Exploiting total unimodularity for classes of random network problems

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Abstract

Network analysis is of great interest for the study of social, biological and technological networks, with applications, among others, in business, marketing, epidemiology and telecommunications. Researchers are often interested in assessing whether an observed feature in some particular network is expected to be found within families of networks under some hypothesis (named conditional random networks, i.e., networks satisfying some linear constraints). This work presents procedures to generate networks with specified structural properties which rely on the solution of classes of integer optimization problems. We show that, for many of them, the constraints matrices are totally unimodular, allowing the efficient generation of conditional random networks by polynomial time interior-point methods. The computational results suggest that the proposed methods can represent a general framework for the efficient generation of random networks even beyond the models analyzed in this paper. This work also opens the possibility for other applications of mathematical programming in the analysis of complex networks.

Key words: Integer Programming, Linear Programming, Total unimodularity, Interior-Point Methods, Complex Networks, Social networks analysis

1. Introduction

Network analysis is an interdisciplinary field which brings together tools and methods from discrete mathematics and computer science with a great concern toward empirical applications, for instance, in business, marketing, epidemiology, engineering and counterterrorism. In the analysis of a complex network the researcher is often interested in assessing the hypothesis of whether a particular network property is likely to appear under a uniform distribution of all networks verifying given constraints, named *conditional random networks* [3]. To perform this hypothesis testing a large sample of conditional random networks satisfying this particular property has to be generated. In this work we introduce a novel procedure to generate this sample, which is based on linear and integer optimization and it outperforms in versatility some currently available approaches.

Following the standard notation [1], a graph $G = (V, E)$ is defined by a finite set V of n nodes, and a set of m pairs of them $E \subseteq V \times V$, named edges or arcs. A graph can be represented by a $n \times n$ binary matrix X, called *adjacency matrix* (AM from now on), whose (i, j)-entry, x_{ij}, is equal to 1 if there is a link between nodes i and j, and 0 otherwise. We will assume the graph has no loops, so that the diagonal of X is null. A network is a graph whose arcs or nodes have associated numerical values (arc costs, arc capacities, node supplies, etc).

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In this work we will make no distinction and the two terms "graph" and "network" will be used as synonyms.

The study of random graphs begins with the seminal work of P. Erdös and A. Rainyi [10], who considered a fixed set of nodes and an independent and equal probability of observing edges among them. There are two closely related variants of the Erdös-Rainyi model:

- *The $G(n,p)$ model.* A network is constructed by connecting nodes randomly with independent probability p.
- *The $G(n,m)$ model.* A network is chosen uniformly at random from the collection of all graphs with n nodes and m edges.

Both models possess the considerable advantage of being exactly solvable for many of their average properties: clustering coefficient, average path length, giant component, etc. In other words, the expectation of many structural properties of networks generated by the Erdös-Rainyi processes is analytically obtainable. Conditional uniform models can be seen as a generalization of the $G(n,m)$ model, when the conditioning information is not necessarily the number of edges but whatever other arbitrary network property. Unfortunately, in this case we have very few analytical results and simulation is required to obtain empirical distributions of their average properties.

Although other Operations Research tools have been used in the context of social networks [2, 11], as far as we know, this work is the first attempt to use integer optimization for the generation of several classes of conditional random graphs. Previous approaches, developed within the fields of *mathematical and computational sociology*, were ad hoc procedures for some particular types of networks, in general difficult to generalize and not very efficient. For instance, the distribution of all networks conditioned to the nodes in- and out-degree have difficult combinatorial properties, as its analytical study involves binary matrices with fixed marginal rows and marginal columns. In this respect, some combinatorial results have been obtained by Ryser [23], who derived necessary and sufficient conditions for two vectors of non-negative integers to constitute the row sums and column sums of some zero-one matrix. On the other hand, ways to generate uniform random networks with given degree distribution were developed in [25, 21, 7, 22, 26].

Snijders [25] considered an enumeration tree representing the AM, which is used to determine whether a particular arc must be created. This method is computationally expensive and prohibitive for very large AMs. A few years later Rao et al. [21] proposed a Markov chain Monte Carlo approach to generate AMs with given in- and out-degrees. The method is based on iteratively interchanging the arcs connecting two or three nodes randomly selected, whenever their degrees are preserved. However, as Robert [22] showed, a particular disadvantage of this procedure is that the arcs connecting the two or three nodes randomly selected in general do not preserve degrees, and many selections are likely to be rejected. The particular importance of the uniform random network model conditioned to the nodes degree is mainly due to the fact that the expectation of the clustering coefficient and the characteristic path length are analytically solvable for uniform undirected networks with given degree distribution. (For more details about network properties, such as the clustering coefficient and the characteristic path length, see Bollobas [3] and Wasserman and Faust [27].)

In practice one would like to go even further in conditioning, which however leads to self-defeating attempts because of combinatorial complexity. This work provides a general methodological framework to generate networks with constraints, representing structural features we wish to control for. Let x_{ij} be entries of the AM of a simple graph (i.e., an undirected graph with no loops or multiple edges). Then, the AM of all simple graphs is an

element of the set of symmetric binary matrices with zero diagonal

$$\begin{aligned} \chi &= \{x_{ij} \in \{0,1\} : x_{ij} - x_{ji} = 0, (i,j) \in H\}, \\ \text{where} \quad H &= \{(i,j) : 1 \leq i \leq n-1, i < j \leq n\}. \end{aligned} \tag{1}$$

As it will be shown in the next section, the constraints matrix associated to the continuous relaxation of χ (the set obtained by replacing $x_{ij} \in \{0,1\}$ with $0 \leq x_{ij} \leq 1$, $i \in H$, in (1)), call it $CR(\chi)$, is totally unimodular (TU, from now on) and its right-hand terms are integer. This fact implies that all extreme points of $CR(\chi)$ are integer. As shown in [13], the next theorem provides sufficient conditions for a matrix to be TU:

Theorem 1. *Let $A \in \{-1,0,1\}^{m \times n}$ be a matrix obtained by elementary operations of $B \in \boldsymbol{Z}^{m \times n}$ and consider a partition of the rows of A in two disjoint sets $\mathcal{J}_1$ and $\mathcal{J}_2$. The following four conditions together are sufficient for B to be TU:*

1. *Every column of A contains at most two non-zero entries, which are either 1 or -1.*
2. *If two non-zero entries in a column of A have the same sign, then the row of one is in $\mathcal{J}_1$, and the other in $\mathcal{J}_2$.*
3. *If two non-zero entries in a column of A have opposite signs, then the rows of both are either in $\mathcal{J}_1$ or $\mathcal{J}_2$.*

The above theorem will be extensively used in next section. More details on unimodularity in integer programming can be found in [24]. As a consequence of total unimodularity, each extreme point of $CR(\chi)$ represents a simple graph. Therefore, it is possible to generate a bunch of simple graphs by merely solving linear programs (LP) with random gradients in the objective function, or by non-degenerated simplex pivoting, starting from a given initial extreme point [19]. Moreover, they can be generated in polynomial time if interior-point methods are used [28].

The paper is organized as follows. Section 2 is devoted to the characterization of the convex hull of polytopes associated to some families of conditional random networks. We will differentiate between families of conditional random networks whose constraints are TU, and those which may provide fractional AMs. Supported by these results, Section 3 presents two particular procedures for the generation of conditional random networks. Section 4 illustrates these techniques using a social network of dolphins living off Doubtful Sound, New Zealand [17].

