FAST NODE VECTOR DISTANCE COMPUTATION WITH LAPLACIAN SOLVERS

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ABSTRACT

Complex networks are a useful tool to investigate various phenomena in social science, economics, and logistics. Node Vector Distance (NVD) is an emerging set of techniques allowing us to estimate the distance and correlation between variables defined on the nodes of a network. One drawback of NVD is its high computational complexity. Here we show that a subset of NVD techniques, the ones calculating the Generalized Euclidean measure on networks, can be efficiently tackled with Laplacian solvers. In experiments, we show that this provides a significant runtime speedup with negligible approximation errors, which opens the possibility to scale the techniques to large networks.

1 Introduction

Complex networks are useful for a number of tasks. One prominent example is tracking the propagation of a phenomenon through a complex system. Examples range from diseases [3, 26, 42], memes/behaviors [19, 47, 16, 14, 22], or product adoption [28, 45] through a social network; productive knowledge in international trade [21, 41]; or goods in network modeling problems in logistics [33].

The Node Vector Distance (NVD) term has been recently used to group these tasks under a common structure [13]. In NVD, the phenomenon is represented as a vector recording one value per node. Then two vectors from different phenomena, or from the same phenomenon at different observation times, can be compared. Specifically, with NVD one can calculate their distance, network variance, or correlation.

Most useful NVD techniques share a drawback: they are computationally complex to calculate. This severely limits their practical applicability to nodes containing a handful thousands of nodes, a far cry from the (tens or hundreds) million of nodes of the most interesting complex networks.

In this paper we focus specifically on those NVD techniques based on the inversion of the graph Laplacian [10]. We do so for two reasons. First, these measures are among the most intuitive available. Second, because it turns out that the most computationally intensive part of calculating such measures is not necessary.

We show how the already existing collection of techniques known as "Laplacian solvers" [37] can be directly applied to the Generalized Euclidean NVD technique, greatly reducing its computational complexity and allowing the analysis of really large complex networks.

In our experiments we show how much runtime we gain in synthetic networks of growing sizes, showing an empirical estimation of the new computational complexity. We also do a brief analysis of the memory consumption. Finally, we show the practical applicability on a number of real world networks. The latter experiments also shows that, even if Laplacian solvers do not provide exact solutions, the approximation they induce is negligible for all practical purposes.

All the experiments we run can be reproduced with the material we provide[1].

[1] https://www.michelecoscia.com/?page_id=1733#nvdfast

2 Related Works

2.1 Node Vector Distance

Node Vector Distance (NVD) is a collection of techniques to estimate the network distance between node vectors – vectors recording one value per node [13]. NVD has a number of applications in network science, it can be used to track disease spreading [3], estimate the complexity of a country's economy [21], or quantify ideological polarization on social media [22]. The techniques at the basis of NVD can also be used to estimate how dispersed a variable is in a network [15], as well as calculating the correlations between node vectors on a network [12].

There are a number of different approaches one can take. One can apply graph signal processing techniques via the graph Fourier transform [35, 36]. Another popular approach is to compute the optimal way to transport the weights of one vector to another with respect to the distance in the network, giving rise to the Earth Mover Distance [33, 50].

In this paper we focus on a different class of solutions, which we label "Generalized Euclidean". In this class, one adapts the classical Euclidean distance to the graph setting. In the case of regular Euclidean distance, the node vectors are embedded in a space where all dimensions contribute equally – here, the distance is induced by the inner product represented by the identity matrix, so there is no distinction between the nodes. In the case of Generalized Euclidean distance, the node vectors are embedded in a complex space represented by the graph; more precisely, the distance between node vectors in this space is given by computing the quadratic product of their difference with the pseudoinverse Laplacian matrix as in Section 3.1. Note that using the pseudoinverse Laplacian is not a unique solution, as there are other ways to take into account the graph structure in the Euclidean formula [10].

Since the pseudoinverse Laplacian is the technique we focus on in this paper, we will provide more details about this approach in Section 3. For the purpose of this section, we only need to mention that pseudoinverting the Laplacian is computationally complex, but not necessary. One can achieve an approximate result by using Laplacian solvers, which we discuss now.

2.2 Laplacian Solvers

Laplacian solvers are a class of solutions to problems in the form $Lx = b$, where L is the Laplacian of an undirected graph [43]. These solvers have a number of applications in graph partitioning and specification.

