AN ALGEBRAIC MONTE-CARLO ALGORITHM FOR THE PARTITION ADJACENCY MATRIX REALIZATION PROBLEM

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ABSTRACT. The graphical realization of a given degree sequence and given partition adjacency matrix simultaneously is a relevant problem in data driven modeling of networks. Here we formulate common generalizations of this problem and the Exact Matching Problem, and solve them with an algebraic Monte-Carlo algorithm that runs in polynomial time if the number of partition classes is bounded.

1. Introduction

In data driven modeling of complex networks one often needs to sample from ensembles of graphs that share characteristics with an observed network. These characteristics act as constraints for the sampling procedure and they may be reproduced exactly (“sharp constraints”) in every sampled graph or in expected value (average constraints) over the ensemble. The most natural such characteristic is the degree sequence. The degree sequence, however, has many graphical realizations in general, with varying properties, e.g., either showing assortativity or disassortativity (the extent to which vertices of similar degrees are connected or not). For example, social networks tend to be assortative, while biological and technical networks tend to be disassortative. Thus, in order to model such situations, one also has to specify the degree correlations. The simplest way of achieving that is via providing the so-called Joint Degree Matrix (JDM), whose entries are the number of edges between degree $i$ and degree $j$ vertices, for all $i$ and $j$ degree values. Note that the JDM also specifies the degree sequence itself, uniquely [5]. The JDM received considerable attention in the literature [1, 2, 5, 9, 7, 21, 23, 25, 27] and it is well understood [1, 2, 5, 21, 27]. Reference [3] presents an exact algorithm for constructing simple graphs with a prescribed JDM.

However, to model real world networks even JDM level constraints are not always sufficient. In particular, Orsini et al. [28] demonstrate this on several networks including the Internet (autonomous systems level), the distributed PGP cryptosystem, US airport network, protein interactions, brain fmri functional networks and an English word adjacency network. To capture most of the “signal” found in the structure of a real-world network they also had to include correlations beyond degree-degree correlations, such as
clustering coefficients, i.e., small subgraph correlations, called collectively as $dk$-series ($1k$ is purely degree distribution, $2k$ is joint degree distribution, etc). When trying to generate and sample graphs with these prescribed correlations, these authors observe that already at the $d = 3$ level the process does not converge and modelling essentially fails. As briefly discussed in [28], this graph generation process can be described as a Boolean constraint satisfaction SAT problem, in which the variables are the elements of the adjacency matrix whose values need to be set (to 0 or 1) such that a set of constraints expressed in terms of functions of the marginals (degrees) are satisfied. From this point of view it is thus expected that the problem eventually becomes NP-complete ($3$-SAT), which indeed was experienced in [28] through the failure of the algorithms to converge.

The graph construction problems above all have their constraints related to some structural properties of the graph. However, in many real world situations there are also externally imposed constraints, such as group membership that is not modelled by the approaches above. For example, one might study a network at different levels of resolution: we may look at a large organization as a network of interactions between teams or departments but also at the connections between the individuals throughout the organization and ask questions related to the performance of the organization as a whole as function of these networks. One can certainly think of the teams and departments as a partitioning of the individuals into groups/classes and the connections between them as a partitioning of the edges. In 2014 the first author introduced the concept of the Partition Adjacency Matrix (PAM), in order to also accommodate such, more general classes of constraints in network modeling [29]. Given a simple graph and a partition of its vertex set, entries of the PAM count the number of edges between, and within the partition classes. If the partition consists of singleton sets of vertices, then it specializes to the familiar Adjacency Matrix of the graph, while the JDM of a graph is a special PAM, with all classes composed of vertices having the same degree.

In contrast with the JDM, however, much less is known about PAMs, which are, as explained above, an important notion in data driven modeling of networks. While a JDM determines the degree sequence of a realizing graph, a PAM does not. Similarly to JDM problems, PAM problems include existence (Is there a simple graph with a given degree sequence and given PAM?), construction (Provide an algorithm that constructs such simple graphs!), sampling (Provide an algorithm that can sample such graphs with prescribed distribution!) and counting problems (How many simple graphs are there to realize a given degree sequence and given PAM?), in increasing order of their difficulty. Here we focus on the realization and construction problems.

