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Generation of networks with prescribed degree-dependent clustering

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Abstract We propose a systematic, rigorous mathematical optimization methodology for the construction, "on demand," of network structures that are guaranteed to possess a prescribed collective property: the degree-dependent clustering. The ability to generate such realizations of networks is important not only for creating artificial networks that can perform desired functions, but also to facilitate the study of networks as part of other algorithms. This problem exhibits large combinatorial complexity and is difficult to solve with off-the-shelf commercial optimization software. To that end, we also present a customized preprocessing algorithm that allows us to judiciously fix certain problem variables and, thus, significantly reduce computational times. Results from the application of the framework to data sets resulting from simulations of an acquaintance network formation model are presented.

Keywords Networks · Graph theory · Mathematical optimization · Clustering

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1 Introduction

Network science research (see [7]) has experienced significant growth in the last decade based on seminal work on random networks, scale-free networks and smallworld networks (see [1,14,37,38,51] and references therein). To a large extent, this was driven by novel technological applications, such as the Internet and modern epidemiology, as well as by national security demands; however, it was also because network science is an integral part of analyzing and engineering many complex systems. The structural properties of networks as diverse as food webs [52], cellular and metabolic networks [28], the Internet backbone [23], coauthorship and citation networks of scientists [35], and social networks [54] to name but a few, have been explored and compared. Measuring the performance and vulnerability [40] of networks, enhancing their capacity for accommodating information or material flow (e.g., [42]), as well as using them in representing massive data sets [9] have all been active research areas. Finally, the effect of network structure on the dynamics of interactions on the network has also been the subject of extensive work—from epidemiology (see, e.g., [11] for the effect of social network structure on epidemic thresholds, or [4] for the effect of population mobility processes in the spreading of infectious diseases), to economy and finance (see, e.g., [15] for how network structure affects the dynamics of employment, or [39] for the containment of a financial crisis) and to opinion formation, culture and language dynamics [3,46,50]. A fundamental question arises: "Why is network anatomy so important to characterize? Because structure always affects *function*" [45].

Elucidating the relationship between the structure of a complex network and its behavior and performance is the crucial first step in analyzing, understanding, designing and controlling many complex systems; and to do this, we *must* be able to construct realizations of networks that have prescribed collective properties. For example, in order to assess how a disease spreading model is affected by a characteristic property of the population, such as its assortativity, we need to create representative population sets for various assortativity levels and apply the model to these sets. In order to simulate a large-scale empirical network such as the Internet, we need to scale it down into some workable size and, for that, we need to construct a test-bed network that is small in size but possesses the relevant features of its larger counterpart. In order to investigate which properties affect the evolution of networks, or be able to computationally accelerate this evolution (e.g., through Coarse Projective Integration [29,30]), we need to have the ability to construct realizations of networks that adhere to prescriptions of some of their macroscopic characteristics.

Existing network generation techniques that give rise to networks with different statistical/structural properties include (but are not limited to): (i) the seminal Erdös–Rènyi model [21] of random graphs, (ii) the Watts–Strogatz model [51] with rewiring probability p, for which the resulting graph degree distribution is Poisson (random) for p=1, uniform (structured) for p=0 and power-law (scale-free) for intermediate values of p, (iii) the Barabási–Albert preferential attachment model [6] which creates networks with a power law degree distribution, (iv) Fu and Liao's [25] extension of the previous model where the probabilities are modified so as to obtain scale-free networks with a power law degree distribution in conjunction with upper bounded, tunable



clustering coefficient, and (v) the R-MAT recursive graph model [16], a procedural algorithm that creates directed graphs. The above techniques focus on the randomness of the results and their adherence to specific probability distributions. One also encounters several algorithms in the literature whose goal is precisely to impart prespecified properties to the graph generated. These include algorithms for (i) networks with given degree distribution (e.g., the Pairing or Configuration model [12,53], the probabilistic Chung–Lu algorithm [17] that creates a random graph with a given expected degree sequence, the deterministic Havel–Hakimi algorithm [26,27] which guarantees a simple graph if the given degree sequence is graphic, and the sequential importance sampling algorithm [8], shown to be amenable to the generation of uniformly distributed graphs with the given degree sequence), (ii) networks with specified degree–degree distribution for nearest neighbors [20], (iii) networks with specified degree distribution and level of clustering [5,31,36,49], and (iv) networks with specified (approximate) degree distribution and degree-dependent clustering [43].

While all these techniques and algorithms—some deterministic, some stochastic, some with convergence guarantees and some without—address several individual aspects of the Network Generation Problem, there is an obvious and important gap in our ability to systematically perform this task, and in hierarchically being able to prescribe several/different collective properties with explicit guarantees of achieving the prescriptions exactly or within bounded deviations. The aim of this paper is to address this gap by proposing a new methodology based on mathematical optimization that can be used to solve the Network Generation Problem with prespecified degree-dependent clustering (see Sect.3.1 for definition). The degree-dependent clustering is an important property of a network that elucidates its inherent hierarchical topology[41,47,48]. Therefore, capturing this property correctly during the derivation of network models is integral for the latter to exhibit dynamics that are consistent with empirical measurements.

In Sect. 2 we present the general outline of our approach and discuss its advantages, its limitations, and potential remedies for overcoming the latter. In Sect. 3 we present in detail the mathematical formulation and a customized preprocessing algorithm required for its efficient solution. Finally, in Sect. 4 we provide computational results for a collection of test data resulting from simulations of social network formation.

