A Additional results

In the following, we provide additional experimental results, namely the number of time-respecting paths in the test graphs along with the required computation time (table 4), the training and inference times for the GCN and the DBGNN model (table 5 and table 6), the optimal order of a k-th order De Bruijn graph model, inferred using the statistical model selection approach from [37] (table 7), additional results for the number of hits among the top-ranked nodes for betweenness and closeness centrality (table 8 and table 9).

Table 4: Computational complexity of path calculations in the test data. All results were obtained on a workstation with AMD Ryzen 9 3900X 12-core CPU and 64 GB RAM

data set	number of time-respecting paths	computation time
ants-1-1	27,308	190.62 s
ants-1-2	1,614	1.24 s
ants-2-1	362	0.24 s
ants-2-2	3,547	6.02 s
company-emails	64,246	285.64 s
eu-email-2	11,599	22.11 s
eu-email-3	2,770	6.37 s
eu-email-4	12,951	48.63 s
sp-hospital	139,724	206.97 s
sp-hypertext	264,300	356.02 s
sp-workplace	7,350	1.04 s
sp-highschool	1,680,651	10,159.71 s
haggle	38,079	4.97 s

Table 5: Training and inference time for betweenness centrality in seconds

experiments	Train		Eval	
	DBGNN	GCN	DBGNN	GCN
ants-1-1	4.525004	3.976138	0.002476	0.002315
ants-1-2	4.415789	4.192388	0.002383	0.002264
ants-2-1	4.333990	4.093549	0.002967	0.002304
ants-2-2	4.316440	4.088560	0.002610	0.003562
company-emails	4.577491	4.918629	0.002660	0.002632
eu-email-2	6.221958	5.719684	0.002624	0.002226
eu-email-3	6.269507	5.765907	0.002470	0.002503
eu-email-4	6.419320	5.738349	0.002483	0.002109
haggle	4.474058	3.991820	0.002908	0.002142
sp-highschool	12.662649	7.989266	0.003281	0.004080
sp-hospital	8.203254	7.664485	0.003546	0.001961
sp-hypertext	13.615240	7.816432	0.002886	0.002269
sp-workplace	8.429780	7.874174	0.002305	0.002002

Table 6: Training and inference time for closeness centrality in seconds

experiments	Train		Eval	
	DBGNN	GCN	DBGNN	GCN
ants-1-1	4.321659	4.092447	0.002468	0.002743
ants-1-2	4.317691	4.237622	0.002660	0.002339
ants-2-1	4.348724	4.054908	0.002440	0.002278
ants-2-2	4.326630	4.243561	0.002483	0.002158
company-emails	4.577662	4.416060	0.003556	0.002216
eu-email-2	6.485234	5.914584	0.002528	0.002099
eu-email-3	6.450350	5.999103	0.002631	0.002527
eu-email-4	7.260510	7.324913	0.003136	0.002314
haggle	4.649249	4.042492	0.002969	0.002297
sp-highschool	12.592707	9.586796	0.003289	0.002356
sp-hospital	8.688761	8.480865	0.002494	0.002364
sp-hypertext	9.988247	8.148300	0.003354	0.002093
sp-workplace	8.595048	7.866499	0.002670	0.002505

Table 7: Result of detection of optimal order based on likelihood ratio test.

data set	K_{opt} train	K_{opt} val
ants-1-1	2	2
ants-1-2	2	2
ants-2-1	1	1
ants-2-2	2	2
company-emails	2	2
eu-email-4	1	1
eu-email-2	2	2
eu-email-3	1	1
sp-hospital	2	2
sp-hypertext	2	2
sp-workplace	2	2
sp-highschool	2	2
haggle	2	2

Table 8: Results for hitsIn5 and hitsIn10 for prediction of temporal betweenness centrality and learning rate for which each experiment performed best

