPROXIMATING – PROBLEM SIZE INFLUENCE
ON NON-MULTITASK MODEL I

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

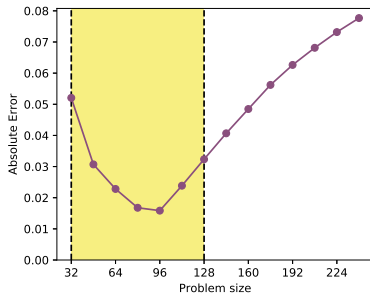
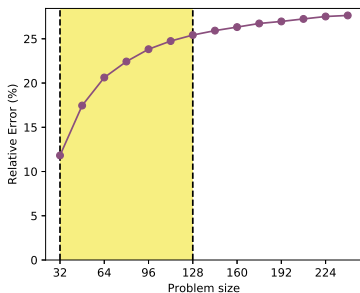


Figure: Overall relative (left) and absolute (right) error for the non-multitasking RN model by number of vertices. Degree (left) and Eigenvector. Source: Author

```

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:    $V^1[i, :] \leftarrow V_{init} \mid \forall v_i \in \mathcal{V}$ 
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:      $\mathbf{M}_{\approx c}[i, j] \leftarrow \text{cmp}_c(\mathbf{V}^{t_{max}}[i, :], \mathbf{V}^{t_{max}}[j, :]) \mid \forall v_i, v_j \in \mathcal{V}$ 
9:      $\mathbf{M}_{> c} \leftarrow M_{\approx c} > \frac{1}{2}$ 
10:  end for
11: end procedure

```

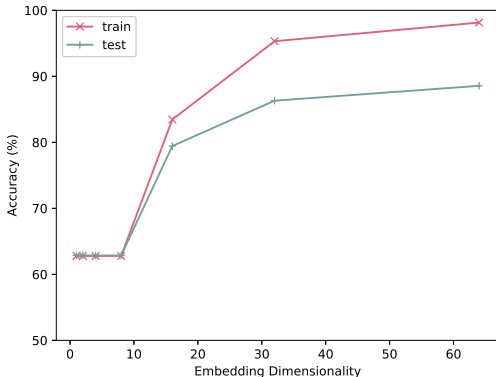

FITTING THE DIMENSIONALITY OF THE
MODEL – COMPARING

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