Throughout the paper we denote the vector of variables associated to the components of the AM with the boldface character $\mathbf{x}^T = [x_{12}, \ldots, x_{1n}, x_{23}, \ldots, x_{2n}, \ldots, x_{(n-1)n}, x_{21}, \ldots, x_{n1}, x_{32}, \ldots, x_{n2}, \ldots, x_{n(n-1)}]$, i.e., the rowwise upper triangle of AM followed by its columnwise lower triangle.

2. Total unimodularity of constraints from some conditional random networks

Let χ be the set of AMs of simple graphs with n nodes defined in (1), and $CR(\chi)$ its continuous relaxation. Using the total unimodularity of the constraints matrix of $CR(\chi)$, next Proposition 1 shows there is a bijection between extreme points of $CR(\chi)$ and simple graphs.

Proposition 1. *Consider the polyhedron $CR(\chi)$. Each graph of n nodes is associated to a unique extreme point of $CR(\chi)$, and conversely each extreme point of $CR(\chi)$ is associated to a unique graph of n nodes.*

Proof. Adding a non-negative slack vector $\mathbf{s} \in \mathbb{R}^{n(n-1)}$, $CR(\chi)$ is given by all $\mathbf{x} \in \mathbb{R}^{n(n-1)}$ verifying the constraints

$$\left[\begin{array}{c|c|c|c} I & -I & & \\ \hline I & & I & \\ \hline & I & & I \end{array}\right] \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] = \left[\begin{array}{c} \mathbf{0} \\ \hline \mathbf{e} \\ \hline \mathbf{e} \end{array}\right]; \qquad \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] \geq \mathbf{0}, \tag{2}$$

where $I \in \mathbb{R}^{n(n-1)/2 \times n(n-1)/2}$ is an identity matrix, and $\mathbf{e} = (1, \ldots, 1)^T \in \mathbb{R}^{n(n-1)/2}$.

The constraints matrix of (2) is easily seen to be TU, by finding a row bipartition in two sets, say $\mathcal{J}_1$ and $\mathcal{J}_2$, in accordance with Theorem 1: set the first $n(n-1)/2$ rows in $\mathcal{J}_1$, the second $n(n-1)/2$ rows in $\mathcal{J}_2$ and the third $n(n-1)/2$ rows in $\mathcal{J}_1$. Therefore, the extreme points of $CR(\chi)$ are all integer and no integer point may be located in its interior (since $CR(\chi)$ is a subset of the unit hypercube). This completes the proof. □

Note that a similar proof is valid for digraphs (we just have to remove the first $n(n-1)/2$ rows of the matrix of (2)).

Therefore each simple graph is a solution of a LP whose feasible region is defined by $CR(\chi)$. However, the importance of Proposition 1 lays on the fact that it can be extended to other interesting families of networks satisfying certain conditions. It is thus possible to generate a bunch of these conditional random networks by exploring the extreme points of their respective polyhedrons. Specifically, this holds for the following families of conditional networks:

1. undirected networks conditioned to the density (i.e., number of edges);
2. directed networks conditioned to the density;
3. undirected networks conditioned to the within & between group densities;
4. undirected networks conditioned to the within group densities;
5. undirected networks conditioned to the between group densities;
6. directed networks conditioned to the within & between group densities;
7. directed networks conditioned to the within group densities;
8. directed networks conditioned to the between group densities;
9. undirected networks conditioned to the within group densities and the density;
10. undirected networks conditioned to between group densities and the density;
11. directed networks conditioned to the within group densities and the density;
12. directed networks conditioned to the between group densities and the density;
13. directed networks conditioned to the nodes in-&-out-degree;
14. undirected networks conditioned to the lower bound of the nodes degree range and density;
15. directed networks conditioned to the dyad count;
16. directed networks conditioned to the number of mutual links.

In some cases there is no bijective relation between a family of conditional random networks and the extreme points of its polyhedron, since some basic solutions may be fractional. However, if we can ensure that no integer solution is in the interior of the polyhedron, this injective relation (i.e., any random network is associated to an extreme point, but not the opposite) is still useful, whenever some kind of acceptance-rejection technique is considered for fractional solutions. TU could not be proved for the following families of conditional random networks:

1. undirected networks conditioned to nodes degree;
2. undirected networks conditioned to the within & between group densities and the degrees;
3. undirected networks conditioned to the within group densities and the nodes degree;
4. undirected networks conditioned to the between group densities and the nodes degree;
5. directed networks conditioned to the within & between group densities and in-&-out-degrees;
6. directed networks conditioned to the within group densities and in-&-out-degrees;
7. directed networks conditioned to the between group densities and in-&-out-degrees;
8. edge-colored undirected networks conditioned to the density;
9. edge-colored undirected networks conditioned to the color densities;
10. edge-colored undirected networks conditioned to the degrees.

The rest of this section is devoted to prove that matrices associated to polyhedrons of some of the aforementioned families of networks are TU. The readers not interested in the proofs can directly jump to Section 3 which describes two LP procedures to randomly generate conditional networks. Acceptation-rejection procedures for the families of networks whose constraints matrices are not TU are empirically evaluated in Section 4, by computing the proportion of fractional solutions.

2.1. Undirected networks conditioned to the density

As mentioned in the introduction, this is the oldest model of random networks [10]. Analytical results [3] show that the expected characteristic path length and clustering coefficients of a uniform random network with n nodes conditioned to density d is $\ln(n)/\ln(2d/n)$ and $2d/n^2$ respectively. However, for non uniform probabilities few analytical results are available.

Proposition 2 below generalizes Proposition 1 for simple graphs conditioned to the density.

Proposition 2. *Let $\varphi = \{\mathbf{x} \in [0,1]^{n(n-1)} : x_{ij} - x_{ji} = 0, (i,j) \in H; \sum_{(i,j)\in H} x_{ij} = d\}$. There is a bijection between the extreme points of φ and the space of simple graphs with n nodes and density d.*

Proof. By adding to (2) the equation $\sum_{(ij)\in H} x_{ij} = d$ we get the constraints of $CR(\varphi)$

$$\left[\begin{array}{c|c|c|c} I & -I & & \\ \hline I & & I & \\ \hline & I & & I \\ \hline \mathbf{e}^T & & & \end{array}\right] \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] = \left[\begin{array}{c} \mathbf{0} \\ \hline \mathbf{e} \\ \hline \mathbf{e} \\ \hline d \end{array}\right], \qquad \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] \geq 0. \tag{3}$$

Let R_j, $j = 1,2,3,4$, be the j^{th} row-block. By performing the elementary operation $R_1 := R_1 - R_2$, the resulting matrix is

$$\left[\begin{array}{c|c|c|c} & -I & -I & \\ \hline I & & I & \\ \hline & I & & I \\ \hline \mathbf{e}^T & & & \end{array}\right] \begin{array}{l} \mathcal{J}_1 \\ \mathcal{J}_1 \\ \mathcal{J}_1 \\ \mathcal{J}_2 \end{array}. \tag{4}$$

By Theorem 1 and the row partition $\mathcal{J}_1$ and $\mathcal{J}_2$ shown in (4), the constraints matrix of (3) is TU and every extreme point is associated to a valid graph. In addition, no integer point may be located in the interior of φ since it is a subset of the unit hypercube, completing the proof. □

The existence of a bijection between the space of directed networks conditioned to the density and the set of extreme points of its polyhedron can be proven in a similar way.

2.2. Undirected networks constrained to the within and between group densities

Suppose a network analyst is studying the (symmetric) friendship relation among high-school students and she has information concerning the number of links between students of the same gender and between students of opposite gender. Nodes of the network are viewed as belonging to one of two groups (male/female) and the interest might be to study the set of all networks having fixed within and between group densities.