	DBGNN			GCN		
Experiment	hitsIn5	hitsIn30	lr	hitsIn5	hitsIn30	lr
ants-1-1	**2.467** ± 0.973	17.533 ± 4.377	0.100	0.400 ± 0.516	17.4 ± 2.757	0.010
ants-1-2	3.2 ± 0.664	**24.133** ± 0.937	0.100	2.5 ± 0.707	17.700 ± 2.058	0.100
ants-2-1	1.633 ± 0.718	18.667 ± 1.295	0.010	1.2 ± 0.919	15.7 ± 1.947	0.010
ants-2-2	1.333 ± 0.711	21.6 ± 1.429	0.100	1.2 ± 0.632	21.5 ± 1.78	0.100
company-emails	0.2 ± 0.484	18.7 ± 1.765	0.100	0.2 ± 0.632	16.3 ± 3.164	0.001
eu-email-4	1.4 ± 0.932	14.233 ± 1.87	0.010	1.1 ± 1.101	11.7 ± 3.889	0.001
eu-email-2	1.233 ± 0.898	14.467 ± 1.717	0.001	1.4 ± 0.966	15.2 ± 2.486	0.001
eu-email-3	2.967 ± 0.615	19.467 ± 1.383	0.001	1.5 ± 1.08	15.3 ± 3.498	0.001
sp-hospital	1.467 ± 0.937	22.767 ± 1.524	0.100	2.1 ± 0.876	23.4 ± 1.43	0.010
sp-hypertext	1.3 ± 0.794	18.833 ± 1.931	0.010	2.1 ± 0.568	19.3 ± 1.337	0.001
sp-workplace	1.7 ± 0.651	19.500 ± 1.28	0.100	2.1 ± 1.101	**22.200** ± 1.135	0.100
sp-highschool	**1.933** ± 0.64	16.167 ± 1.859	0.010	1.000 ± 0.0	16 ± 1.247	0.001
haggle	1.633 ± 0.809	24.933 ± 1.015	0.010	2.8 ± 1.033	23.9 ± 1.969	0.001

Table 9: Results for hitsIn5 and hitsIn10 for prediction of temporal closeness centrality and learning rate for which each experiment performed best

	DBGNN			GCN		
Experiment	hitsIn5	hitsIn30	lr	hitsIn5	hitsIn30	lr
ants-1-1	**3.700** ± 0.535	**25.200** ± 0.925	0.100	0.600 ± 0.966	15.700 ± 1.947	0.010
ants-1-2	**3.933** ± 0.365	**27.100** ± 0.662	0.100	1.600 ± 0.516	16.900 ± 2.283	0.001
ants-2-1	**5.000** ± 0.0	**28.200** ± 0.407	0.100	2.400 ± 1.506	20.200 ± 2.741	0.100
ants-2-2	**3.767** ± 0.568	**26.367** ± 0.556	0.001	0.700 ± 0.675	20.100 ± 2.234	0.001
company-emails	**3.467** ± 0.507	**26.333** ± 0.606	0.100	1.500 ± 0.85	14.700 ± 2.406	0.001
eu-email-4	**4.167** ± 0.461	**26.833** ± 0.913	0.100	1.400 ± 1.174	10.700 ± 3.433	0.001
eu-email-2	**4.833** ± 0.379	**25.133** ± 0.73	0.100	0.900 ± 1.287	9.700 ± 3.234	0.100
eu-email-3	**4.000** ± 0.0	**27.000** ± 0.0	0.100	1.300 ± 0.949	20.600 ± 1.506	0.100
sp-hospital	**2.667** ± 0.711	**23.800** ± 0.847	0.100	1.300 ± 0.483	20.800 ± 0.422	0.001
sp-hypertext	**4.100** ± 0.481	**26.033** ± 0.765	0.001	0.800 ± 0.422	19.600 ± 0.843	0.001
sp-workplace	3.2 ± 0.551	**24.500** ± 0.572	0.010	1.7 ± 1.059	20.400 ± 1.897	0.001
sp-highschool	**2.967** ± 0.615	**21.733** ± 1.081	0.001	0.000 ± 0.0	8.300 ± 1.16	0.001
haggle	**4.333** ± 0.479	**28.433** ± 0.504	0.100	0.400 ± 0.699	17.700 ± 7.304	0.010

B Model architecture and Details on Hyperparameters

Layer	Input dimensions	Output dimensions	Activation Function
GCNConv	$\|V\|$	16	Sigmoid
GCNConv	16	8	ELU
Linear layer	8	1	ELU

