Scalable Dyadic Independence Models with Local and Global Constraints

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Abstract

An important challenge in the field of exponential random graphs (ERGs) is the fitting of non-trivial ERGs on large networks. By utilizing matrix block-approximation techniques, we propose an approximative framework to such non-trivial ERGs that result in dyadic independence (i.e., edge independent) models, while being able to meaningfully model local information (degrees) as well as global information (clustering coefficient, assortativity, etc.) if desired. This allows one to efficiently generate random networks with similar properties as an observed network, scalable up to sparse graphs consisting of millions of nodes. Empirical evaluation demonstrates its competitiveness in terms of accuracy with state-of-the-art methods for link prediction and network reconstruction.

1. Introduction

Network modeling is typically concerned with the following setting: given measurements on certain structural properties of a real-life network, such as node degrees, clustering coefficient, density, and so forth, one wishes to find a model for the network where samples generated by the model have similar values of the measured properties. Prominent examples include stochastic block models (Airoldi et al., 2009), graphons (Borgs et al., 2014) and exponential random graphs (ERGs) (Holland & Leinhardt, 1981).

ERGs have received significant attention in numerous research areas (Holland & Leinhardt, 1981; Frank & Strauss, 1986; Snijders et al., 2006; Robins et al., 2007), as they provide a well-founded probabilistic framework to network modeling; their study has been described as the “statistical mechanics of networks” (Park & E. J. Newman, 2005). They arise naturally as the solution to the problem of finding the maximum entropy distribution over a set of graphs, while respecting constraints that a probabilistic statistic must equal an observed statistic in expectation. Equivalently, the parameters of an ERG can be determined by maximum likelihood estimation of an exponential distribution for explaining the observed statistics in a principled manner. The advantage of ERGs is that they can represent a wide range of structural tendencies, such as transitivity and degree heterogeneity, by capturing complicated dependence patterns that are not easily modeled by simpler probabilistic models.

The downside of classically specified ERGs is their limited scalability (Goodreau, 2007). Inferring the parameters of an ERG is often intractable for networks of even moderate size, because computing the partition function may require evaluating a summation over all $2^{O(n^2)}$ for graphs with $n$ nodes. The common approach is to approximately infer the parameters by MCMC sampling, after which a goodness of fit is measured by generating random networks from the ERG and comparing statistics with the observed network. Besides limited scalability, MCMC methods often have the problem of degeneracy (Handcock, 2003), assigning most probability mass to either near-empty or near-full graphs, for example when one is counting Markov neighborhood properties such as triangles (Snijders et al., 2006). ERGs typically lose efficiency when they aim to model global constraints that suggest dependencies between edges, such as degree assortativity or the existence of many triangles. Modeling such information is important in practice: e.g. if the number of triangles is large as compared to other graphs with the same local properties, this may indicate that edge formation is a result of a triadic closure process, which can be an important property to understand and model.

Addressing this challenge, in this paper we utilize matrix block-approximation techniques to derive intelligible and scalable approximations to non-trivial ERGs for large sparse graphs ($>10^6$ nodes). The resulting models are dyadically independent, while still meaningfully incorporating local information (degrees) and global information (triangles, assortativity, etc.).

Contributions and roadmap.

- Discussion of a general dyadic independence model that is able to incorporate arbitrary (structural) features between pairs of nodes (Section 2).
- Depending on the incorporated features, fitting the model parameters may not be scalable. We propose fast
matrix block-approximation techniques to provide scalable approximations to the general model (Section 3).

- An empirical comparison with several state-of-the-art (embedding) methods on two applications: link prediction and network reconstruction (Section 4).

2. MaxEnt models with structural constraints

**Notation.** Let \( G = (V, E) \) be a graph with \(|V| = n\) nodes and \(|E| = m\) edges. The neighborhood of node \( i \) is denoted as \( \mathcal{N}(i) \). The adjacency matrix of an observed graph \( G \) is denoted as \( \hat{A} = [\hat{A}_{ij}] \in \mathcal{A} \), where \( \mathcal{A} = \{0, 1\}^{n \times n} \) is the set of square matrices of size \( n \). A random matrix is denoted as \( A \in \mathcal{A} \). The transpose of a matrix \( A \) is denoted as \( A^T \) and the Frobenius norm is denoted as \( \|A\|_F \). The expected value operator related to a distribution \( P \) is denoted as \( \mathbb{E}_P[\cdot] \). The focus in this paper is restricted to undirected graphs, where \( d \) is infeasible to compute, because of edge dependencies introduced by the assortativity constraint. As such, the parameters of the distribution are intractable to compute exactly. This is in contrast to a MaxEnt model subject to only degree constraints. As observed by different authors (Park & E. J. Newman, 2005; De Bie, 2011; Parisi et al., 2018), in this case \( P \) is a dyadic independence model: it factorizes as a product of independent Bernoulli distributions, one for each node pair \((i, j) \in V \times V\). Moreover, in a degree-only model, the number of unique parameters to be optimized over is fully determined by the number of unique degrees in \( G \). As shown by De Bie (2011), for sparse \( G \) (where \( m = O(n) \)), the problem has in fact only \( O(\sqrt{n}) \) free variables instead of the \( O(n) \) original variables (one original variable for each degree constraint), making inference possible on very large networks. In Section 3, we show that we can do a similar reduction in variables also for more complex models.

One way to approximate (1) is to replace the row- and column sums of random variables \( \sum_e A_{ic} \) by their expectation:

\[
\sum_c A_{ic} \approx \mathbb{E}_P[\sum_c A_{ic}] = d_i.
\]

The approximated model of (1) then becomes

\[
\arg \max_{P(A)} -\mathbb{E}_P[\log P(A)], \quad \text{s.t.} \quad \mathbb{E}_P[\sum_{i,j} A_{ij} \sum_c A_{ic} \sum_r A_{rc}] = c, \quad \mathbb{E}_P[\sum_{i,j} A_{ij}] = d_i, \quad \forall i, \quad \mathbb{E}_P[\sum_{i,j} A_{ij}] = d_j, \quad \forall j.
\]

We omit the details, but it is easy to show that the solution to (2) is again a dyadic independence model, and the complexity depends on the number of unique degrees in \( G \).