More generally, suppose we have g different groups, $\gamma_i, \ldots, \gamma_g$ and let Γ be the set of such groups. Consider a function, $\theta : V \times V \to \Gamma \times \Gamma$, associating to each pair of nodes the pair of groups they belong to. The density constraint between group γ_k and γ_h, $1 \leq k \leq g$, $k \leq h \leq g$, is $\sum_{(i,j)\in H:\theta(i,j)=(\gamma_k,\gamma_h)} x_{ij} = d_{kh}$, where d_{kh} is a non-negative integer. Note that when $k = h$ we have a within group density constraint, otherwise a between group density constraint.

Proposition 3. *Let* $\varphi = \{\mathbf{x} \in [0,1]^{n(n-1)} : x_{ij} - x_{ji} = 0, (i,j) \in H; \sum_{(i,j)\in H:\theta(i,j)=(\gamma_k,\gamma_h)} x_{ij} = d_{kh}, 1 \leq k \leq g, k \leq h \leq g\}$. *There is a bijection between the extreme points of* φ *and the space of all simple graphs with* n *nodes and within and between group densities* d_{kh}.

Proof. The constraints of $CR(\varphi)$ are obtained by adding to (2) the equations $\sum_{(i,j)\in H:\theta(i,j)=(\gamma_k,\gamma_h)} x_{ij} = d_{kh}, 1 \leq k \leq g, k \leq h \leq g$:

$$\left[\begin{array}{c|c|c|c} I & -I & & \\ \hline I & & I & \\ \hline & I & & I \\ \hline F & & & \end{array}\right] \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] = \left[\begin{array}{c} \mathbf{0} \\ \hline \mathbf{e} \\ \hline \mathbf{e} \\ \hline \mathbf{d} \end{array}\right], \qquad \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] \geq 0, \tag{5}$$

where $\mathbf{d} = (d_{kh\ 1\leq k\leq g, k\leq h\leq g})^T \in \mathbb{Z}_{+\cup\{0\}}^{g(g+1)/2}$, $\mathbf{x}$ and $\mathbf{s}$ have the same definition as in (2), and $F \in \{0,1\}^{g(g+1)/2 \times n(n-1)/2}$ is the matrix related to within and between group density constraints. Note that columns of F have only a single $+1$. Subtracting the second row-block of (5) to the first row-block, and considering the following row partition $\mathcal{J}_1$ and $\mathcal{J}_2$

$$\left[\begin{array}{c|c|c|c} & -I & -I & \\ \hline I & & I & \\ \hline & I & & I \\ \hline F & & & \end{array}\right] \begin{array}{l} \mathcal{J}_1 \\ \mathcal{J}_1 \\ \mathcal{J}_1 \\ \mathcal{J}_2, \end{array} \tag{6}$$

by Theorem 1 the constraints matrix of (5) is TU. The proof is completed by noting that no integer point may be located in the interior of φ since it is a subset of the unit hypercube. □

2.3. Undirected networks conditioned to the lower bound of the degrees range and density

Let $\varphi = \{\mathbf{x} \in \{0,1\}^{n(n-1)} : x_{ij} - x_{ji} = 0, (i,j) \in H; \sum_{1\leq j\leq n, j\neq i} x_{ij} = f_i, i = 1 \ldots n\}$, where f_i is the degree of node i. The constraints of $CR(\varphi)$ are

$$\left[\begin{array}{c|c|c|c} I & -I & & \\ \hline I & & I & \\ \hline & I & & I \\ \hline F & & & \end{array}\right] \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] = \left[\begin{array}{c} \mathbf{0} \\ \hline \mathbf{e} \\ \hline \mathbf{e} \\ \hline \mathbf{d} \end{array}\right], \qquad \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] \geq 0, \tag{7}$$

where $F \in \mathbb{R}^{n\times n(n-1)}$ is the submatrix associated to $\sum_{1\leq j\leq n, j\neq i} x_{ij} = f_i, i = 1 \ldots n$. Although every column of F contains only a single $+1$, there is no way to transform the matrix

of (7) by elementary operations to satisfy Theorem 1. Indeed, the polytope associated to $CR(\varphi)$ has fractional extreme points.

However, if we only add the constraints associated to the degrees of two particular nodes—with optionally the constraint associated to the number of edges (density)—the resulting matrix is TU, as shown by next Proposition. The information we are conditioning in this case can be seen as a lower bound of the distance between the maximum and minimum degrees.

Proposition 4. *Let $i_1, i_2 \in V$ be two nodes with degrees f_{i_1} and f_{i_2}, $\widetilde{f}_{i_1}$ and $\widetilde{f}_{i_2}$ their degrees without considering the arcs (i_1, i_2) and (i_2, i_1), and d the total number of edges in the network. Let $J(k,h) = \{j : 1 \leq j \leq n, j \neq h, j \neq k\}$ and $\varphi = \{\mathbf{x} \in [0,1]^{n(n-1)} : x_{ij} - x_{ji} = 0, (i,j) \in H; \sum_{(i,j)\in H} x_{ij} = d; \sum_{j\in J(i_1,i_2)} x_{ij} = \widetilde{f}_i, i = i_1, i_2\}$. There is a bijection between the extreme points of the polyhedron φ and the space of all simple graphs with n nodes, d edges and degree range greater than or equal to $|f_{i_1} - f_{i_2}|$. This same result holds if the density constraint $\sum_{(i,j)\in H} x_{ij} = d$ is removed from φ.*

Proof. First, we note that if a network satisfies $\sum_{j\in H(i_1,i_2)} x_{ij} = \widetilde{f}_i, i = i_1, i_2$ and $x_{ij} = x_{ji}$ $(i,j) \in H$ then $|f_{i_1} - f_{i_2}| = |\sum_{1\leq j\leq n, j\neq i_1} x_{i_1,j} - \sum_{1\leq j\leq n, j\neq i_2} x_{i_2,j}| = |\sum_{j\in J(i_1,i_2)} x_{i_1,j} + x_{i_1,i_2} - \sum_{j\in J(i_1,i_2)} x_{i_2,j} - x_{i_2,i_1}| = |\widetilde{f}_{i_1} - \widetilde{f}_{i_2}|$.

By adding to (2) the extra constraints $\sum_{(i,j)\in H} x_{ij} = d$, $\sum_{j\in J(i_1,i_2)} x_{ij} = \widetilde{f}_i, i = i_1, i_2$, the resulting system is

$$\left[\begin{array}{c|c|c|c} I & -I & & \\ \hline I & & I & \\ \hline & I & & I \\ \hline F & & & \end{array}\right] \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] = \left[\begin{array}{c} \mathbf{0} \\ \hline \mathbf{e} \\ \hline \mathbf{e} \\ \hline \mathbf{d} \end{array}\right], \qquad \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] \geq 0, \tag{8}$$

where $\mathbf{d} = [\widetilde{f}_{i_1}, \widetilde{f}_{i_2}, d]^T$, $\mathbf{x}$, $\mathbf{e}$ and $\mathbf{s}$ are as in (2), and $F \in \{0,1\}^{3\times n(n-1)}$ is associated to the degree equations of nodes i_1 and i_2 and the density constraint. Since the $+1$s of F are located in the positions associated to either x_{ij} or x_{ji} —not both, since the network is undirected—, and $x_{ij} = x_{ji}$, F may be rearranged such that the $+1$s only appear at positions x_{ij}, $j > i$. Therefore (8) can be rewritten as