**Partition Adjacency Matrix realization problem:** Given a set $W$ and natural numbers $d(w)$ associated with $w \in W$, a $W_i : i \in I$ partition of $W$, and natural numbers $c(W_i, W_j)$ associated with unordered pairs of partition classes, is there a simple graph on the vertex set $W$ with degree $d(w)$ for every $w \in W$, and with exactly $c(W_i, W_j)$ edges with endpoints in $W_i$ and $W_j$?

**Partition Adjacency Matrix construction problem:** Construct such a graph, if the answer to the realization problem is affirmative.
Reference [8] conjectures that the realization problem is NP-complete, and here we also support this conjecture. The skeleton of a PAM is the graph, whose vertices are the partition classes, and two partition classes, \( W_i \) and \( W_j \) are joined by an edge, if \( c(W_i, W_j) > 0 \). Reference [8] found polynomially solvable instances of the realization problem for two partition classes (\(|I| = 2\)), and also for loopless unicyclic skeleton graphs. In the Bipartite PAM problem the skeleton graph is bipartite and loopless.

A stronger version of the problems above is when there is also a forbidden subgraph that all graphical realizations must avoid. Such problems arise in part for algorithmic reasons in direct construction algorithms that add edges sequentially: the existing edges forbid the addition of further edges between the same pairs of vertices in the graph being constructed [14], [3]. Thus, we formulate:

**Partition Adjacency Matrix realization/construction problems in the presence of a blue graph:** In addition to the contraints of the PAM realization problem, a graph \( B \) (the blue graph) is given on the vertex set \( W \). Is there a realization that is not using any edges from \( B \)? If yes, construct such a graph.

To simplify the discussion, we assume that for any PAM realization/construction problem, the obvious and easy-to-check necessary conditions that \( d \) is the degree sequence of a simple graph, and that

\[
\sum_{v \in W_i} d(v) = c(W_i, W_i) + \sum_j c(W_i, W_j),
\]

\[
\sum_v d(v) = \sum_i c(W_i, W_i) + \sum_i \sum_j c(W_i, W_j)
\]

hold. In an earlier version of this manuscript [6], we gave an algebraic Monte-Carlo algorithm for the blue graph version of Bipartite PAM realization problem. This algorithm runs in polynomial time if the number of partition classes is bounded. We are indebted to András Frank (Budapest), who kindly called our attention to the analogous Exact Matching Problem [32], and asked if the two problems admit a common generalization, i.e. a third problem, of which the first two problems are specific instances, such that third problem allows algorithmic solution like the first two. Let us recall the

**Exact Matching Problem:** Given a graph \( G \), whose edges are colored red or green, is there a perfect matching with exactly \( m \) red edges in the matching?

The Exact Matching Problem originates from Papadimitriu and Yannakakis [20], and Lovász proposed a Monte-Carlo algorithm for it. Lovász’ algorithm, which he never published, is based on the general ideas in his paper [15], and is described by Mulmuley, Vazirani and Vazirani in [19] pp. 111. No deterministic polynomial time algorithm is known for the Exact Matching Problem. Here we provide the promised common generalization:

**Dominating \( f \)-factor Problem:** Given a graph \( G \) on \( n \) vertices, disjoint subsets \( E_1, ..., E_k \subseteq E(G) \), integers \( m_1, ..., m_k \), and prescribed degrees \( d_1, ..., d_n \) associated with the vertices \( v_1, ..., v_n \) of \( G \), is there a subgraph \( G' \) of \( G \), such that \( v_i \) has degree \( d_i \) in \( G' \) for all vertices, and \( G' \) has at least \( m_j \) edges from the edge set \( E_j \), for all \( j = 1, ..., k \)?
Dominating Matching Problem: Given a graph $G$, disjoint subsets $E'_1, ..., E'_k \subset E(G)$, integers $m_1, ..., m_k$, is there a perfect matching in $G$, which uses at least $m_j$ edges from the edge set $E'_j$, for all $j = 1, ..., k$?