Laplacian solvers make use of a number of techniques to solve the $Lx = b$ problem in near linear time [37, 38, 39, 40]. Examples include sparse approximate Gaussian elimination [27], building a chain of progressively sparser graphs [24, 25], and recursive graph preconditioning [40].

One major drawback of the methods cited so far is that they only work with undirected graphs. However, there is a collection of techniques that work on directed graphs as well [8, 7].

3 Methods

3.1 Generalized Euclidean

Let us assume we are working with a graph $G = (V, E)$, with V being the set of nodes and $E \subseteq V \times V$ the set of edges – pairs of nodes. For this paper we assume to work with undirected graphs: if $u, v \in V$ and $(u, v) \in E$, then $(u, v) = (v, u)$. The graphs can be weighted, i.e. each edge can have a positive real weight $w > 0$ – although, in this paper, we ignore weights (including them does not change any of our conclusions).

We can define a number of useful matrices. A is the adjacency matrix of G, with $A_{uv} = 1$ if $(u, v) \in E$ and $A_{uv} = 0$ otherwise. D is the degree matrix, the degree being the number of connections a node has. D contains the degree of a node in the main diagonal and zero elsewhere. The Laplacian matrix is defined as $L = D - A$, i.e. it contains the degree of a node on the main diagonal and $L_{uv} = -1$ if $(u, v) \in E$.

The Laplacian is useful to solve a number of problems. For instance, it can be used to solve the discrete heat exchange problem. If h contains the heat value for each node of the network, we can use the Laplacian to estimate how heat propagates through the graph. This is done by solving the differential equation $\frac{\partial h}{\partial t} = -Lh$ [9]. It can also be used for spectral clustering [44].

It follows that the Laplacian is helpful to understand the relationships between nodes. Previous work has exploited this fact to use the Laplacian as the matrix defining the space in which a Generalized Euclidean (GE) distance measure lives. If we are given two vectors a and b, each with $|V|$ entries, then their network distance is:

$$\delta_{G,a,b} = \sqrt{(a-b)^T L^\dagger (a-b)}.$$

where $L^\dagger$ is the (Moore–Penrose) pseudoinverse of L. L cannot be inverted directly, because it is singular. To calculate $L^\dagger$ one needs to perform a singular value decomposition (SVD) of L. Herein lies the main issue with this measure: SVD requires $\mathcal{O}(|V|^\alpha)$ time to be solved, with α larger than 2 and smaller than 3. This makes GE intractable for all but trivially sized graphs.

3.2 Laplacian Solvers

A Laplacian solver is a technique that is able to solve systems of linear equations in the form of $Lx = b$ in near linear time. To explain each Laplacian solver techniques in depth goes beyond the scope of this paper. In Section 2.2 we provide further references. In this section, we briefly mention how some of these solvers work.

Sparse approximate Gaussian elimination [27] works by performing an approximate sparse Cholesky decomposition. The Cholesky decomposition is an efficient algorithm for solving systems of linear equations. The issue is that, locally, L does not satisfy the sparsity assumption for the Cholesky decomposition – e.g. in case of large cliques. Thus, cliques need to be sampled and then the regular Cholesky decomposition can be applied.

Spectral graph sparsification [24, 25] works by taking G and sparsify it to G' in such a way that G and G' have very similar spectra. This is done iteratively via a preconditioning chain. After the first spectral sparsification, G' is then contracted by eliminating nodes of degree 1 and 2. This can be done efficiently, because the spectrum of the Laplacian is related to the cut problem, and it is possible to sparsify the graph while preserving its cuts.

Recursive graph preconditioning [40] puts together the previous two approaches by recursively sparsifying G via a partial Cholesky factorization, ensuring a low condition number at every step in the recursion.

4 Experiments

4.1 Setup Details

4.1.1 Implementation

We implement the GE function in Julia (version 1.8.0). We use the Laplacians.jl package[2] for Julia to access implementations of the Laplacian solvers (version 1.3.0). We use the methods' names provided in the package to refer to the various methods we use here. We run our code on a Intel Xeon Platinum 8358 at 2.60GHz.