$$\left[\begin{array}{c|c|c|c} I & -I & & \\ \hline I & & I & \\ \hline & I & & I \\ \hline F' & & & \end{array}\right] \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] = \left[\begin{array}{c} \mathbf{0} \\ \hline \mathbf{e} \\ \hline \mathbf{e} \\ \hline \mathbf{d} \end{array}\right], \qquad \left[\begin{array}{c} \mathbf{x} \\ \hline \mathbf{s} \end{array}\right] \geq 0, \tag{9}$$

where

$$F' = \left[\begin{array}{c} \mathbf{w}^T_{(i_1,i_2)} \\ \mathbf{w}^T_{(i_2,i_1)} \\ \mathbf{e}^T \end{array}\right] \tag{10}$$

and $\mathbf{w}^T_{(i,k)} \in \mathbb{R}^{n(n-1)/2}$ is a vector derived from the degree equation of node i, with $+1$s in the positions associated to $x_{ij}, j > i, j \neq k$ and zeros elsewhere. Since the intersection of columns with $+1s$ in $\mathbf{w}^T_{(i_1,i_2)}$ and $\mathbf{w}^T_{(i_2,i_1)}$ is empty, by subtracting the first and second rows of F' to its third row, we obtain a matrix F'' with only a single $+1$ at each column. Subtracting the second row-block of (9) to its first row-block we get

$$\left[\begin{array}{c|c|c|c} & -I & -I & \\ \hline I & & I & \\ \hline & I & & I \\ \hline F'' & & & \end{array}\right] \begin{array}{l} \mathcal{J}_1 \\ \mathcal{J}_1 \\ \mathcal{J}_1 \\ \mathcal{J}_2. \end{array} \tag{11}$$

The row partition shown in (11) satisfies Theorem 1, thus it is TU and every extreme point is associated to a valid graph. In addition, no integer point may be located in the interior of φ since it is a subset of the unit hypercube, completing the proof.

If the density constraint is removed from φ, the same proof is valid by noting that F' only contains the first two rows in (10), and thus (11)—replacing F'' by F'—with the same row partitioning also satisfies Theorem 1.

□

2.4. Directed networks conditioned to the dyad count

Holland and Leinhardt [14] initiated the study and application of uniform models for directed networks constrained to the dyad count, i.e., the numbers of mutual, asymmetric, and null dyads. Denoting by f^M and f^N the number of, respectively, mutual and null dyads, and considering (i) binary variables $x_{ij}, x_{ji},\ (i,j) \in H$ associated to the $n(n-1)$ non-diagonal components of the AM, and (ii) binary variables y_{ij}^M and $y_{ij}^N,\ (i,j) \in H$—which are 1 if nodes i and j are, respectively, a mutual or null dyad, and 0 otherwise—, this problem can be formulated as

$$x_{ij} \geq y_{ij}^M \quad (i,j) \in H \tag{12a}$$
$$x_{ji} \geq y_{ij}^M \quad (i,j) \in H \tag{12b}$$
$$y_{ij}^M \geq x_{ij} + x_{ji} - 1 \quad (i,j) \in H \tag{12c}$$
$$1 - x_{ij} \geq y_{ij}^N \quad (i,j) \in H \tag{12d}$$
$$1 - x_{ji} \geq y_{ij}^N \quad (i,j) \in H \tag{12e}$$
$$y_{ij}^N \geq 1 - (x_{ij} + x_{ji}) \quad (i,j) \in H \tag{12f}$$
$$\sum_{(i,j)\in H} y_{ij}^M = f^M \tag{12g}$$
$$\sum_{(i,j)\in H} y_{ij}^N = f^N \tag{12h}$$
$$x_{ij}, x_{ji}, y_{ij}^M, y_{ij}^N \in \{0,1\} \quad (i,j) \in H. \tag{12i}$$

From (12c), $y_{ij}^M = 0$ implies that x_{ij} and x_{ji} cannot be both equal to 1, whereas $y_{ij}^M = 1$ implies that both x_{ij} and x_{ji} must be equal to 1 (constraints (12a)–(12b)). Similarly, when $y_{ij}^N = 0$ one has that x_{ij} and x_{ji} cannot be both equal to 0 (constraint (12f)), whereas, when $y_{ij}^N = 1$, both x_{ij} and x_{ji} must be equal to 0 (constraints (12d)–(12e)). Thus, (12g) and (12h) force the number of mutual dyads and null dyads to be f^M and f^N, respectively. Consequently, $n(n-1)/2 - \sum_{(i,j)\in H}(y_{ij}^M + y_{ij}^N)$ represents the number of asymmetric dyads. Next proposition shows the constraints matrix of the linear relaxation of (12) is TU.

Proposition 5. *Let φ be the polytope associated to the continuous relaxation of (12). The constraints matrix associated to this polytope is TU, and then there exists a bijection between the space of digraphs conditioned to the dyad counts and the set of extreme points of φ.*

Proof. By adding slacks, the constraints matrix of the linear relaxation of (12) in standard

form can be recast as

$$
\begin{array}{l}
\text{(12a)}\\ \text{(12b)}\\ \text{(12c)}\\ \text{(12d)}\\ \text{(12e)}\\ \text{(12f)}\\ - - -\\ - - -\\ - - -\\ - - -\\ \text{(12g)}\\ \text{(12h)}
\end{array}
\left[\begin{array}{cccccccccccccc}
I & & -I & -I & & & & & & & & & & \\
 & I & -I & & -I & & & & & & & & & \\
I & I & -I & & & I & & & & & & & & \\
I & & & & & & I & I & & & & & & \\
 & I & & & & & I & & I & & & & & \\
I & I & & & & & I & & & -I & & & & \\
I & & & & & & & & & & I & & & \\
 & I & & & & & & & & & & I & & \\
 & & I & & & & & & & & & & I & \\
 & & & & & & I & & & & & & & I \\
 & & \mathbf{e}^T & & & & & & & & & & & \\
 & & & & & & \mathbf{e}^T & & & & & & &
\end{array}\right]
\left[\begin{array}{c}
\mathbf{x}\\ \hline \mathbf{y}^M\\ \hline \mathbf{s}^{M1}\\ \hline \mathbf{s}^{M2}\\ \hline \mathbf{s}^{M3}\\ \hline \mathbf{y}^N\\ \hline \mathbf{s}^{N1}\\ \hline \mathbf{s}^{N2}\\ \hline \mathbf{s}^{N3}\\ \hline \mathbf{u}^x\\ \hline \mathbf{u}^M\\ \hline \mathbf{u}^N
\end{array}\right]
=
\left[\begin{array}{c}
0\\ \hline 0\\ \hline \mathbf{e}\\ \hline \mathbf{e}\\ \hline \mathbf{e}\\ \hline \mathbf{e}\\ \hline \mathbf{e}\\ \hline \mathbf{e}\\ \hline \mathbf{e}\\ \hline \mathbf{e}\\ \hline f^M\\ f^N
\end{array}\right] \tag{13}
$$

$$
\mathbf{x}, \mathbf{y}^M, \mathbf{s}^{M1}, \mathbf{s}^{M2}, \mathbf{s}^{M3}, \mathbf{y}^N, \mathbf{s}^{N1}, \mathbf{s}^{N2}, \mathbf{s}^{N3}, \mathbf{u}^x, \mathbf{u}^M, \mathbf{u}^N \geq 0, \tag{14}
$$

where $\mathbf{x}$, $\mathbf{u}^x \in \mathbb{R}^{n(n-1)}$ and $\mathbf{y}^M$, $\mathbf{s}^{M1}$, $\mathbf{s}^{M2}$, $\mathbf{s}^{M3}$, $\mathbf{y}^N$, $\mathbf{s}^{N1}$, $\mathbf{s}^{N2}$, $\mathbf{s}^{N3}$, $\mathbf{u}^M$, $\mathbf{u}^N \in \mathbb{R}^{n(n-1)/2}$.