Let us provide some intuition on the solution of (2). First, because the distribution has maximum entropy, it is the unique distribution that injects no side information on properties that were not taken into account as constraints (Cover & Thomas, 2006). Secondly, if the degree assortativity cannot be explained by a model that is inferred using only degree constraints, for example if \( c \) is larger than expected under a model where only degrees are constrained, then the optimum of (2) will on average assign higher probabilities between pairs of high degree nodes and between pairs of low degree nodes, at the expense of pairs of nodes where one has a large and the other a low degree. This results in a more accurate fit of the observed graph.

An example of a highly disassortative network is the Karate dataset (Zachary, 1976). It has a negative assortativity coefficient (Newman, 2002) of \(-0.48\), and thus nodes with similar degrees are less often connected. This is confirmed in a visualization of the network in Figure 1a. The dataset essentially consists of two Karate club teachers (the two highest-degree nodes), mostly connected to their own students, with few edges between the two communities. Most connections are between a high-degree node and a low-degree node, and the two teachers themselves are not connected.

Figure 1b shows the edge probabilities between all pairs of nodes, when the network is modeled by a MaxEnt model with a constraint on the expectation of each individual node degree. Connections between high degree nodes are more likely, and thus it assigns most probability mass in the top
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Figure 1. (a) The Karate network (b) MaxEnt edge success probabilities with constraints on degrees (c) MaxEnt edge probabilities with constraints on degrees, and a global constraint on degree assortativity as given by (2). In both heatmaps, nodes are sorted in descending degree order (highest degree in the top left corner).

On the other hand, Figure 1c shows the MaxEnt model with an additional assortativity constraint as given by (2). It builds on the degree-only model by taking into account the network’s disassortativity, and as such it lowers the edge probabilities between nodes of similar degree and increases the edge probabilities between nodes with dissimilar degrees. Note that it correctly assigns a low probability for a connection between the two Karate teachers.

2.2. Generalizing to arbitrary features

Building on the previous example, we can view (2) as a model that takes into account observed features \( f_{ij} \equiv d_i d_j \). Instead of taking the product of two node degrees, we can simply extend this to arbitrary observed features.\(^2\) Denote \( \mathbf{F} = [f_{ij}] \in \mathbb{R}^{n \times n} \) as an induced pairwise feature matrix. For example, the degree matrix of a node \( i \) is a matrix with ones on the \( i \)-th row and zeros elsewhere. The common neighbor matrix (triangle counting) is given by \( \mathbf{F}_{\text{CN}} \equiv \hat{\mathbf{A}}^2 = \|N(i) \cap N(j)\| \). Counts of different types of graphlets besides triangles can be incorporated as well, e.g., by using so-called ‘weighted motif graphs’ (Ahmed et al., 2016; Rossi et al., 2018) as feature matrices.

Given \( M \) of these feature matrices \( \mathbf{F}_l \equiv [f_{ij}^l] \) with \( l = 1, \ldots, M \), we aim to solve

\[
\arg \max_{P(A)} -\mathbb{E}_P[\log P(A)],
\]

s.t. \( \mathbb{E}_P[\sum_{i,j} f_{ij}^l A_{ij}] = c_l \) \( \forall l = 1, \ldots, M \).

Where \( c_l = \sum_{i,j} f_{ij}^l \hat{A}_{ij} = \sum_{(i,j) \in E} f_{ij}^l \) are the observed statistics. Solutions to the class of models defined by (3) have the convenient property that the partition function (the normalizing constant) factorizes as a product over all possible edges. As such (3) is again a dyadic independence model, with a Bernoulli success probability for a node pair \((i,j)\):

\[
P(A_{ij} = 1) = \frac{\exp(\sum_{l=1}^{M} f_{ij}^l \lambda_l)}{1 + \exp(\sum_{l=1}^{M} f_{ij}^l \lambda_l)},
\]

where \( \lambda_l \) denotes the Lagrange multiplier associated with the \( l \)-th constraint in (3). These are found by unconstrained minimization of the convex Lagrange dual function:

\[
L(\lambda_1, \ldots, \lambda_M) = \sum_{i,j} \log(1 + \exp(\sum_{l=1}^{M} f_{ij}^l \lambda_l)) - \sum_{l=1}^{M} c_l \lambda_l.
\]

The partial derivatives \( \forall l = 1, \ldots, M \) are computed as

\[
\frac{\partial L}{\partial \lambda_l} = \sum_{i,j} f_{ij}^l \cdot \frac{\exp\left(\sum_{l=1}^{M} f_{ij}^l \lambda_l\right)}{1 + \exp\left(\sum_{l=1}^{M} f_{ij}^l \lambda_l\right)} - c_l.
\]

\(^2\) Such a generalization is often less well-founded than the case of degree assortativity (where we replaced a sum of random variables with the sum of their expectations), but these models still turn out to be useful.

Figure 2. MaxEnt edge success probabilities on the Dolphins network (a), when different kinds of constraints are taken into account; (b) MaxEnt with degrees (c) MaxEnt with only a global constraint on \( \mathbf{F}_{\text{CN}} \) (c) MaxEnt with a combined constraint on both the degrees and \( \mathbf{F}_{\text{CN}} \), demonstrating that combining local and global information results in a superior model.
Instead of counting exact specifications in the original ERG, the models (3) can be seen as applying a ‘linear mask’ in order to approximately count the specifications. In fact, they are often identical to expressions found by pseudo likelihood estimation (Strauss & Ikeda, 1990; Duijn et al., 2009). Pseudo likelihood is mainly used for estimation of the original ERG parameters (He & Zheng, 2015), but we argue that dyadic independence models can be valuable by themselves. For the exact derivations and a discussion regarding the pseudo likelihood, we refer to Appendix A.