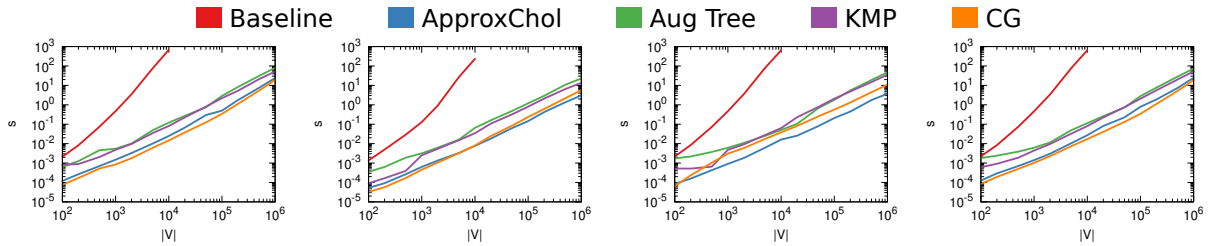
4.1.2 Synthetic Data

We test the Laplacian solvers on a number of synthetic networks, which allow us to vary both the number of nodes $|V|$ and the graph's density by changing the average degree. We use different models because each of them can reproduce some of the common properties we find in real world networks. Specifically, we use:

- Erdős–Rényi (ER): this is a $G_{n,m}$ model where we create a graph with $|V| = n$ and $|E| = m$. The edges are assigned uniformly at random by extracting two random node ids. This network model reproduces well the small world feature of real networks – the resulting networks have small diameters [11].
- Barabási-Albert (BA): we grow this network by adding one node at a time. Each node connects to k already existing nodes, with k being a parameter. Existing nodes receive new connections with a probability directly proportional to their degree. This network reproduces well both small world property and broad degree distributions [4].
- Watts-Strogatz (WS): this network starts from a circle graph where nodes are connected to all of their k closest neighbors. Then, each edge is rewired randomly with probability p, with k and p as parameters. This model reproduces the high clustering and small world features [46].
- Stochastic Blockmodel (SBM): in this model, as an input, the user partitions nodes into groups and specifies two probabilities. p_{in} determines the probability of connecting to a node inside the same group, and p_{out} regulates the connections to nodes outside the group. This model can generate network communities [23].

For all models, we make sure to directly compare networks with roughly the same number of edges.

[2] `https://danspielman.github.io/Laplacians.jl/dev/`



(a) Erdős–Rényi (b) Barabási-Albert (c) Watts-Strogatz (d) Stochastic Blockmodel

Figure 1: The running time (y axis) against $|V|$ (x axis) for all the methods (line color) on different synthetic networks.

4.1.3 Real World Data

For our applications section (Section 5) we also make use of real world data, to showcase the usefulness of GE – and, as a consequence, the need for efficient ways to estimate it. Specifically we use:

- Section 5.1 (US Congress): networks from the roll call votes in the House of Representatives – one network per congress edition –, using data from Voteview.com [31]. Each node is a representative and they are connected if the two representatives have co-voted on bills more often than the average same-party pair. The procedure to build these networks has been used multiple times in the literature [1, 22].
- Section 5.2 (Various): networks that come from a variety of papers, retrieved via the network catalogues SNAP [30] and Netzschleuder [32].

We use small networks in Section 5.1 because we want to show how accurate the Laplacians solvers can be in quantifying the GE values against the exact result obtained via SVD – thus we need to be able to run SVD. The larger networks in Section 5.2 are used to showcase the possibilities opened by the Laplacian solvers that are not available to the exact solutions via the Laplacian pseudoinverse.

4.2 By Network Size

In this section we test the effect of the size of the network on the running time and memory consumption of the Laplacian solvers against the baseline using the pseudoinversion via SVD. We split the size test first by increasing the number of nodes while keeping the density of the network constant, and then by keeping the number of nodes fixed but increasing the network density.

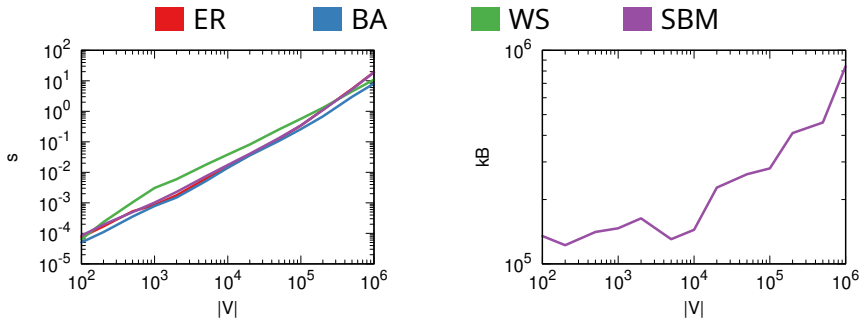
4.2.1 Runtimes ($|V|$)

For the runtimes, we exclude outlier runs which took more than twice the average runtime. This is done to exclude compilation time from the estimate – this issue only affects very small input sizes where compilation could take significantly longer than running time. All plots report average runtimes over ten independent runs. The exception is Baseline, for which we make a single run for $|V| = 10^4$ and we do not run for larger $|V|$ at all, due to its excessively long runtimes.