Let C_i and R_j be respectively the i-th column-block (a $(5n(n-1)+2) \times (n(n-1)/2)$ matrix) and j-th row-block (a $(n(n-1)/2) \times (7n(n-1))$ matrix, for $j \leq 10$) of (13). By performing the following elementary operations: $C_3 := C_3 - C_4 - C_5 + C_6$, $C_7 := C_7 - C_8 - C_9 + C_{10}$ and $R_3 := R_3 - R_2 - R_1$, $R_6 := R_6 - R_4 - R_5$, $R_1 := R_1 - R_7$, $R_2 := R_2 - R_8$, the resulting matrix is.

$$
\left[\begin{array}{cccccccccccccc}
 & & & -I & & & & & & & -I & & & \\
 & & & & -I & & & & & & & -I & & \\
 & & & I & I & I & & & & & & & & \\
I & & & & & & & I & & & & & & \\
 & I & & & & & & & I & & & & & \\
 & & & & & & & -I & -I & -I & & & & \\
I & & & & & & & & & & I & & & \\
 & I & & & & & & & & & & I & & \\
 & & I & & & & & & & & & & I & \\
 & & & & & & I & & & & & & & I \\
 & & \mathbf{e}^T & & & & & & & & & & & \\
 & & & & & & \mathbf{e}^T & & & & & & &
\end{array}\right]
\begin{array}{c}
\mathcal{J}_1\\ \mathcal{J}_1\\ \mathcal{J}_1\\ \mathcal{J}_2\\ \mathcal{J}_2\\ \mathcal{J}_2\\ \mathcal{J}_1\\ \mathcal{J}_1\\ \mathcal{J}_1\\ \mathcal{J}_1\\ \mathcal{J}_2\\ \mathcal{J}_2
\end{array} \tag{15}
$$

By Theorem 1 and the row partition $\mathcal{J}_1$ and $\mathcal{J}_2$ shown in (15), the constraints matrix of (13) is TU. In addition, no integer point may be located in the interior of φ since it is a subset of the unit hypercube, completing the proof. □

2.5. Conditional edge-colored networks

The study of edge-colored graphs has given rise to important developments during the last few decades. From the point of view of applicability, problems arising in molecular biology are often modeled using edge-colored graphs [20], and the problem of interpersonal ties in social networks might be also modeled considering different types of arcs [12].

Let $\mathcal{C}$ be a given set of colors, $|\mathcal{C}| \geq 2$. Formally, an edge-colored graph is a tuple $G_{\mathcal{C}} = (V, E, \tau)$, where V and E are the sets of nodes and edges, respectively, and $\tau : E \longrightarrow \mathcal{C}$

a function assigning a color to each edge. They are, in some sense, related to multicommodity networks. Edge-colored graphs can be modeled as

$$\begin{array}{ll} \sum_{c=1}^{|\mathcal{C}|} x_{ij}^c \leq 1 & (i,j) \in H \\ x_{ij}^c, x_{ji}^c \in \{0,1\} & (i,j) \in H, c = 1, \ldots, |\mathcal{C}| \end{array} \tag{16}$$

where x_{ij}^c is 1 if an arc with color c from node i to node j exists, and 0 otherwise, and H was defined in (1). If the graph is forced to be symmetric, the set of constraints $x_{ij}^c = x_{ji}^c,\ (i,j) \in H, c = 1, \ldots, |\mathcal{C}|$, must be added. In the case of edge-colored networks conditioned to having f_c edges per color c, the constraints $\sum_{(i,j)\in H} x_{ij}^c = f_c,\ c = 1, \ldots, |\mathcal{C}|$ should be included.

The first set of constraints of (16)—multicommodity or generalized upper bounding constraints—complicate the structure of the constraints matrix for some structural properties, such as the total number of edges, the number of edges per color, and the lower bound of the degree range. Proving the total unimodularity of the resulting matrices for some of these cases is part of the further work to be done.

2.6. Other families of networks associated to extreme points of polytopes

Based on the reasoning used in the previous subsections, one can prove the constraints associated to the following families of networks are TU:

1. undirected networks conditioned to the within group densities and the lower bound of the degree range;
2. undirected networks conditioned to the between group densities and the lower bound of the degree range;
3. directed networks conditioned to the in-&-out-degrees;
4. directed networks conditioned to the within & between group densities and to the in-&-out-degrees;
5. directed networks conditioned to the within group densities and in-&-out-degrees;
6. directed networks conditioned to the between group densities and in&out-degrees;
7. undirected networks constrained to the within group densities;
8. undirected networks constrained to the between group densities;
9. directed networks constrained to the within and between group densities;
10. directed networks constrained to the within group densities;
11. directed networks constrained to the between group densities;
12. undirected networks constrained to the within group densities and the density;
13. undirected networks constrained to the between group densities and the density;
14. directed networks constrained to the within group densities and the density;
15. directed networks constrained to the between group densities and the density.

3. Procedures for the generation of random networks

The previous section provided an algebraic characterization of a vast amount of families of networks by linear constraints. From a constructive point of view, this section proposes LP-based polynomial-time methods to generate instances of networks with given structural properties.

3.1. Generating random networks by Linear Programming

Let $\varphi = \{\mathbf{x} \in [0,1]^{n'} : A\mathbf{x} = \mathbf{b}\}$ be a polytope whose set of extreme points is bijectively related to a given family of networks, where $A \in \mathbb{R}^{m' \times n'}$, $\mathbf{b} \in \mathbb{R}^{m'}$. Given a $\mathbf{c} \in \mathbb{R}^{n'}$, by the Fundamental Theorem of Linear Programming, there exists a network $\mathbf{x}$ such that $\mathbf{x} \in \arg\min_{\mathbf{y}} \mathbf{c}^T\mathbf{y}$, s.to $\mathbf{y} \in \varphi$. Therefore, if $\mathbf{c}$ is a properly defined random vector, the probability distribution of a simple graph can be derived from the transformation associating to a given $\mathbf{c} \in \mathbb{R}^{n'}$ the set $\{\mathbf{x} \in \varphi : \mathbf{x} \in \arg\min_{\mathbf{y}} \mathbf{c}^T\mathbf{y}\}$. To specify this transformation, let us introduce the parameterized function $\mathbf{G}_{[\mathbf{c},\mathbf{x}]} : \mathbb{R}^{m'} \times \mathbb{R}^{2n'}_{+\cup\{0\}} \longrightarrow \mathbb{R}^{3n'}$,

$$\mathbf{G}_{[\mathbf{c},\mathbf{x}]}(\mathbf{y},\mathbf{z},\mathbf{w}) = \begin{bmatrix} A^T\mathbf{y} + \mathbf{z} - \mathbf{w} - \mathbf{c} \\ XZ\mathbf{e} \\ (I - X)W\mathbf{e} \end{bmatrix}, \tag{17}$$