In this paper, we focus on combining individual local constraints (degrees) with a limited number of global structural constraints. Figure 2 shows an example of the predictive power of combining constraints on degrees with a global structural constraint $F_{CN}$ on the Dolphins dataset (Lusseau et al., 2003). Figure 2a shows the connectivity of the dataset. Figure 2b shows the edge probabilities according to a MaxEnt model with just degree constraints. It assigns higher probability to edges between two high degree nodes, but it fails to capture any form of local community structure. Figure 2c is a MaxEnt model fitted with just the structural constraint $F_{CN}$. Although it captures community structure, it fails to make good predictions about the actual edges in the network. Indeed, most observed edges have a low probability of being present, and all node pairs with zero common neighbors are assigned a probability of 1/2 of being connected. Figure 2d shows the model when combining degree constraints and the structural constraint $F_{CN}$. It leads to a remarkably good fit of the original network, while still leaving room for prediction and inference.

2.3. Scalability issues

Inference on large graphs is typically not possible when we have $M = O(n)$ constraints, as is the case when combining degree constraints with a limited number of global constraints. Minimizing (4) can be viewed as a classical learning setting with $n^2$ training examples and $O(n)$ weights. Standard gradient methods need $\Omega(n^2)$ computations per iteration and $F$ needs to be stored in memory. To resolve both issues, in Section 3 we propose to block-approximate the feature matrices. In particular, Theorem 1 shows that number of variables to be optimized can be reduced from $O(n)$ to $O(\sqrt{n})$. At the same time, block-approximated matrices are efficiently maintained in memory.

2.4. Label leakage & degeneracy

To avoid overfitting, it is crucial to avoid ‘label leakage’. More concretely, when predicting whether or not an edge exists, one should avoid making direct use of the actual existence of that edge while fitting the model. Indeed, if one selects $F = \hat{A}$, the only solution to (3) is exactly $P(\hat{A}) = 1$. In other words, the model of the network is the network itself, rendering it completely useless for tasks like link prediction. In contrast, $F_{CN}$ is an excellent candidate for a link prediction feature matrix, since the number of common neighbors between two nodes is not directly related to the existence of that edge, and if it is the case, the model will actually learn the relation. Remarkably, other methods often overlook this fact. For example, the method by Zhang et al. (2018) considers embeddings defined by a truncated singular value decomposition of the adjacency matrix $\hat{A}$. The Katz centrality measure (Katz, 1953) is another such example. Nevertheless, for other tasks that require a closer fit to the observed network (e.g., network reconstruction), it might become arbitrarily close to the observed network. For example, $F = \hat{A} + \beta \hat{A}^2$ with small $\beta > 0$ was used in Section 4.2 to obtain a close fit to the Facebook network.

The other side of degeneracy, i.e. assigning most probability mass to near-empty graphs, is seemingly avoided by incorporating degree constraints into the model. For example, compare Figure 2c with Figure 2d.

3. Block-approximating feature matrices

3.1. Motivation

Prior work on improving the scalability of fitting a general MaxEnt model (3) looks for permutations of $\lambda_i, \ldots, \lambda_M$ that leave the Lagrangian dual function $L$ (4) invariant. The convexity of $L$ then implies that if there is a permutation that maps $\lambda_i$ to $\lambda_j$, then there necessarily exists an optimum of (4) where $\lambda_i = \lambda_j$ (Adriaens et al., 2019). Similarly as in (Adriaens et al., 2019), we look for equivalent Lagrange multipliers associated with the degree constraints. Equivalent Lagrange multipliers are equated and the reduced model is solved by standard convex optimization methods.

However, for general feature matrices equivalences are rare. Thus, in this paper we propose to block-approximate the feature matrices. Let $\tilde{F} \in \mathbb{R}^{n \times n}$ be a block-approximation of $F$, represented by a structure with $k \times k$ blocks, with each block being a submatrix with constant values. Theorem 1 below shows that for sparse graphs, the number of free variables in the reduced model of (4) has $O(\sqrt{kn})$ variables instead of the original $O(n)$ variables. It exploits the limited number of unique degrees in sparse graphs, as given by Lemma 1. Proofs can be found in Appendix A.

Lemma 1. If $\hat{A}$ is sparse, symmetric and the nodes are partitioned into $k$ disjoint groups, then the sum over all groups of the number of unique degrees inside each group is $O(\sqrt{kn})$.

Theorem 1. If $\hat{A}$ is sparse, symmetric and $\tilde{F}$ can be represented by a $k \times k$ block matrix, with constant values in each block, then (3), with constraints on each individual degree and a constraint as given by $\tilde{F}$, can be solved by optimizing an unconstrained convex problem with $O(\sqrt{kn})$ variables.
3.2. Methods