Clearly the Dominating Matching Problem is a special case of the Dominating $f$-factor Problem, where every degree is one. In Section 2, we will show using the Tutte gadget that the Dominating $f$-factor Problem can be solved through solving a Dominating Matching Problem on about $n^2$ vertices. The Exact Matching problem is an instance of the Dominating Matching Problem, where $k = 2$, $E_1$ is the set of red edges, $E_2$ is the set of green edges, $m_1 = m$, $m_2 = |E(G)| - m$. The PAM realization problem is an instance of the Dominating $f$-factor Problem in the following way: $G$ is the complement of the blue graph $B$, the disjoint edge subsets are $E_{ij} = \{\{u, v\} \in E(G) : u \in W_i, v \in W_j\}$ for $i \leq j$ (assuming without loss of generality that $I$ is an ordered set), $m_{ij} = c(W_i, W_j)$ for $i < j$ and $m_{ii} = c(W_i, W_i)$.

Here we provide an algebraic Monte-Carlo algorithm for the Dominating Matching Problem, and hence for the Dominating $f$-factor Problem, which runs in polynomial time under the assumption that

$$\prod_{i \in I} (m_i + 1) = O(\text{polynomial}(n)).$$

This assumption certainly holds if $|I|$ stays bounded, while $n$ grows. If the algorithm returns TRUE, then the sought-after graph exists, if the algorithm returns FALSE, then with high probability (whp) such a graph does not exist. The correctness of the algorithm hinges on the Schwartz-Zippel Lemma [26]. The realization algorithm and its correctness are described in Section 3. We will also conclude that constructing an actual solution is not harder than the decision problem. We conclude the paper with some complexity results in Section 4.

2. The Tutte gadget

Clearly, the standard degree sequence realization problem is a relaxation of the PAM problem, where we do not care for satisfying the $c_{ij}$ conditions. Havel [13] and Hakimi [12] solved the degree sequence realization problem and Ryser [24] solved the bipartite degree sequence realization problem. We next use a result of Tutte [31] to connect degree sequence realization to the existence of a perfect matching in a bigger graph, the Tutte gadget.

Initially, we are given a degree sequence realization problem on the vertices in $V$, i.e. for each $v \in V$ we are given a proposed degree $d(v)$. We are also given a set of blue – or forbidden – edges $B$ that our realization is not allowed to use. For a vertex $v \in V$, let $N_B(v) = \{u : \{u, v\} \in B\}$ denote the set of blue neighbors of $v$, and $S_v = V \setminus (\{v\} \cup N_B(v))$ denote the set of allowed neighbors. Without restrictions in the degree sequence realization problem, we have $S_v = V \setminus \{v\}$. The setup of this problem implies that $u \in S_v$ iff $v \in S_u$, and we will also assume further that for each $v \in V$ $|S_v| \geq d(v)$ holds (otherwise a realization obviously cannot exist).
The Tutte gadget of the degree sequence realization problem with a set $B$ of blue edges is a graph $T$ such that

$$V(T) = \{v^u : v \in V, u \in S_v\} \cup \{a^v_i : i = 1, 2, \ldots, |S_v| - d(v) : v \in V\}$$

and

$$E(T) = \{\{v^u, a^v_i\} : v \in V, u \in S_v, i = 1, 2, \ldots, |S_v| - d(v)\}.$$

For the degree sequence realization problem, with $B = \emptyset$, for each $v \in V$, $S_v = V \setminus \{v\}$ and the degree condition becomes $d(v) \leq |V| - 1$. The Tutte gadget is a graph with $2n(n - 1) - \sum_v d(v)$ vertices.

The Tutte gadget is relevant for the following property: it has a perfect matching if and only if a graph solves the corresponding degree sequence realization problem; furthermore, if some $\{w^v, w^u\}$ edges are present in the perfect matching, then the corresponding $\{w, u\}$ edges provide a graph solving this degree sequence realization problem, and if some $\{w, u\}$ edges provide a graph solving the degree sequence realization problem, then the corresponding $\{w^v, w^u\}$ edges in $T$ are part of a perfect matching of $T$. This property is well-known and is also easy to verify.