associated with the KKT conditions of the optimization problem, where $\mathbf{x} \in \varphi$ are the primal variables and $(\mathbf{y}^T, \mathbf{z}^T, \mathbf{w}^T) \in \mathbb{R}^{m'} \times \mathbb{R}^{2n'}_{+\cup\{0\}}$ are the Lagrange multipliers for the equations $A\mathbf{x} = \mathbf{b}$, $\mathbf{x} \geq 0$ and $\mathbf{x} \leq 1$, respectively. The KKT optimality conditions ensure that a given $\mathbf{x}_0 \in \varphi$ minimizes $\mathbf{c}^T\mathbf{x}$ if $\exists\,(\mathbf{y}^T, \mathbf{z}^T, \mathbf{w}^T)$ such that $\mathbf{G}_{[\mathbf{c},\mathbf{x}_0]}(\mathbf{y},\mathbf{z},\mathbf{w}) = \mathbf{0}$. The probability of a given network $\mathbf{x}_0$ (represented by the vector of AM components) is thus defined as

$$P(\mathbf{x}_0) = \int_{\Omega} P(\mathbf{c})d\mathbf{c}, \tag{18}$$

where $\Omega = \{\mathbf{c} \in \mathbb{R}^{n'} : \exists\,\mathbf{y}, \mathbf{z} \geq 0, \mathbf{w} \geq 0 \text{ such that } \mathbf{G}_{[\mathbf{c},\mathbf{x}_0]}(\mathbf{y},\mathbf{z},\mathbf{w}) = \mathbf{0}\}$, so that the integral is taken over all $\mathbf{c}$ for which $\mathbf{x}_0$ is optimal. The notation $P(\mathbf{x}|\mathbf{x} \in \chi)$ is used to refer to the probability of a network $\mathbf{x}$, conditioned to the fact that it belongs to the family χ. Clearly, if each network is an optimal solution of a LP with randomly generated objective function, we cannot state that $P(\mathbf{x}|\mathbf{x} \in \chi)$ is uniform for all $\mathbf{x} \in \chi$, as $P(\mathbf{x}|\mathbf{x} \in \chi)$ depends on the geometry of the associated polytope. It seems in any case reasonable to assume that $P(\mathbf{x}|\mathbf{x} \in \chi)$ does not depend on any structural property of the network, except for the ones defining the family χ.

3.2. The constraints matrix structure of the LPs

The amount of computation required to solve a LP is related to its constraints structure, apart from its size. Specialized versions of the simplex method, interior point methods and decomposition techniques have been proposed to face several different structures [4, 8]. It can be shown that, under a proper row and column permutation, all LPs associated to the families of networks of Section 2 can be reformulated as a primal block-angular problem of the form

$$\min \quad \sum_{h=0}^{k} (c^h)^T x^h \tag{19a}$$

$$\text{subject to} \quad \begin{bmatrix} N_1 & & & & \\ & N_2 & & & \\ & & \ddots & & \\ & & & N_k & \\ L_1 & L_2 & \dots & L_k & I \end{bmatrix} \begin{bmatrix} x^1 \\ x^2 \\ \vdots \\ x^k \\ x^0 \end{bmatrix} = \begin{bmatrix} b^1 \\ b^2 \\ \vdots \\ b^k \\ b^0 \end{bmatrix} \tag{19b}$$

$$0 \leq x^h \leq u^h \quad h = 0, \dots, k. \tag{19c}$$

Matrices $N_h \in \mathbb{R}^{m_h \times n_h}$ and $L_h \in \mathbb{R}^{l \times n_h}$, $h = 1, \dots, k$, respectively define the block-diagonal and linking constraints, k being the number of blocks. Vectors $x^h \in \mathbb{R}^{n_h}, h = 1, \dots, k$,

are the variables for each block. $x^0 \in \mathbb{R}^l$ are the slacks of the linking constraints. $b^h \in \mathbb{R}^{m_h}, h = 1, \ldots, k$, is the right-hand side vector for each block of constraints, whereas $b^0 \in \mathbb{R}^l$ is for the linking constraints. The upper bounds for each group of variables are defined by $u^h, h = 0, \ldots, k$; in our problems $u^h = \mathbf{e}$, i.e., a vector of ones.

The specialized interior point method of [5, 6] is an efficient procedure for the solution of (19). Briefly, it requires the solution at each interior point iteration of the system

$$
\begin{aligned}
A\Theta A^T \Delta_y &= \left[\begin{array}{ccc|c} N_1\Theta_1 N_1^T & & & N_1\Theta_1 L_1^T \\ & \ddots & & \vdots \\ & & N_k\Theta_k N_k^T & N_k\Theta_k L_k^T \\ \hline L_1\Theta_1 N_1^T & \ldots & L_k\Theta_k N_k^T & \Theta_0 + \sum_{h=1}^k L_h\Theta_h L_h^T \end{array}\right] \Delta_y \\
&= \left[\begin{array}{cc} B & C \\ C^T & D \end{array}\right] \left[\begin{array}{c} \Delta_{y_1} \\ \Delta_{y_2} \end{array}\right] = g,
\end{aligned}
\tag{20}
$$

where Δ_y is the direction of movement for the dual variables, $\Theta_h = ((I - X_h)^{-1} W_h + X_h^{-1} Z_h)^{-1}$ $h = 0, \ldots, k$, are diagonal matrices, and g is some right-hand side. By eliminating Δ_{y_1} from the first group of equations of (20), we obtain

$$
(D - C^T B^{-1} C)\Delta_{y_2} = g_1 \tag{21a}
$$

$$
B\Delta_{y_1} = g_2, \tag{21b}
$$

for a proper partition of the right-hand side into g_1 and g_2. Systems involving B are solved by k Cholesky factorizations. The system (21a)—of dimension l, the number of linking constraints—is solved by a preconditioned conjugate gradient. In [4] a very efficient preconditioner was introduced for multicommodity flows (a type of block-angular problems), which was later extended to general primal block-angular problems [5, 6].

In our particular problems, matrices N_h $h = 1, \ldots, k$, are shown to be row vectors, and then B is diagonal. For instance, for problems associated to undirected networks, whose decision variables are the out-diagonal components of the AM, the number of blocks is $k = n(n-1)/2$, and matrices $N_h \in \mathbb{R}^{1\times 2}$ and $\Theta_h \in \mathbb{R}^{2\times 2}$, $h = 1, \ldots, k$, associated to arcs x_{ij} and x_{ji}, are

$$
N_h = [1 \; -1] \qquad \Theta_h = \left[\begin{array}{cc} \dfrac{x_{ij}(1-x_{ij})}{x_{ij}w_{ij} + (1-x_{ij})z_{ij}} & \\ & \dfrac{x_{ji}(1-x_{ji})}{x_{ji}w_{ji} + (1-x_{ji})z_{ji}} \end{array}\right], \tag{22}
$$

such that

$$
B = \left[\begin{array}{ccc} \mathrm{Tr}(\Theta_1) & & \\ & \ddots & \\ & & \mathrm{Tr}(\Theta_k) \end{array}\right], \tag{23}
$$

where $\mathrm{Tr}(M)$ denotes the trace of matrix M. Systems involving (23) are directly solvable.

Note that, despite the suitable matrix structure, the underlying amount of operations can still be high, as the generation of networks requires the solution of a large number of independent LPs. Such an amount of computation might however be significantly reduced if we allow the computation of related extreme points. Two particular procedures are presented in next two subsections.