3.2.1. Spectral Clustering Adjacency Polynomials

A principled way of block-approximating a feature matrix $\mathbf{F}$ is to first spectral cluster $\mathbf{F}$ and then replacing rows with centroids. Assuming $\mathbf{F}$ is real and symmetric, spectral clustering first calculates a truncated eigenvalue decomposition to get an optimal low-rank approximation of $\mathbf{F}$, after which $k$-means is used to cluster the nodes in the low dimensional space (Luxburg, 2004). A block-approximation of $\mathbf{F}$ is then found by

$$\mathbf{F} \approx \mathbf{U} \mathbf{S} \mathbf{U}^T \approx \mathbf{U}_c \mathbf{S} \mathbf{U}_c^T,$$

with $\mathbf{U}, \mathbf{U}_c \in \mathbb{R}^{n \times d}$ and $\mathbf{S} \in \mathbb{R}^{d \times d}$ a diagonal matrix containing the signs of the largest $d$ positive eigenvalues of $\mathbf{F}$. The matrix $\mathbf{U} = \mathbf{V} \sqrt{\Sigma}$ consists of the rescaled eigenvectors $\mathbf{V}$ corresponding to the top $d$ eigenvalues, where $\Sigma$ denotes a diagonal matrix with the absolute values of these eigenvalues. The matrix $\mathbf{U}_c$ is defined by replacing each row of $\mathbf{U}$ by its respective cluster centroid. Notice that symmetry of $\mathbf{F}$ is maintained by both of the approximations in (5). Now let $\mathbf{F} \triangleq \mathbf{U}_c \mathbf{S} \mathbf{U}_c^T$. The following proposition gives a bound on the expected distance between $\mathbf{F}$ and $\mathbf{F}$ (the proof can be found in Appendix A).

**Proposition 1.** Let $|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_d|$ be the $d$ largest eigenvalues of $\mathbf{F}$. Let $\phi_{OPT,k}$ denote the optimal clustering objective value with $k$ clusters. Using k-means++ as a (randomized) clustering algorithm, the expected error $\mathbb{E} \left[ \| \mathbf{F} - \hat{\mathbf{F}} \| \right]$ is at most

$$2\sqrt{\sum_{i=1}^{d} |\lambda_i| \cdot O(\log(k)) \cdot \phi_{OPT,k}}$$

additively larger than any optimal rank $d$ approximation of $\mathbf{F}$.

The bound from Proposition 1 gives insight in how the dimension $d$ and number of bins $k$ affect the block-approximation (5). Increasing $k$ will benefit the approximation since $\hat{\mathbf{F}}$ becomes closer to the optimal rank $d$ approximation. However, for fixed $k$, increasing $d$ does not always benefit the block-approximation. Indeed, as the clustering approximation gets worse with increasing dimension $d$ (Arthur & Vassilvitskii, 2006), the effect on the overall block-approximation could potentially be detrimental, which is confirmed in practice. As a practical guideline, we advise to keep $d$ small, and selecting a high $k$ while maintaining tractable computational complexity (Section 3.3).

Since $\mathbf{F}$ is often dense, directly calculating $\mathbf{F}$ and performing a top $d$ eigendecomposition is not scalable both memory and time wise. Instead, for higher-order proximity matrices, i.e. matrices that are expressed as polynomials of $\hat{\mathbf{A}}$ with positive coefficients, one can directly use a (fast) eigendecomposition of $\hat{\mathbf{A}}$ (which is typically sparse) to get the top $d$ eigendecomposition (Higham & Tisseur, 2003; Zhang et al., 2018). Indeed, if $\mathbf{F}$ is of the form

$$\mathbf{F}_p \triangleq \text{poly}(\hat{\mathbf{A}}) = q_1 \hat{\mathbf{A}} + \ldots + q_n \hat{\mathbf{A}}^n \quad q_i \geq 0,$$

then it’s trivial to see that if $\alpha$ is an eigenvalue with eigenvector $x_\alpha$ of $\hat{\mathbf{A}}$ then $\text{poly}(\alpha)$ will be an eigenvalue of $\mathbf{F}_p$ with the same eigenvector $x_\alpha$. Hence eigenvalues are rescaled, and eigenvectors are preserved. The only difficulty is that this rescaling does not preserve the ordering. More precisely, the top $d$ eigenvalues of $\mathbf{F}_p$ are in general not equal to the rescaled top $d$ eigenvalues of $\hat{\mathbf{A}}$. To get the top $d$ eigenvalues of $\mathbf{F}_p$ one needs to calculate $l > d$ eigenvalues of $\hat{\mathbf{A}}$, where $l$ denotes the index of the $d$-th positive eigenvalue of $\hat{\mathbf{A}}$, when sorted according to absolute value. This is true since $q_i \geq 0$ guarantees that the ordering is preserved only for the positive eigenvalues of $\mathbf{A}$. In practice $l$ is often not significantly larger than $d$. For example, for sufficiently large Erdos-Renyi graphs $l \approx 2d$ due to the semicircle law (Erdos et al., 2013).

3.2.2. Resource Allocation Index (RAI) and Adamic-Adar (AA)

One is not limited to polynomials of $\hat{\mathbf{A}}$ for scalable block-approximation. For other practical feature matrices $\mathbf{F}$, we can still utilize an eigendecomposition of $\hat{\mathbf{A}}$ to get a fast block-approximation of $\mathbf{F}$. One such matrix often used in the complex networks community is the so-called Resource Allocation Index (RAI) (Zhou et al., 2009). The RAI defines a similarity score $r$ between two nodes $u$ and $v$ as $r_{uv} = \sum_{k \in N(u) \cap N(v)} 1/d_k$. The induced matrix $\mathbf{F}_{\text{RAI}} \triangleq [r_{uv}]$ can be written in terms of the adjacency matrix $\hat{\mathbf{A}}$:

$$\mathbf{F}_{\text{RAI}} = \hat{\mathbf{A}} \mathbf{D}^{-1} \hat{\mathbf{A}},$$

where $\mathbf{D}$ is a diagonal matrix containing the degree of each node. Assume $\hat{\mathbf{A}}$ is connected, such that $d_k > 0$ and (6) is well-defined. Given a top $d$ eigendecomposition of $\hat{\mathbf{A}} \approx \mathbf{V} \Lambda \mathbf{V}^T$, with orthonormal columns of $\mathbf{V} \in \mathbb{R}^{n \times d}$, one obtains a rank $d$ approximation of $\mathbf{F}_{\text{RAI}}$ as follows:

$$\mathbf{F}_{\text{RAI}} \approx \mathbf{V}(\mathbf{V}^T \mathbf{D}^{-1} \mathbf{V} \Lambda) \mathbf{V}^T = \tilde{\mathbf{V}} \tilde{\mathbf{V}}^T,$$

where $\tilde{\mathbf{V}} \triangleq \mathbf{V}(\Lambda^{1/2} \mathbf{V}^T \mathbf{D}^{1/2} \mathbf{V} \Lambda)^{1/2} \in \mathbb{R}^{d \times d}$. These expressions are well-defined, since the positive definiteness of $\mathbf{V}^T \mathbf{D}^{-1} \mathbf{V} \in \mathbb{R}^{d \times d}$ implies positive definiteness of $\Lambda^{1/2} \mathbf{V} \Lambda \in \mathbb{R}^{d \times d}$, hence the principal root exists and is unique. To obtain a block-approximation $\mathbf{F}_{\text{RAI}}$, simply cluster the rows of $\tilde{\mathbf{V}}$ into bins and replace the rows by centroids.

The Adamic-Adar Index (AA) (Adamic & Adar, 2003) can be block-approximated in a very similar fashion. It is defined similarly as (6), by substituting $d_k$ by $\log(d_k)$. Nodes
with \( d_k = 1 \) lead to an ill-defined \( \mathbf{D}^{-1} \) matrix, but since they never occur as a common neighbor of two other nodes, these nodes are omitted in the calculations.

3.2.3. Preferential Attachment (PA)

The preferential attachment feature matrix (Grover & Leskovec, 2016a; Parisi et al., 2018) is defined as \( \mathbf{F}_{\text{PA}} \triangleq ||N(i) : |N(j)| || \) i.e., the matrix induced by the product of the degrees. By definition \( \mathbf{F}_{\text{PA}} \) is already rank one; it is the outer product of a vector of degrees with itself. For reasons discussed in the proof of Theorem 1, the natural way to block-approximate (in this case, exactly) \( \mathbf{F}_{\text{PA}} = \mathbf{F}_{\text{PA}} \) is by considering the unique degrees in the network.

3.2.4. Cross/Skeleton decompositions

Alternatively, general methods from the vast literature on scalable low-rank approximations (Goreinov et al., 1997; Achlioptas & Mesherry, 2007; Markovsky, 2012; Kumar & Schneider, 2017; Indyk et al., 2019) can be utilized. The most scalable methods (Cross/Skeleton decompositions) essentially sample rows and columns to obtain a low-rank decomposition. We did not utilize these methods. Instead, we restricted ourselves to the feature matrices defined above, for which a fast top \( d \) eigendecomposition of \( \hat{\mathbf{A}} \) was sufficient to obtain qualitative block-approximations.

3.3. Overall running time

Computing the top \( l \) eigendecomposition of \( \hat{\mathbf{A}} \) is efficient for sparse symmetric matrices using iterative methods (Lehoucq & Sorensen, 1996; Stewart, 2001), scaling linearly with \( n \) for a fixed number of iterations. Moreover, this is only computed once. Running the kmeans++ algorithm for \( t \) iterations has time complexity \( O(t nk d) \) (Arthur & Vassilvitskii, 2007). There are known instances (Arthur & Vassilvitskii, 2006) for which \( t = 2^{\Theta(\sqrt{n})} \) until convergence, but the \( O(\log(k)) \) approximation ratio in expectation is valid even after the initialization of the clustering \( (t = 1) \). Hence, overall running time is linear in \( n \) for fixed \( t \), \( k \) and \( d \).

Optimizing the reduced Lagrange dual function. Theorem 1 shows that the final computational step is to solve an unconstrained convex optimization problem with \( O(\sqrt{kn}) \) variables. The computational complexity for computing the gradient as well as the Hessian is \( O(kn) \). Space complexity for storing the gradient is \( O(\sqrt{kn}) \) and \( O(kn) \) for the Hessian, which roughly (for small \( k \)) equals the space complexity of storing the graph in sparse representation. In Appendix C we compare three different optimization strategies, and conclude that L-BFGS (Liu & Nocedal, 1989) is particularly well-suited for this objective function. This has been observed before, as L-BFGS has been described as the ‘algorithm of choice’ for fitting log-linear (i.e., maximum entropy) models (Malouf, 2002; Andrew & Gao, 2007).

3.4. Combining multiple feature matrices

Theorem 1 is formulated for the case of only one block-approximation matrix \( \mathbf{F}_i \). Combining multiple block-approximations \( \mathbf{F}_1, \ldots, \mathbf{F}_s \) can be done by considering the greatest lower bound of the node binning. Each \( \mathbf{F}_i \) defines a partition \( B_i \) on the set of nodes. A partition \( B_i \) is a refinement of a partition \( B_j \) if each element of \( B_i \) is a subset of some element in \( B_j \). This relation \( B_i \leq B_j \) defines a partial order (Birkhoff, 1967) and the set of all partitions form a lattice. A given set of partitions \( \{B_1, \ldots, B_s\} \) thus has a greatest lower bound \( b \leq B_i \). Theorem 1 still holds for multiple \( \mathbf{F}_i \) matrices, if ones replaces \( k \) with \( |b| \). Assuming an equal number of bins \( k \) for each \( \mathbf{F}_i \), worst-case this amounts to a lower bound with \( |b| = \min\{k^n, n\} \) bins. However, for a limited number of global constraints \( \gamma \) and small \( k \), we already obtain qualitative and scalable results in practice (Section 4).