We start by analyzing the runtimes for increasing number of nodes. Figure 1 reports the results. The first evident result is that any Laplacian solver has both a constant running time advantage and a better asymptotic complexity. Even for tiny networks of 100 nodes, regardless of the network topology, all Laplacian solvers are at least one order of magnitude faster than the baseline. From these plots we can infer that the empirical asymptotic complexity of the baseline is $\sim \mathcal{O}(|V|^{2.6})$. For the Laplacian solvers the exact combination of solver and topology matters, but in general the empirical asymptotic complexity is between $\mathcal{O}(|V|^{1.2})$ and $\mathcal{O}(|V|^{1.4})$, in all cases decisively below $\mathcal{O}(|V|^2)$.

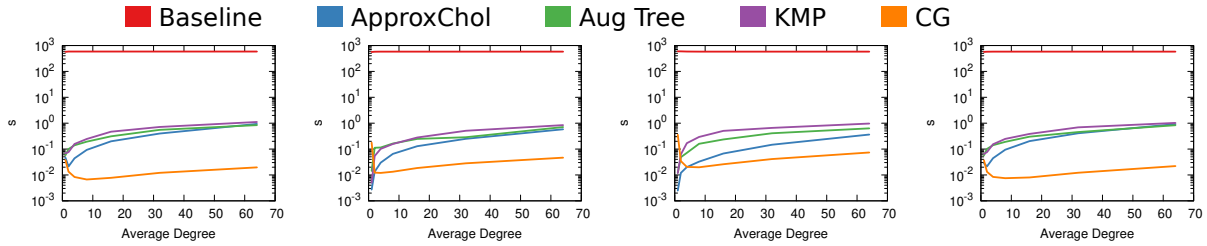
The practical result is that the baseline takes at least one order of magnitude more time to compute a $|V| = 10^4$ network than any Laplacian solver takes for a network two orders of magnitude larger.

Among the Laplacian solvers there is no clear overall winner. CG is the fastest for the Erdős–Rényi and SBM topologies, but it ties with ApproxChol for the Barabási-Albert model, while ApproxChol is also fastest for Watts-Strogatz. The topology in general has different effects on different solvers. Picking CG as an example, Figure 2(a) shows that indeed CG runs slower for Watts-Strogatz than it does for all other topologies. Other solvers also experience different strengths and weaknesses depending on the topology – not shown here for space issues.



(a) Runtime (b) Memory

Figure 2: Time and memory consumption (y axis) against $|V|$ (x axis) for all synthetic networks (line color) for the CG Laplacian solver.



(a) Erdős–Rényi (b) Barabási-Albert (c) Watts-Strogatz (d) Stochastic Blockmodel

Figure 3: The running time (y axis) against average degree (x axis) for all the methods (line color) on different synthetic networks.

4.2.2 Runtimes (Density)

Efficient Laplacian solvers exploit, among other things, the sparseness of a graph. It is interesting to investigate what happens to the runtime when the graphs we investigate get denser and denser. In this experiment, we fix $|V| = 10,000$, and we increase the average degree of the network from 1 to 64. The vast majority of real world networks have low average degrees in the single digit realm [17], thus this domain covers the most realistic scenarios. Also in this case we report the average of ten runs, taking out outliers and ignoring compilation time.

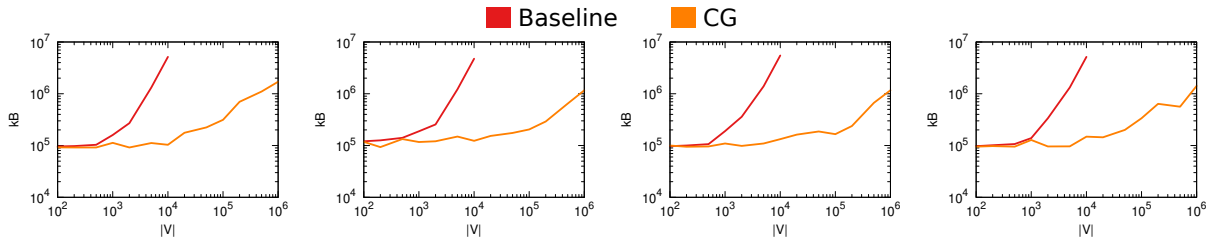
Figure 3 shows the results. Since the baseline works with dense matrices anyway, there is no real effect of density on its running time, which is roughly constant. Most Laplacian solvers have longer runtimes for denser networks – as expected. All Laplacian solvers are orders of magnitude faster than the baseline, and thus represent a significant advantage.