Algorithm 1 r-blocks

Let $k = 0$, $\mathbf{x}^0$ be an initial extreme point;
repeat
  Randomly select $i \in \{1, \ldots, r\}$ and $\mathbf{c} \in \mathbb{R}^{n'-t_i}$;
  Let $\mathbf{x}^k_{F_i}$ and $\mathbf{x}^k_{C_i}$ be the vectors of fixed and changing components respectively;
  Let $A^k_{F_i}$ and $A^k_{C_i}$ be the associated coefficient matrices;
  Solve (24) and let $\mathbf{y}^*$ be its optimal solution;
  $\mathbf{x}^{k+1}_{C_i} = \mathbf{y}^*$, $\mathbf{x}^{k+1}_{F_i} = \mathbf{x}^k_{F_i}$;
  $k := k + 1$;
until $k \geq \bar{k}$

3.3. Sequential r-blocks algorithm

Let χ be one of the families of networks associated to extreme points of polytopes of the form $\varphi = \{\mathbf{x} \in [0,1]^{n'} : A\mathbf{x} = \mathbf{b}\}$, $A \in \mathbb{R}^{m' \times n'}$. As we noted in Subsection 3.1, given a $\mathbf{c} \in \mathbb{R}^{n'}$, we can compute a network by solving $\min_{\mathbf{y}} \mathbf{c}^T\mathbf{y}$, s.to $\mathbf{y} \in \varphi$. Similarly, if we have a given extreme point $\mathbf{x}_0$ of φ, we might obtain another extreme point $\mathbf{x}_1$ of φ, by fixing $t < n'$ variables and optimizing, with a given objective cost vector $\mathbf{c} \in \mathbb{R}^{n'-t}$, the remaining $n' - t$ variables.

Formally, if we partition the set of variables in r blocks of dimensions t_i, $i = 1, \ldots, r$, $\sum_{i=1}^{r} t_i = n'$, and denote by $\mathbf{x}_{F_i} \in \mathbb{R}^{t_i}$ and $\mathbf{x}_{C_i} \in \mathbb{R}^{n'-t_i}$ the fixed and *changing* components of $\mathbf{x}$ associated to block i, and by A_{F_i} and A_{C_i} the submatrices of A associated to $\mathbf{x}_{F_i}$ and $\mathbf{x}_{C_i}$, the new extreme point is obtained by solving

$$\begin{array}{ll} \min & \mathbf{c}^T\mathbf{y} \\ \text{s.to} & \\ & A_{C_i}\mathbf{y} = \mathbf{b} - A_{F_i}\mathbf{x}_{F_i} \\ & \mathbf{0} \leq \mathbf{y} \leq \mathbf{1} \end{array} \tag{24}$$

for some random vector $\mathbf{c} \in \mathbb{R}^{n'-t_i}$ and $i \in \{1, \ldots, r\}$. Algorithm 1 shows how to obtain $\bar{k}$ random networks by iteratively applying this procedure.

3.4. Sequential s-pivots algorithm

Considering again the polytopes $\varphi = \{\mathbf{x} \in [0,1]^{n'} : A\mathbf{x} = \mathbf{b}\}$, where $A \in \mathbb{R}^{m' \times n'}$, $m' < n'$, we know from LP that there is an equivalence between extreme points and basic solutions, which can be written as $\mathbf{x}^T = [\mathbf{x}_B^T, \mathbf{x}_N^T]$, $\mathbf{x}_B \in \mathbb{R}^{m'}$, $\mathbf{x}_N \in \mathbb{R}^{n'-m'}$, $A = [B\ N]$, $B \in \mathbb{R}^{m' \times m'}$, $N \in \mathbb{R}^{m' \times (n'-m')}$, for a suitable permutation of the variables. Since the extreme points of φ have been proved to be all integer, it turns out that all basic variables must be at their limits (either at 0 or 1), as well as the non-basic variables. The basic solutions are thus fully degenerate.

Denoting by e_q the q-th column vector of the identity matrix, and by B_k and N_k the basic and nonbasic submatrices of A, given a basic solution $\mathbf{x}^k$ we can obtain another one by moving along the simplex-like direction

$$\Delta_k(q) = \begin{bmatrix} -B_k^{-1}N_k e_q \\ e_q \end{bmatrix}. \tag{25}$$

If the nonbasic variable q is 0, then the iteration performed is $\mathbf{x}^{k+1} = \mathbf{x}^k + \lambda\Delta_k(q)$, for some non-negative step-length λ. On the other hand if $\mathbf{x}^k_{N_q} = 1$ then we apply $\mathbf{x}^{k+1} = \mathbf{x}^k - \lambda\Delta_k(q)$.

Algorithm 2 s-pivots

Let $\mathbf{x}^0$ be an extreme point computed with some initial cost vector $\mathbf{c}$; $k = 0$;
repeat
  if $((k+1) \bmod s) > 0$ **then**
    repeat
      Randomly select $q \in \{1, \ldots, n' - m'\}$;
      Compute step-length $\lambda \in \{0, 1\}$ associated with $\pm\Delta_k(q)$;
    until $\lambda \neq 0$
    Compute $\mathbf{x}^{k+1} = \mathbf{x}^k \pm \lambda\Delta_k(q)$ and update B_k and N_k;
    $k = k + 1$;
  else
    Generate cost vector $\mathbf{c} \in \mathbb{R}^{n'}$ and compute a new extreme point $\mathbf{x}^k$;
    $k = k + 1$;
  end if
until $k \geq \bar{k}$

It can be easily verified that in both cases $A\mathbf{x}^{k+1} = A\mathbf{x}^k = b$, i.e., the new point satisfies the linear constraints. In addition, since the constraints matrices of Section 2 are TU, the step-lengths λ—computed by a ratio test—are always either 0 or 1. It is thus possible to generate a new basic solution (i.e., a new random graph) by randomly selecting $q \in \{1, \ldots, n' - m'\}$ and computing $\mathbf{x}^{k+1} = \mathbf{x}^k \pm \lambda\Delta_k(q)$. A sample of $\bar{k}$ networks can be obtained by iteratively applying this procedure. Since the resulting sample may be claimed to be quite local, every s iterations we can jump to an independent extreme point of the polytope by generating some random cost vector, and solving the associated LP. A drawback of this procedure is that many iterations may be degenerate, i.e., $\lambda = 0$, so no new point is obtained. Algorithm 2 summarizes this procedure.

4. Computational analysis

This section provides numerical results comparing the efficiency of the r-blocks and s-pivots procedures, both in terms of CPU time and analysis of specified network features. The dataset used to carry out the analysis is a 62 nodes undirected graph, representing the social network of frequent associations between dolphins in a community living off Doubtful Sound, New Zealand [15, 16]. Animal social networks are substantially harder to study than networks of human beings because animals do not give interviews or fill out questionnaires, and network data must be gathered by direct observation of interactions between individuals. Nonetheless, it has recently been possible to determine behaviourally meaningful measures of association in a number of species. Early studies of animal social networks showed striking similarities to human networks [9].

The following subsections evaluate three particular aspects of the r-blocks and s-pivots procedures. The LPs have been solved using the specialized interior-point algorithm for block-angular problems of [5, 6], which happened to be much more efficient than state-of-the-art solvers in our application. The s-pivots procedure makes use of a Matlab implementation of the Simplex pivoting. The runs were carried out on a Fujitsu Primergy RX300 server with 3.33 GHz Intel Xeon X5680 CPUs (24 cores) and 144 GB of RAM, under a GNU/Linux operating system (Suse 11.4), without exploitation of multithreading capabilities.