Table 10: Overview of proposed model architecture for simple GCN

Layer	Input dimensions	Output dimensions	Activation Function
GCNConv first order	$\|V\|$	16	Sigmoid
GCNConv second order	$\|E\|$	16	Sigmoid
Bipartite layer	16	8	ELU
Linear layer	8	1	ELU

Table 11: Overview of proposed model architecture for DBGNN

C Static vs temporal centralities

Let $G = (V, E)$ be a (static) graph, where V is a set of vertices or nodes and $(v, w) \in E$ are potentially directed edges or links from node v to w. Let us further consider weighted graphs, where we have a function $w : E \to \mathbb{N}$ that assigns integer weights to edges. In a static network $G = (V, E)$, we define a path (or walk) of length l from v_0 to v_l as any sequence of nodes $v_0, \ldots, v_l$ iff $(v_{i-1}, v_i) \in E$ for $i = 1, \ldots, l$. If every node occurs only once in the sequence, we call the sequence a *simple* path. A shortest path between two nodes v and w is a (not necessarily unique) path of legth l such that all other paths from v to w have length $l' \geq l$.

In static networks, shortest paths between pairs of nodes allow us to define *path-based nodes centralities*, which can be used to identify influential nodes. Here, we briefly introduce two important path-based centrality measures, namely *betweenness and closeness centrality*. For static networks without temporal interactions the betweenness centrality of a node v is calculated as

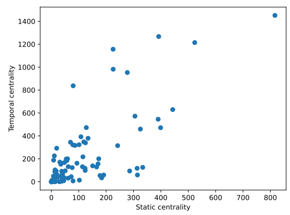
$$c_B(v) = \sum_{s \neq v \neq t \in V} \frac{\sigma_{s,t}(v)}{\sigma_{s,t}}$$

where $\sigma_{s,t}$ is the number of the shortest paths between nodes s and t and $\sigma_{s,t}(v)$ is the number of such paths that pass through node v. In other words the node is considered central if there are many shortest paths that pass through the node. The closeness centrality on the other hand is defined as

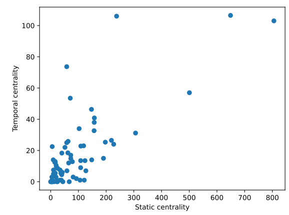
$$c_C(v) = \frac{1}{\sum_{u \in V} d(u, v)}$$

where $d(u, v)$ describes the distance (length of the shortest path) of node u to node v. Thus, in terms of closeness a node is considered more central if the overall distance to all other nodes in the graph is relatively small.

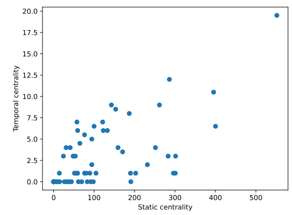
To contrast the temporal path-based centralities defined in section 2 with the corresponding static centralities defined above, in fig. 2 and fig. 3 we plot the temporal vs. static betweenness and closeness centralities of all nodes for all 13 empirical temporal graphs considered in our work (cf. table 1).