CG shows a peculiar pattern: it takes longer for extremely sparse networks – with average degree close to one – then gets faster and faster for middle values of average degree between four and eight. After this, the runtimes increase with density as expected. This pattern is consistent, independently from the topology of the network. It seems that, for extremely sparse networks with average degree lower than four, CG might not be the best choice. For denser networks, however, CG can be one or two orders of magnitude faster than the other Laplacian solvers.

4.2.3 Memory

For the memory test we show only a single run per method, due to limitations in memory benchmarking. However, memory consumption should not be variable across runs and the results of a single run are still indicative of the overall trends. We also run a single Laplacian solver, CG, because the memory consumption for all solvers is indistinguishable in all cases.

From Figure 4 we can see that there is a basic memory consumption coming from simply running the program. For $|V| = 10^4$, the Laplacian solvers do not add any memory consumption to this basic rate. However, the baseline needs to shift from sparse to dense matrix representations to calculate the pseudoinverse of the Laplacian. This means that its memory consumption is already between 5 and 6GB in our implementation even for these small networks. If we exclude the warm-up phase for $|V| < 10^3$, the memory consumption of the baseline scales exponentially.



(a) Erdős–Rényi (b) Barabási-Albert (c) Watts-Strogatz (d) Stochastic Blockmodel

Figure 4: Memory consumption (y axis) against $|V|$ (x axis) for all the methods (line color) on different synthetic networks.

Method	85th	105th	113th
Baseline	1.006	3.664	8.330
ApproxChol	$2.1e^{-14}$	$2.1e^{-14}$	$1.3e^{-13}$
Aug Tree	$6.9e^{-9}$	$1.1e^{-14}$	$5.0e^{-14}$
KMP	$4.4e^{-16}$	$2.7e^{-15}$	$1.1e^{-13}$
CG	$4.9e^{-10}$	$2.7e^{-15}$	$2.1e^{-13}$

Table 1: The polarization scores for three US Congress networks (top row) and the difference between exact and approximate solution using a specific Laplacian solver (bottom four rows).

This is not true for Laplacian solvers, here represented by CG. The total memory consumption at $|V| = 10^4$ is still in the neighborhood of the basic cost of running the program. Even for $|V| = 10^6$, the memory required is below 2GB in all but one case. Asymptotically, the best function describing the growth in memory consumption by CG is linear, not exponential. Figure 2(b) does not show any significant difference in memory consumption for CG depending on the topology of the network.

5 Applications

5.1 Polarization

The GE measure can be used to estimate polarization on social media, or any networked system where we have information about the opinions of the nodes [22]. This is done by calculating the distance between the vector recording the opinions of nodes on one side of the spectrum – e.g. Democrats – with the one recording the opinions of the nodes on the other side of the spectrum – e.g. Republicans.

For this task we use the Congress networks described in Section 4.1.3. Specifically, we focus on the 85th, 105th, and 113th Congress, since they show the lowest, average, and highest value of polarization, respectively. Table 1 shows the result. First, the Baseline method confirms the differences in scores between the three networks. Then we show how the four Laplacian solvers estimate the level of polarization to be practically identical to the exact one we compute via the Baseline. The largest error is in the neighborhood of 10^{-8}, which is far below the level of precision required for such an analysis.

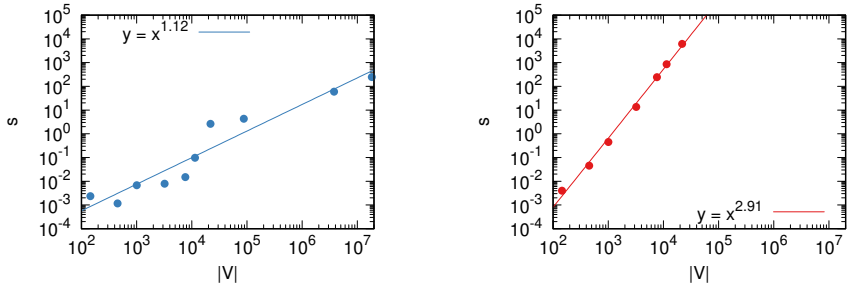
5.2 Various

We look at a variety of networks which would all benefit from a GE analysis, in increasing size to show the speedup of the Laplacian solvers in real world scenarios. We simplify all networks to an undirected, unweighted, simple graph version, even if the original network was either directed, weighted, or multilayer. All runtimes exclude I/O operations and preprocessing, so they ignore the time it takes to read the graph from disk. Below we briefly explain what the node vectors are in each case.