Furthermore, if an edge $\{u, v\} \in E(G)$ belongs to an edge set $E_i$, put the edge $\{w^v, w^u\} \in E(T)$ into $E'_i$, when solve the Dominating f-factor Problem from the Dominating Matching Problem using the Tutte gadget.

### 3. The Dominating Matching Problem

Let $A$ be a skew-symmetric matrix, i.e. $A = -A^T$, and assume that $A$ has an even order $2n$. The Pfaffian of $A$ is defined as

$$\text{Pf}(A) = \sum_{\pi} \text{sign}(\pi) \cdot i_{i_1} j_{j_1} \cdot i_{i_2} j_{j_2} \cdots i_{i_n} j_{j_n},$$

where $\pi$ runs through permutations of the form

$$\pi = \begin{pmatrix} 1 & 2 & 3 & 4 & \ldots & 2n - 1 & 2n \\ i_1 & j_1 & i_2 & j_2 & \ldots & i_n & j_n \end{pmatrix}$$

under the assumptions $i_1 < j_1, i_2 < j_2, \ldots, i_n < j_n$ and $i_1 < i_2 < \cdots < i_n$, and $\text{sign}(\pi) = \pm 1$, the sign of the permutation $\pi$. For more background on the Pfaffian, see [16]. Cayley [4] and Muir [17, 18] proved that $(\text{Pf}(A))^2 = \det(A)$. Note that the summation for $\pi$ can be thought of as a summation over the perfect matchings of $2n$ elements.

Assume now that we are given a graph $G$ for the Dominating Matching Problem. We will assume that the graph has an even number of vertices, say $2n$, otherwise it cannot have a perfect matching. Fix an arbitrary orientation $\overrightarrow{G}$ of the graph $G$. For the arc $i \to j$ introduce a variable $x_{ij}$, and define $A$ by

$$i[A]_j = \begin{cases} x_{ij} & \text{if } i \to j \\ -x_{ij} & \text{if } j \to i \\ 0 & \text{otherwise.} \end{cases}$$
The variables $x_{ij}$ are independent of each other. It is clear that $G$ has a perfect matching if and only if the polynomial $\text{Pf}(A)$ is not termless, i.e., not the zero polynomial, as cancellation of terms is not possible. Tutte’s theorem [30], that $G$ has a perfect matching if and only if the polynomial $\text{det}(A)$ is not the zero polynomial follows from Cayley’s theorem. Introduce now additional new variables, $z_i$ associated with the edge set $E'_\ell$, for $\ell = 1, 2, \ldots, k$. Define the matrix $A^*$ by the substitutions $x_{ij} \leftarrow x_{ij} z_\ell$ for all $\{i, j\} \in E'_\ell$ in $A$, and not changing $x_{ij}$ if $\{i, j\} \notin \bigcup_{\ell=1}^k E'_\ell$. A matching that defines a term in $\text{Pf}(A)$ solves the Dominating Matching Problem if and only if for every $\ell$, the exponent of $z_\ell$ is at least $m_\ell$, for $\ell = 1, 2, \ldots, k$.

Now we need some properties of the difference operator acting on multivariate polynomials. For a polynomial $f(x, y, z, \ldots)$, set

$$ \nabla_x f = f(x, y, z, \ldots) - f(x - 1, y, z, \ldots). $$

We will use products of these operators to indicate juxtaposition, and consequently $\nabla^k_x$ will denote the repetition of the operator $\nabla_x$ $k$ times. $\nabla_x^0$ is the identity operator. Note that unless $f$ is identically zero, applying $\nabla_x$ strictly decreases the degree of $x$ in the polynomial. Therefore, if the degree of $x$ in $f$ is less than $k$, then $\nabla^k_x f$ is identically 0, and $\nabla_x^k x^k = k! \neq 0$. It is well-known that