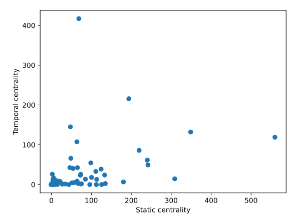
(a) ants-1-1



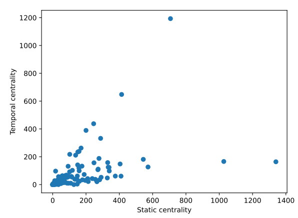
(b) ants-1-2



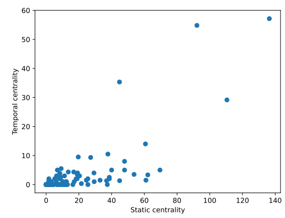
(c) ants-2-1



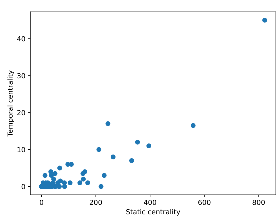
(d) ants-2-2



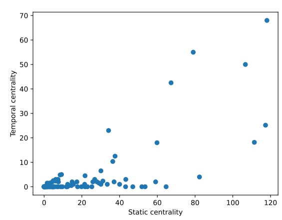
(e) company-emails



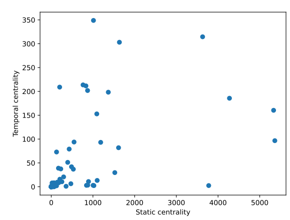
(f) eu-email-2



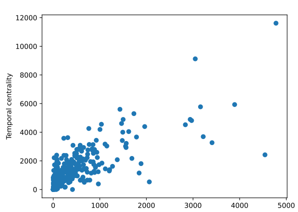
(g) eu-email-3



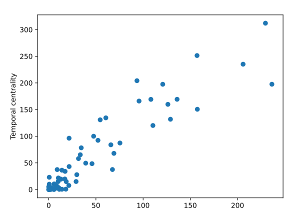
(h) eu-email-4



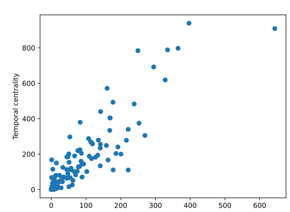
(i) haggle



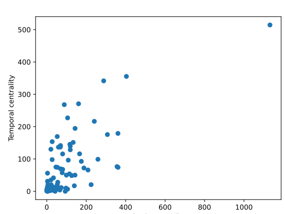
(j) sp-highschool



(k) sp-hospital

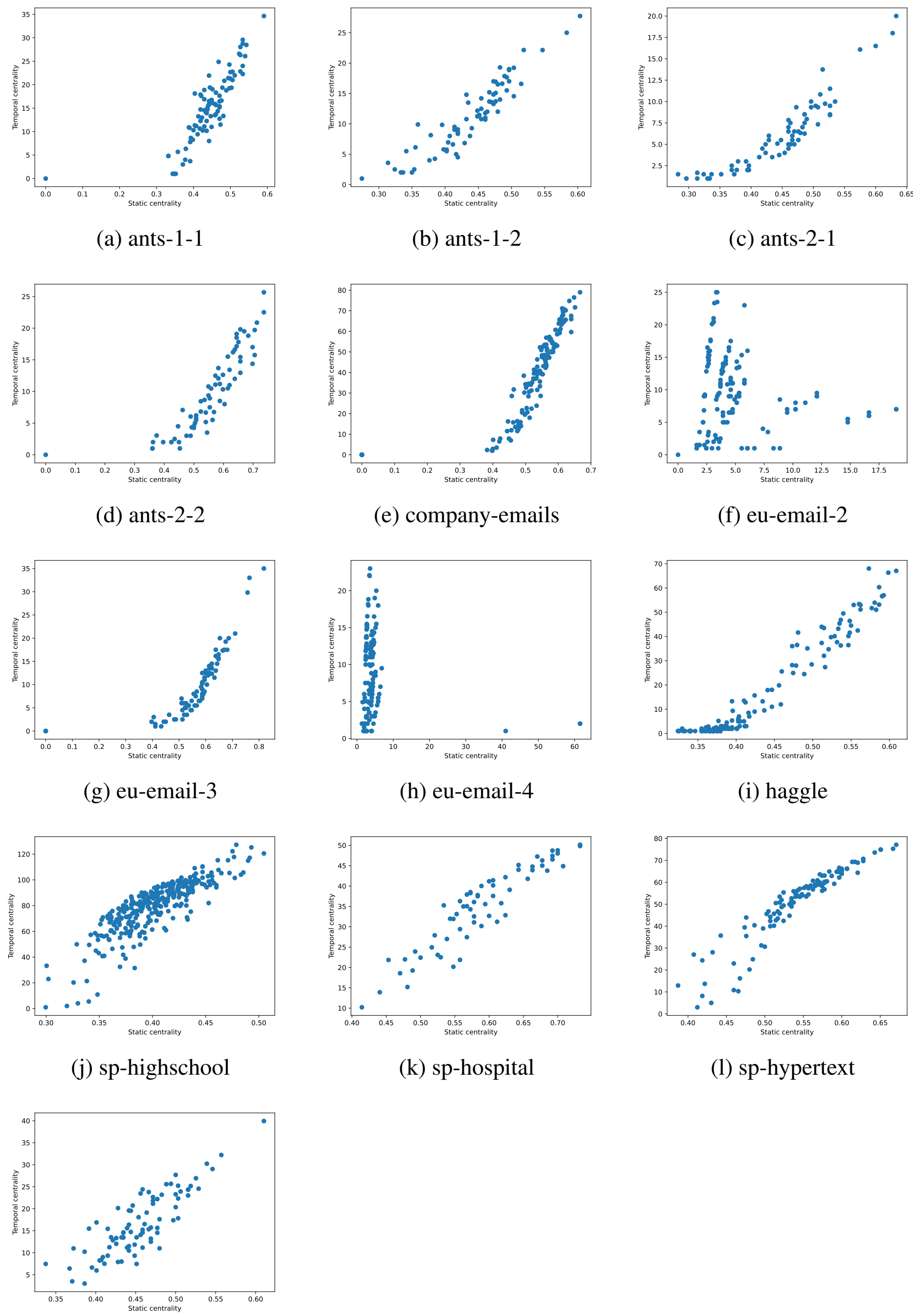


(l) sp-hypertext



(m) sp-workplace

Figure 2: Static vs temporal betweenness centralities of all nodes in 13 empirical dynamic graphs



(a) ants-1-1 (b) ants-1-2 (c) ants-2-1

(d) ants-2-2 (e) company-emails (f) eu-email-2

(g) eu-email-3 (h) eu-email-4 (i) haggle

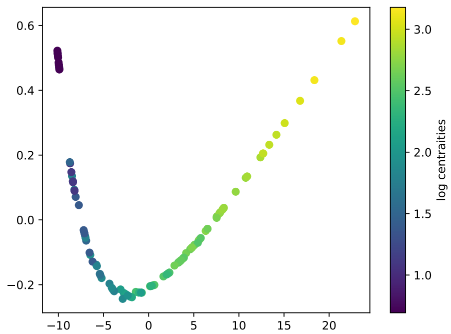
(j) sp-highschool (k) sp-hospital (l) sp-hypertext