- *Hiring*: we can calculate the distance between the region in which a university is located, by analyzing the hiring patterns.
- *EUAir*: we can calculate the distance between airlines depending on which airports they serve.
- *EUCore*: we have communities based on email exchange, and GE could tell the distance between community pairs.

Network	$\|V\|$	$\|E\|$	Dens	ApproxChol (s)	Baseline (s)	Ref
Hiring	145	2,266	0.2170	0.0023	0.0040	[6]
EUAir	450	2,953	0.0292	0.0011	0.0454	[5]
EUCore	1,005	16,064	0.0318	0.0068	0.4496	[29]
Open Flights	3,214	18,858	0.0036	0.0079	13.623	[32]
LastFm	7,624	27,806	0.0009	0.0149	244.20	[34]
Wiki RFA	11,381	194,592	0.0030	0.0976	853.00	[48]
Fly Brain	21,739	2,897,925	0.0122	2.6151	6181.3	[49]
Twitter15m	87,569	4,708,274	0.0012	4.3299		[18]
Patents	3,774,768	16,518,947	$2.31e^{-6}$	59.311		[20]
DBpedia	18,268,992	136,537,566	$8.18e^{-7}$	247.10		[2]

Table 2: The runtimes of the ApproxChol solver against the exact solution in number of seconds for a collection of networks of different sizes (in number of nodes $|V|$ and edges $|E|$). We terminate the process after one hour, thus we do not report runtimes longer than that.



(a) ApproxChol (b) Baseline

Figure 5: Runtime (y axis) on real networks by number of nodes (x axis).

- *Open Flights*: we can calculate the distance between countries based on how the airlines connect their airports.
- *LastFm*: we can calculate the distance between countries – a metadata we have about the users – based on their friendships on the platform.
- *Wiki RFA*: we can calculate the distance between admins and non-admins in the voting network.
- *Fly Brain*: we can calculate the distance between neuron types in the neural network.
- *Twitter15m*: we can measure the distance between two hashtags in the user network.
- *Patents*: we can measure the distance between patent categories in the patent citation patterns.
- *DBpedia*: we do not have node metadata, so we calculate distances between random vectors, but this network could be used, e.g., to calculate distances between different page categories in the encyclopedia, whose pages are connected by hyperlinks.

Table 2 reports the running times. These are also summarized in Figure 5. For comparison purposes, we estimate the scaling of the two methods with a power relation with the number of nodes. The best function approximating the runtime of ApproxChol is $\mathcal{O}(|V|^{1.12})$ (Figure 5(a)). On the other hand, the best function approximating the runtime of the exact SVD-based solution is $\mathcal{O}(|V|^{2.91})$ (Figure 5(b)).

However, it would be more appropriate to estimate the scaling of the Laplacian solver with the number of edges. This is is because their advantage becomes less and less relevant the more the network is dense. Note the difference in runtimes, e.g., in Hiring and EUAir. Notwithstanding the fact that Hiring has fewer nodes and fewer edges, it is much more dense than EUAir (21% dense vs 3% dense) and thus the Laplacian solvers actually take longer to run on this smaller network. On the other hand, it is remarkable that the Laplacian solver can process the DBpedia network (18M nodes) in the same time it takes the baseline to process LastFm (7.6k nodes).

6 Conclusions

In this paper we showed that using Laplacian solvers will bring massive speedups in the calculation of the Generalized Euclidean measure and other related measures in the Node Vector Distance class of problems. The speedup is relative

to calculating an exact solution via the pseudoinverse of the Laplacian. Since Laplacian solvers scale with the number of edges, these speedups are more noticeable for sparse networks. Besides an improved time efficiency, these methods also require fewer resources in terms of memory, since the process to obtain the pseudoinverse of the Laplacian involves using dense matrices, while all Laplacian solvers work with sparse structures.

We failed to notice significant differences between different Laplacian solvers in synthetic networks. As the network grows in number of nodes, they all increase their runtimes approximately at the same rate. The only potential difference comes when we densify the network. The CG solver is the slowest for very sparse networks, but it scales better as the network becomes denser and denser.

This paper can be used as an argument to use Laplacian solvers to efficiently solve GE and related NVD problems.

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