4. Evaluation

Performance is tested on two important applications: link prediction (Section 4.1) and network reconstruction (Appendix B). To ensure reproducibility, we utilize the EvalNE library (Mara et al., 2019). Model implementations, as well as customized configuration files describing the experiments, are publicly available.3 Section 4.2 evaluates our proposed models on a social network using a goodness-of-fit approach. Detailed runtime experiments and optimization strategies are discussed in Appendix C. Datasets are listed in Table 2. Experiments were conducted on a Linux server with two Intel Xeon Gold processors and 256GB of RAM.

4.1. Link Prediction

In link prediction the aim is to identify missing links from a given network. In this task, we randomly remove 50% of the edges such that the remaining network is still connected. The reduced network is used for training, the removed edges are used for testing. We compare with eight state-of-the-art network embedding methods and five common heuristics. Method descriptions, parameter tuning and further details on the experimental setup are discussed in Appendix B.

MaxEnt (full). First, we evaluate an exact model according to (3) with constraints on node degrees, and global constraints on \( \mathbf{F}_{\text{CN}}, \mathbf{F}_{\text{RAI}} \) and \( \mathbf{F}_{\text{PA}} \). This model is denoted as MaxEnt (full) in Table 1.

MaxEnt (blocked). Secondly, two block-approximated models where both \( \mathbf{F}_{\text{CN}} \) (Section 3.2.1) and \( \mathbf{F}_{\text{RAI}} \) (Sec-

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3 www.dropbox.com/sh/ok9xn98xjgs2jnv/AADJnax6r5pMedok3b4zzcY2a?dl=0
The idea is to compare a set of higher-order network statistics, preferably statistics that are not directly modeled, with a range of the same statistics obtained by simulating random graphs from the model. We test on the Facebook dataset, and use three statistics that have been previously proposed to evaluate social network models (Hunter et al., 2008): i) Minimum geodesic distance; ii) the distribution of the number of edges between a set of three nodes. iii) Local and global constraints (Section 3.2.2) are binned into \( k \in \{5, 100\} \) bins and with \( d = 128 \). The matrix \( F \) is naturally binned by the unique degrees (Section 3.2.3). These models are denoted as MaxEnt (\( k = 5 \)) and MaxEnt (\( k = 100 \)) in Table 1.

In Table 1 we present the average Area Under the ROC Curve (AUC) over three experiment repeats with different train/test splits for all methods. We use \( \times \) to indicate that a method did not finish within a pre-set time of 4 hours. Best results for each dataset are highlighted in bold.

| Dataset | Category | \(|V|\) | \(|E|\) |
|---------|----------|-------|-------|
| StudentDB (Goethals et al., 2010) | Relational | 395 | 3,423 |
| Facebook (Leskovec & Krevl, 2015) | Social | 4,039 | 86,234 |
| PPI (Breidtrenz et al., 2007) | Biological | 3,862 | 37,844 |
| Wikipedia (Mahoney, 2011) | Language | 4,777 | 92,295 |
| GR-QC (Leskovec & Krevl, 2015) | Collaboration | 4,158 | 26,844 |
| BlogCatalog (Zafarani & Liu, 2009) | Social | 10,312 | 333,983 |
| YouTube (Mislove et al., 2007) | Social | 1,138,409 | 2,990,443 |
| Flickr (Leskovec & Krevl, 2015) | Social | 80,511 | 11,799,764 |
| DBLP (Leskovec & Krevl, 2015) | Collaboration | 317,080 | 1,049,866 |

Figure 3. Total execution times for the link prediction task on the StudentDB, Facebook, PPI, Wikipedia and GR-QC datasets.
of the actual degree distribution. However, they fail to capture any form of community structure which the dataset most surely has. The dataset is essentially a combination of social circles (communities), combined with individual ego-networks.

Figure 4 shows the goodness-of-fit plots. Both MaxEnt models with global constraints capture the triad census and edge-wise shared partners distributions quite well. The geodesic distances are less well captured by the block-approximated MaxEnt model. The block-approximated model captures the community structure, but it still assigns a decent amount of probability mass to inter-community edges, reducing distances between nodes in different communities. As expected, the exact model fitted with the polynomial constraint is a very close fit to the original network (Section 2.4).

5. Related Work & Concluding Discussion

Although ERGs have a long history (Frank & Strauss, 1986; Newman, 2003) and have been successfully used as network models (Goodreau, 2007; Hunter et al., 2008; Koskinen et al., 2010), they usually suffer from limited scalability and degeneracy (Handcock, 2003). A theoretical explanation for degeneracy is given by Chatterjee & Diaconis (2013) for dense graphs. Snijders et al. (2006) propose a set of ERG specifications less prone to degeneracy than Markov graphs. Karwa et al. (2016) try to resolve degeneracy by limiting the support of an ERG. Recently, Byshkin et al. (2018) proposed slightly more scalable parameter estimates by exploiting properties of Markov chains at equilibrium, allowing for inference on a network with $10^5$ nodes. Our paper circumvents both shortcomings by approximating independence models by using block-approximated feature matrices, allowing for qualitative inference on sparse graphs with millions of nodes. With sensible feature selection, degeneracy can be avoided (Section 2.4), and block-approximating typically results in additional probability smoothing.