(m) sp-workplace

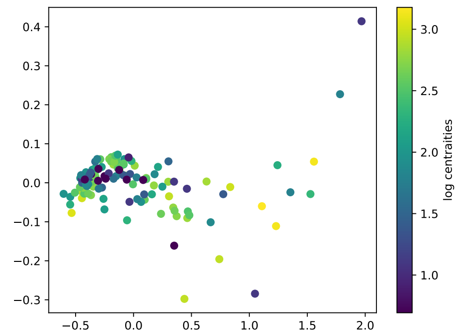
Figure 3: Static vs temporal closeness centralities of all nodes in 13 empirical dynamic graphs

D Visualization of Node embeddings

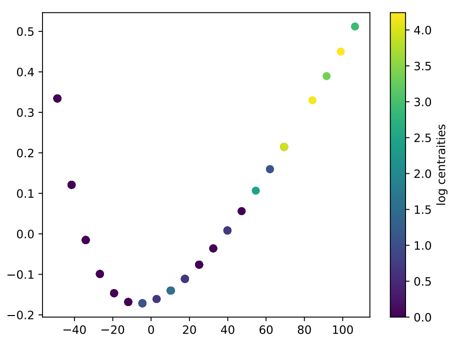
The plots in appendix D show the node emebddings obtained for a GCN and DBGNN model trained to predict temporal closeness centrality (a, b) as well as temporal betweenness centrality (c, d) for the `eu-email-4` data set.



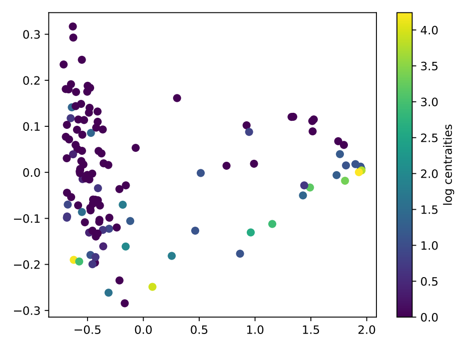
(a) Embedding of nodes based on DBGNN model trained for prediction of temporal closeness centrality in eu-email-4



(b) Embedding of nodes based on GCN architecture trained for prediction of temporal closeness centrality in eu-email-4



(c) Embedding of nodes based on DBGNN model trained for prediction of temporal betweenness centrality in eu-email-4



(d) Embedding of nodes based on GCN architecture trained for prediction of temporal betweenness centrality in eu-email-4