4.1. Degeneracy in the s-pivots procedure

Graph conditioned to ...	bases	CPU time
total density	1220	16
within group densities	131	12
lower bound of the degrees range and density	1475	17

Table 1: Number of bases visited to compute 100 extreme points with the s-pivots method for the three specified polytopes

r	mean CC	std. CC	mean AC	std. AC	CPU
10	0.0940859	0.03345999	-0.0238137	0.06698295	19
20	0.0920425	0.02761306	-0.0365208	0.08673276	65
40	0.0829533	0.02535695	-0.0280215	0.07502490	138
80	0.0844383	0.02453850	-0.0467273	0.07477907	315
160	0.0821106	0.02053597	-0.0364258	0.07088100	756

Table 2: Numerical results using the r-blocks method for generating 1000 networks

Consider the binary and symmetric network of 62 dolphins introduced in the beginning of this section and the following families of networks:

1. undirected networks conditioned to the density;
2. undirected networks conditioned to the within and between group densities;
3. undirected networks conditioned to the lower bound of the degree sequence range and density.

These three models are specified by the observed parameters of the dolphin's social network. The within group densities are obtained from the community structure of the observed network, computed by the *walk trap* community search algorithm of [18]. Table 1 shows the number of basic solutions explored by the s-pivots procedure to generate 100 different networks, and the required CPU time. The results confirm the high degeneracy of the s-pivots procedure.

4.2. Utility and efficiency of r-blocks and s-pivots procedures

We consider the simple uniform random network conditioned to the density model, which allows comparing computationally obtained with available analytical results for many network features. In particular, we will focus on two network features: clustering coefficient (CC) and assortativity coefficient (AC). The CC of a network is the average CC of all the nodes, as a measure of how dense is the neighborhood of each node. The AC is the Pearson correlation coefficient of degree between pairs of linked nodes. Positive values of AC indicate a correlation between nodes of similar degree, while negative values indicate relationships between nodes of different degree.

Table 2 shows the sample mean and standard deviation of the CC and AC over 1000 networks obtained using the r-blocks method for different r values. Last column reports the CPU time in seconds. Likewise, Table 3 shows the same information for 1000 networks generated with the s-pivots methods, for different s values.

Theoretical results [3] state that the expected clustering coefficient of a uniform random network with n nodes conditioned to d edges is CC$= 2d/n^2$, which in our case is $2 \cdot 159/62^2 = 0.08272633$. This is approximately what we obtained by averaging over 1000 networks in

s	mean CC	std. CC	mean AC	std. AC	CPU
10	0.0829844	0.02659200	-0.0332546	0.06904464	1278
20	0.0916872	0.03159023	-0.0336965	0.06959257	788
40	0.0899651	0.03985421	-0.0409772	0.07413242	519
80	0.0979905	0.05035389	-0.0505990	0.06839814	386
160	0.1118884	0.06435935	-0.0546719	0.08368978	320

Table 3: Numerical results using the s-pivots method for generating 1000 networks

tables 2 and 3 for $r = 160$ and $s = 10$, respectively. It is worth remarking that this kind of simulations are normally divided into pre- and post-convergence periods, where the pre-convergence part, known as *burn-in*, is discarded and the post-convergence part is used for inference. The sample means in tables 2 and 3 have been calculated without discarding the burn-in period, so they may include some bias.

The local behaviour of the s-pivots procedure is observed from the autocorrelation functions of CC and AC (not plotted to save space) for the 1000 networks obtained in each of the runs of tables 2 and 3. We observed that the autocorrelations are close to 0 when s is small and r is large. In general, r-blocks outperforms s-pivots: it provides less autocorrelated networks with less computational effort. For instance, the sample of 1000 networks obtained with 80-blocks in 315 seconds has an autocorrelation similar to that of the sample obtained with 10-pivots in 1270 seconds.

As already mentioned, the study of uniform random networks conditioned to the density by the s-pivots or r-blocks methods are quite unreasonable, since plenty of theoretical results for this model are available [3]. However this simple model allowed us to validate our procedures. For more complicated models, as the one of next subsection, this LP-based network generation procedures are instrumental.

4.3. Application to models with non-TU constraints matrices

In [15, 16] it was shown that the social network of dolphins exhibits a remarkable level of community structure, i.e., dolphins can be easily grouped into (potentially overlapping) sets such that each set of nodes is densely connected internally. Characterizing those communities is in general a difficult task. We used two of the several algorithms for community finding, the walk trap community and the fast greedy community, as implemented in the `igraph` library of the `R` package. The first algorithm finds densely connected subgraphs by simulating random walks on the graph, which tend to stay inside communities. The second algorithm identifies (using the betweenness measure) edges in a network that lie between communities and then removes them, leaving behind just the communities themselves. Both algorithms found almost the same four communities.

Using the above four groups, the goal is to decide whether the CC and AC of our social network of dolphins is likely to have been randomly obtained from the distribution of undirected networks conditioned to the observed within-community-densities and degree nodes. As noted in Section 2 the constraints matrix of this model is not TU. However, we can still use the r-blocks procedure, discarding the fractional solutions found. We generated 10100 networks, removing the first 100 ones as burn-in period. A value $r = 250$ was used, which guarantees an uncorrelated sample.

The resulting empirical distribution of CC and AC is shown in the density plot of Figure 1. Table 4 shows the sample mean and standard deviation of the CC and AC over the 10000 generated networks, the observed values in the dolphins social network, and the associated

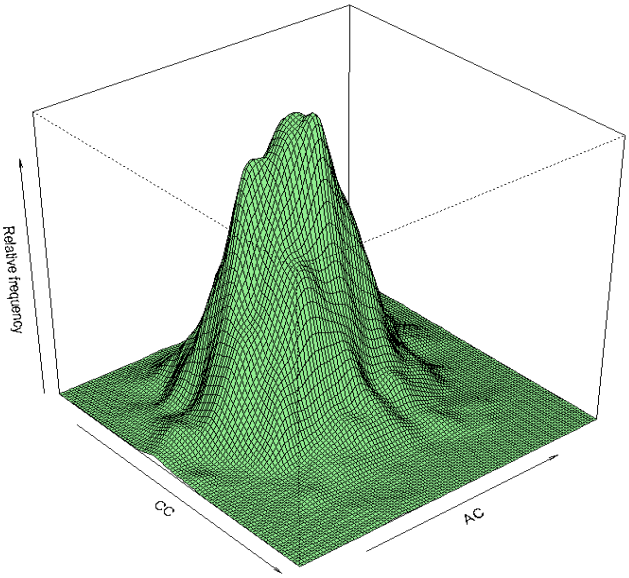

Figure 1: Empirical distribution of CC and AC obtained with the 250-blocks procedure

	sample mean	sample std.	observed value	one tail p-value
CC	0.199145	0.01949775	0.2901595	0.0112000
AC	-0.065980	0.07585131	-0.0436017	0.6941203
Fractional solutions:	335			

Table 4: Numerical results from the sample obtained with the 250-blocks method

p-values. From these p-values we conclude hat the CC cannot be explained by only using the information concerning the within-community-density and the degree nodes. On the other hand, the AC seems instead to be likely induced by the fixed structural properties we considered. The last row of Table 4 reports the number of fractional solutions obtained. In this case only a 3.3% of the solutions were fractional, making the r-blocks procedure still very efficient for this non-TU model.

5. Conclusions

The constraints matrices associated to several classes of random graph problems have shown to be TU. The resulting MILP problems are thus efficiently solved as LPs, by using specialized interior point algorithms for block-angular problems. Two particular procedures, r-blocks and s-pivots, are used to generate large samples of random graphs. Using a real-world dataset, it was shown that both methods produce the same results for different values of r and s. We also observed that the autocorrelation of network features decreases monotonically with r and increases monotonically with s, for the two respective methods. This work shows how mathematical programming tools can be efficiently used for the analysis of complex networks, and it opens the possibility for other applications in this field.

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