Duijn et al. (2009) argued that the properties of the pseudo likelihood for analyzing social networks are poorly understood. A possible explanation of the strength of the proposed models is the combination of both local role-based similarities (degrees) (Rossi et al., 2019), with community information. Leveraging other graphlets counts, e.g., by considering weighted common graphlet counts as features, is a promising avenue for further work. Recent methods (Rossi et al., 2018; Rossi et al., 2019) have been proposed to obtain approximative low-rank decompositions of such matrices. Another indication is the recent success of graphons (Borgs et al., 2014; Choi & Wolfe, 2012), which are essentially dyadic independence models for dense graphs. A further investigation of the relationship with graphons is a second interesting avenue for further work.
A. Model Derivation & Proofs

Partition function & Pseudo Likelihood. When considering the Lagrangian $L$ of the entropy optimization problem defined by (3), and setting derivatives with respect to $P(A)$ equal to zero, one obtains the following form for $P(A)$

$$P(A) = \frac{\exp(\sum_i \lambda_i \sum_{i,j} f^i_{ij} A_{ij})}{Z} = \prod_{i,j} \exp(\sum_i \lambda_i f^i_{ij} A_{ij}),$$

(7)

where $Z = Z(\lambda_1, \ldots, \lambda_M)$ is the partition function (i.e., the normalizing constant). Evaluating $Z$ yields

$$Z = \sum_{A \in \{0,1\}^{n \times n}} \prod_{i,j} \exp(\sum_i \lambda_i f^i_{ij} A_{ij})$$

$$= \prod_{i,j} \sum_{A_{ij} \in \{0,1\}} \exp(\sum_i \lambda_i f^i_{ij} A_{ij})$$

$$= \prod_{i,j} (1 + \exp(\sum_i \lambda_i f^i_{ij})).$$

Hence $P(A)$ factorizes as a product of independent Bernoulli distributions. The pseudolikelihood of an ERG with parameters $\theta_i$ and related statistics $s^l$ is equal to (Duijn et al., 2009; He & Zheng, 2015)

$$P_{\text{pseudo}}(A) = \prod_{i,j} \frac{\exp(\sum_i \theta_i \Delta s^l_{ij} A_{ij})}{1 + \exp(\sum_i \theta_i \Delta s^l_{ij})},$$

where $\Delta s^l_{ij}$ denotes the change in the statistic $s^l$ when going from a realization of $A$ without the edge $(i, j)$ to a realization of $A$ that includes the edge $(i, j)$. Hence $P_{\text{pseudo}}$ is identical to (1), when the $f^i_{ij}$ features are chosen to be equal to $\Delta s^l_{ij}$, as will be the case for statistics that are counts of certain graph related properties (degrees, triangles, etc.). For example, consider the out-degree of node $i$ as a statistic. Then $\Delta s^l_{kj} = 1$ when $k = i$ and $j \neq i$, and $\Delta s^l_{kj} = 0$ elsewhere. This is exactly equal to the $f^l_{ij}$ degree-features defined in Section 2.2.

Lemma 1. Let $\text{nnz}(\hat{A})$ be the number of ones in $\hat{A}$. The nodes are partitioned into $k$ disjoint groups. Denote $\text{nnz}(i)$ as the number of ones in the rows of $\hat{A}$, when restricted to the nodes in group $1 \leq i \leq k$. Let $u_i$ denote the number of unique degrees in group $i$. Then it holds that (De Bie, 2011):

$$u_i \leq \sqrt{2 \cdot \text{nnz}(i)}$$

Summating over the $k$ groups:

$$\sum_{i=1}^{k} u_i \leq \sqrt{2 \cdot (\sqrt{\text{nnz}(1)} + \ldots + \sqrt{\text{nnz}(k)})}.$$ 

Utilizing $\text{nnz}(1) + \ldots + \text{nnz}(k) = \text{nnz}(\hat{A})$, the concavity of $\sqrt{x}$ and Jensen’s inequality:

$$\sqrt{\text{nnz}(1)} + \ldots + \sqrt{\text{nnz}(k)} \leq k \cdot \sqrt{\frac{\text{nnz}(\hat{A})}{k}}.$$ 

Hence $\sum_{i=1}^{k} u_i = O(\sqrt{km})$ for sparse matrices. \hfill \square

Theorem 1. When $F$ is represented by a blockmatrix, observe that the convex Lagrange dual function (4) is invariant if one swaps two degree Lagrange multipliers $\lambda_i$ and $\lambda_j$, when $i$ and $j$ are part of the same block and have the same degree $d_i = d_j$. This implies there exists an optimum where $\lambda_i = \lambda_j$ (Adriaens et al., 2019, Section 4.2). As such, the number of free variables is determined by the number of unique degrees in each block. By Lemma 1, the total number of unique degrees summated over $k$ blocks is $O(\sqrt{km})$. \hfill \square

Proposition 1. Invoking the triangle inequality, and since $USU^T$ is the optimal rank $d$ approximation of $F$, we can write

$$\|F - USU^T\| \leq \|F - U_cS_c^T\| \leq \|F - USU^T\| + \|USU^T - U_cS_c^T\|.$$
The latter term can again be bounded with the triangle inequality
\[
\|USU^T - U_cSU_c^T\| \\
\leq \|USU^T - U_cSU^T\| + \|U_cSU^T - U_cSU_c^T\| \\
= \|(U - U_c)SU^T\| + \|U_cS(U^T - U_c^T)\|. 
\]
(8)

Observe that we can write \(U_c = CU\), where \(C \in \mathbb{R}^{n \times n}\) denotes a matrix with in each row entries equal to \(1/n_i\) for nodes that are in the same bin, and zero otherwise. Here, \(n_i\) denotes the size of a cluster \(i\), i.e. \(C\) is a matrix that replaces each row in \(U\) by its cluster centroid. It’s easy to see that \(C\) is an orthogonal projection matrix, in the sense that \(C^2 = C\) and \(C = C^T\). As such, for any matrix \(B\) it holds that \(\|CB\| \leq \|B\|\). Applying the second term in (8) yields
\[
\|(U - U_c)SU^T\| + \|U_cS(U^T - U_c^T)\| \\
\leq \|(U - U_c)SU^T\| + \|US(U^T - U_c^T)\| \\
\leq 2\sqrt{\sum_{i=1}^{d} |\lambda_i|} \cdot \|U - U_c\|.
\]