$$ \nabla^k_x f(x) = \sum_{\ell=0}^{k} (-1)^\ell \binom{k}{\ell} f(x - \ell). $$

Furthermore, as

$$ \nabla_x \nabla_y f = f(x, y, z, \ldots) - f(x - 1, y, z, \ldots) - f(x, y - 1, z, \ldots) + f(x - 1, y - 1, z, \ldots) = \nabla_y \nabla_x f, $$

the order of $\nabla$ operators associated with different variables is freely interchangeable. For any function $f$ in variables $z_\ell$, and possibly other variables not shown, the following iterated difference, which is put into product notation, can be computed formally:

$$ \left( \prod_{\ell=1}^{k} \nabla_{z_\ell}^{m_\ell} \right) f(z_1, \ldots, z_\ell, \ldots, z_k) = $$

$$ \sum_{u_1=0}^{m_1} \cdots \sum_{u_\ell=0}^{m_\ell} \cdots \sum_{u_k=0}^{m_k} \left( \prod_{\ell=1}^{k} (-1)^{u_\ell} \binom{m_\ell}{u_\ell} \right) f(z_1 - u_1, \ldots, z_\ell - u_\ell, \ldots z_k - u_k). $$

We are ready to claim the key fact behind our algorithm: the polynomial

$$ \left( \prod_{\ell=1}^{k} \nabla_{z_\ell}^{m_\ell} \right) \text{Pf}(A^*(z_1, \ldots, z_k)) = $$

$$ \sum_{u_1=0}^{m_1} \cdots \sum_{u_\ell=0}^{m_\ell} \cdots \sum_{u_k=0}^{m_k} \left( \prod_{\ell=1}^{k} (-1)^{u_\ell} \binom{m_\ell}{u_\ell} \right) \text{Pf}(A^*(z_1 - u_1, \ldots, z_\ell - u_\ell, \ldots z_k - u_k)) $$

is not identically 0 if and only if the Dominating Matching Problem has a solution, as no monomial can be a multiple of another. Thus, the Dominating Matching Problem boils
down to checking whether the polynomial \( (2) \) is identically zero or not. Make random substitutions into all variables of \( (2) \), if this polynomial is not identically zero, then whp after a number of substitutions we obtain a nonzero value. In this case the answer to the problem is a (correct) \textsc{true}. If we always get zero values, the answer returned is a \textsc{false}, and it is correct whp. (We give a more detailed analysis below.) From a computational point of view, the issue is whether we can compute substituted values of \( (2) \) in polynomial time. Note that the Pfaffian with integer entries (or with entries from an integral domain) can be evaluated efficiently, similarly to the evaluation of a determinant \[10\].

While the polynomial \( \text{Pf}(A^\star) \) is not computable in polynomial time, the result of substituting numbers into all variables is. Indeed, \( (2) \) expanded in \( (1) \) with \( f(z_1, \ldots, z_{\ell}, \ldots, z_k) = \text{Pf}(A^\star) \) is just a weighted sum of values of \( \text{Pf}(A^\star) \) after the substitutions \( z_\ell \leftarrow z_\ell - u_\ell \) \((\ell = 1, 2, \ldots, k)\) for every \( 0 \leq u_\ell \leq m_\ell \). In other words, for every attempt to substitute random numbers, we have to evaluate \( \prod_{\ell=1}^k (m_\ell + 1) \) numerical Pfaffians, a polynomial number of steps in \( n \).

Recall the Schwartz-Zippel Lemma \[26\], where non-zero polynomial means that at least one term comes with nonzero coefficient.

**Lemma 1.** For a field \( \mathbb{F} \), let \( f \in \mathbb{F}[x_1, x_2, \ldots, x_t] \) be a non-zero polynomial of degree \( d \) and \( \Omega \subseteq \mathbb{F} \) a finite set, \( |\Omega| = N \). Let \( Z(f, \Omega) \) denote the set of roots from \( \Omega^n \), i.e.

\[
Z(f, \Omega) = \{(\alpha_1, \alpha_2, \ldots, \alpha_t) \in \Omega^n : f(\alpha_1, \alpha_2, \ldots, \alpha_t) = 0\}.
\]

Then \( |Z(f, \Omega)| \leq dN^{t-1} \), and the probability that \( f \) vanishes on randomly and independently selected uniformly random elements of \( \Omega \) is at most \( d/N \).