The result follows by noting that \(\|U - U_c\|\) is the k-means objective function and applying the bound in expectation for the kmeans++ algorithm (Arthur & Vassilvitskii, 2007).

\[\Box\]

B. Experimental setup LP & Network Reconstruction

The sets of train and test edges are topped with equal amounts of non-edges drawn uniformly at random from the original graph. The train set is further divided in 90% train and 10% validation for hyper-parameter tuning. The link prediction heuristics and embedding methods AROPE, CNE and MaxEnt provide node similarities which can be directly interpreted as probabilities of linking nodes. For the remaining methods we apply Logistic Regression with 5-fold cross validation on the edge embeddings to obtain link predictions. We set \(d = 128\) for all methods. The following method parameters were tuned using grid search: for DeepWalk and Struc2vec window sizes \{5, 10, 20\}, for Node2vec and Role2vec \(p = q \in \{0.5, 1, 2\}\) and window sizes \{5, 10, 20\}, for LINE learning rate \(\rho \in \{0.01, 0.025\}\) and number of negative samples \{5M, 10M\}, for SDNE \(\beta \in \{2, 5, 10\}\), for AROPE higher-order proximities of orders 1 up to 4 and for CNE the learning rate \(\alpha \in \{0.01, 0.05\}\). Most methods require a binary operator that transforms node embeddings into edge embeddings. We use the same operators proposed in (Grover & Leskovec, 2016b), and tuned them as additional method hyper-parameters.

Deepwalk (Perozzi et al., 2014) computes node embeddings using truncated random walks and the Skipgram model approximated by hierarchical softmax.

Node2vec (Grover & Leskovec, 2016b) is a generalization of DeepWalk which approximates the Skipgram model by means of negative sampling. The model uses two parameters \(p\) and \(q\) that interpolate between the importance of BFS/DFS random walk strategies.

Struc2vec (Ribeiro et al., 2017) extracts structural information from the graph through node pair similarities for a range of neighbourhood sizes. This information is then summarized as a multi-layer weighted graph. A random walk on this graph is used to generate the embeddings.

Role2vec (Ahmed et al., 2018) is a space-efficient random walk based approach which learns embeddings for different types of nodes.

LINE (Tang et al., 2015) is a probabilistic approach which computes node embeddings based on first and second order similarities between network nodes.

SDNE (Wang et al., 2016) uses a deep auto-encoder to generate embeddings which capture first and second order proximities.

CNE (Kang et al., 2019) uses a Bayesian approach to generate embeddings using structural graph properties as priors.

AROPE (Zhang et al., 2018) proposes embeddings as found by the truncated singular value decompositions of higher order proximities.

In addition to the embedding methods, we consider the following well-known heuristics: Common Neighbours (CN), Adamic-Adar Index (AA), Jaccard Coefficient (JC), Preferential Attachment (PA) and Resource Allocation Index (RAI). We refer to (Sarkar et al., 2011) for more details.
Network Reconstruction. The goal is to evaluate how accurately a model captures the actual link structure of a network. As with LP, we train all embedding methods and tune their hyper-parameters using grid search. In contrast to LP, however, method training and parameter tuning are performed on the complete input graph. We randomly select 10% of all possible node pairs and computing their similarity. The highest ranked pairs are used to reconstruct the network and results are evaluated in terms of precision@\( N_p \), defined as the number of node pairs correctly recovered within the first \( N_p \) pairs with highest similarity. Figure 5 presents the precision@\( N_p \) for a range of \( N_p \) values on the StudentDB, Facebook, and GR-QC datasets. We use the same MaxEnt models as used in the LP experiment. MaxEnt (\( k = 100 \)) and MaxEnt (full) perform well across all datasets. The good performance exhibit by AROPE is potentially due to the fact that the adjacency matrix \( \hat{A} \) is used as one of the polynomials in the grid search (see Section 2.4 for a discussion of label leakage).

C. Detailed runtime testing

First, we generate synthetic Erdos-Renyi graphs of different sizes \( n \in \{1, 5, 25, 125, 625\} \cdot 10^3 \) with edges \( m \approx 10n \), test the influence of the graphsize \( n \) on scalability, and compare three optimization strategies. We solve a MaxEnt model with constraints on degrees and a block-approximated \( F = \hat{A}^2 \) (\( d = 20 \) and \( k = 100 \)). We try three different optimizers using the minFunc optimization package (Schmidt, 2005): i) a full Newton’s method, with analytical Hessian provided. ii) a diagonal quasi-Newton’s method, with an approximative Hessian consisting of the diagonal elements of the exact Hessian. iii) L-BFGS, a well-known and popular quasi-Newton method for parameter estimation in machine learning (Liu & Nocedal, 1989). All optimizers use the same Wolfe line-search criteria to ensure global convergence. Figure 6a shows the time needed to reach a norm gradient tolerance of \( 10^{-3} \), showing the superior performance of L-BFGS. Figure 6b shows the overall time needed to block-approximate \( F \), and then fitting the reduced model with L-BFGS. K-means++ was repeated 5 times per instance, and each try was given a 100 iterations. Because of the small number of bins \( k = 100 \), and thus a small number of variables, the overall fitting time is mostly dominated by the eigendecomposition of \( \hat{A} \) and the k-means clustering.

Secondly, we generate 10 Erdos-Renyi graphs with graphsize \( n = 10^5 \) and \( m \approx 10n \). The number of bins \( k \) are varied according to \( 200 \leq k \leq 2000 \), in steps of 200. Figure 6d shows the average running time needed for L-BFGS to reach a gradient norm tolerance of \( 10^{-3} \). Figure 6c shows the average sum of the number of unique degrees across all the bins,
which is a measure of the number of variables that need to be optimized over (Section 3.3). Theorem 1 shows that this number scales as $O(\sqrt{kn})$ and Figure 6c indeed provides slight evidence for this.

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