The polynomial \( (2) \) has degree at most \( 2n \). Let \( p \) be a prime number, such that \( p \geq 2n^2 \). One can find such a prime using Bertrand’s Postulate (better estimates on gaps between primes exist) and prime testing the numbers one after the other. Set \( \mathbb{F} = \Omega = \mathbb{GF}(p) \). We compute \( (2) \) in \( \mathbb{GF}(p) \), i.e. we do the calculations mod \( p \). Note that the polynomial \( (2) \) is non-zero over \( \mathbb{GF}(p) \) as well if a solution to the Dominating Matching Problem exists, since after taking the derivatives we get coefficients at the terms that are products of numbers at most \( 2n \).

Substituting randomly and uniformly selected elements of \( \mathbb{GF}(p) \) into the variables of \( A^\star \) and its translates, the probability of getting a 0 value for the expression \( (2) \) if it is not the identically 0 polynomial, is at most \( 2n/N = 2n/p \leq 1/n \), according to the Lemma.

**Theorem 2.** There is a Monte-Carlo algorithm for the Dominating Matching Problem and the Dominating f-factor Problem, which runs in polynomial time under the assumption that \( \prod_{i \in I}(m_i + 1) = O(\text{polynomial}(n)) \), which certainly holds if \( |I| \) stays bounded. If the algorithm returns \textsc{true}, then the sought after graph exists, if the algorithm returns \textsc{false}, then with high probability (whp) such a graph does not exist.

An actual solution easily can be found by testing iteratively whether an edge can be included in the matching in a modified problem, a standard approach \[19, 14\]. In the first version of this manuscript \[6\] we provided a pseudocode for the Bipartite PAM realization and construction problems.
Theorem 3. There is a Monte-Carlo algorithm to construct a solution for the Dominating Matching Problem or the Dominating f-factor Problem, which runs in polynomial time under the assumption that \( \prod_{i \in I} (m_i + 1) = O(\text{polynomial}(n)) \), which certainly holds if \(|I|\) stays bounded. If the algorithm returns a construction, then it is a correct solution, and if a correct solution exists, a construction is found whp.

4. Concluding remarks

Our algorithm for the Dominating Matching Problem, if specialized for the Exact Matching Problem, is different from from Lovász’ algorithm [19]. We believe, however, that the same techniques may also be used to solve the Dominating Matching Problem.

Here we did not attempt to optimize and estimate the running time of the algorithms, as they are very far from practical. We repeat here that no deterministic polynomial time algorithm is known for the Exact Matching problem, not even for bipartite graphs. Hence no deterministic polynomial time algorithm is known for the Dominating f-factor and Dominating Matching Problems.

We are thankful to Stefan Lendl (Graz) for bringing to our attention reference [22]. Ref. [22] shows that given a bipartite graph \( G \) and a partition \( V_1, ..., V_s \) and \( U_1, ..., U_\ell \) of the paritite classes, the decision problem whether a perfect matching \( M \) exists with at most 1 edge between any pair of partition classes is NP-complete. It is easy to see that this problem is equivalent to the following instance of the Dominating f-factor Problem: the graph is \( G \), the prescribed degree is \( d_G(v) - 1 \) for vertex \( v \), the \( E_{ij} \) edge sets are \( E(G) \cap (V_i \times U_j) \), and \( m_{ij} = |E(G) \cap (V_i \times U_j)| - 1 \). Hence the Dominating f-factor Problem is also NP-complete.

Ref. [11] noted that 3-dimensional perfect matching problem in 3-partite graphs can be reduced to the problem of finding a multicolored perfect matching in an \( n \)-colored bipartite graph \( K_{n,n} \). This gives another proof for the fact that the Dominating Matching Problem is NP-complete. Reference [8] conjectures that the PAM realization problem (with empty blue graph) is already NP-complete.

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