2 Proposed framework

Mathematical optimization has been successfully used in the past to solve many combinatorial problems. In the area of biological networks [13], it has been applied to identify critical nodes in protein–protein interaction networks [10] as well as motifs in DNA sequences [32,55]. In the context of Network Generation, mathematical optimization approaches offer a number of advantages when compared to traditional methods, as a number of additional goals may be pursued. For example, in addition to identifying a network that possesses an ensemble of desired properties, an optimization-based framework would be suitable to: (i) certify if no such network exists, (ii) identify multiple, or even all, non-isomorphic such networks, (iii) identify the network that is most similar—under a suitable metric—to a given network, (iv) identify the network



that minimizes/maximizes some objective, (v) determine the smallest size N_0 for a network to admit all properties, (vi) construct networks that approximately satisfy the properties within given tolerances.

A mathematical optimization framework is versatile enough to accommodate prescriptions that involve various types of network properties and characteristic features of networks. These include among others the degree distribution, global and average clustering coefficient, distribution of local clustering coefficients, absolute number of distinctive patterns, or "motifs," such as triplets, triangles, squares, stars, etc. It may be required that the above properties be imposed on a network individually, or in any suitable combination. They may also be collectively and independently imposed on subsets of nodes, called *classes*. An example of this concept is the requirement to impose degree-dependent clustering coefficients, that is, to identify a network where the total number of triangles involving nodes of a given degree (the *degree class*) is pre-specified.

In general, the Network Generation Problem calls for the identification of the connections (arcs) that need to exist between its N nodes. To that end, we define a collection of binary variables x_{ij} , i < j to indicate the existence or not of these connections:

$$x_{ij} = \begin{cases} 1 & : \text{ if arc } (i, j) \text{ exists in the solution} \\ 0 & : \text{ otherwise.} \end{cases}$$
 (1)

For computational tractability, the aim is to always express the problem as a Mixed-Integer Linear Problem (MILP) [24,34], that is, through a formulation of the general form (2–3).

$$\min_{x,x'} \alpha^T x + \beta^T x' \tag{2}$$

$$s.t. \ Ax + Bx' \le c \tag{3}$$

where x' is a generic set of auxiliary variables that could be either binary or continuous.

The two major challenges of the Network Generation Problem are its large combinatorial complexity and the potential isomorphism of the solutions. Both of these challenges make instances with even a small number of nodes to be intractable for off-the-shelf commercial optimization software. In order to address such challenges, the proposed mathematical optimization approach is based on efficient representation (modeling) of the problem and effective model reduction procedures.

Typically, we aim at formulating the various requirements of the prescription using few variables and involving expressions that have as tight LP-relaxations as possible. We also focus on modularity of the model, that is, we attempt to describe each property with a stand-alone set of equations that can be included—like a "building block"—in an overall formulation, whenever the property is part of the prescription. This allows us to easily move from one formulation to another, making heavy use of results at hand (e.g., use a network that satisfies property A to initialize the search process for a network that satisfies both properties A and B).

Furthermore, since most of the times one is interested in only feasible solutions (not necessarily optimal in terms of an objective function), we can reduce the combinatorial



search space by a priori postulating the existence of certain arcs as part of the solution, e.g., by postulating some sub-network as an unnegotiable part of the network under construction. In principle, this requires thoughtful analysis of the particular prescription at hand, as one needs to rank-order the set of possible network arcs in terms of their likelihood to participate in feasible solutions. However, if performed well, such a step would reduce the size of the MILP formulation and possibly bring the remaining problem—which can be of significantly smaller complexity than the original—within the capabilities of available optimization software. By providing the possibility to relax some of the postulated arcs in an iterative fashion, the overall scheme inherits the exactness of the approach and can still guarantee the identification of a solution, when one exists, in all cases.

3 Degree-dependent clustering

We begin by providing a few definitions:

Definition 1 The degree of a node equals the number of nodes with which it is connected.

Definition 2 Node A forms a triplet with nodes B and C if the connections (A, B) and (A, C) exist.

Definition 3 Node A forms a triangle with nodes B and C if the connections (A, B), (A, C) and (B, C) exist.

Definition 4 The local clustering coefficient of a node equals the number of triangles divided by the number of triplets it forms with other nodes.

Definition 5 A degree class is the collection of all nodes in a network that have the same degree.

3.1 Optimization formulation

Consider a set of N nodes and a prescription d_i , $i=1,2,\ldots,N$, for the degree sequence. We aim at constructing a network where each node i attains degree d_i . Let index q loop over all the degree classes thus defined. Degree-dependent clustering calls for imposing—in addition to the degree sequence—an allowable range on the number of triangles, $T_q \in [T_q^L, T_q^U]$, $\forall q$, that can be collectively formed by all nodes of degree class q. This is equivalent to imposing an allowable range on the average local clustering coefficient across all nodes of the same degree. The problem is formulated as a feasibility problem. Formulation (4-8) applies.

$$\min_{\substack{x_{ij} \in \{0,1\}\\0 \le tr_{ijk} \le 1\\sd_i^+, sd_i^-, st_q^+, st_q^- \ge 0}} \sum_{i} (sd_i^+ + sd_i^-) + \sum_{q} (st_q^+ + st_q^-)$$
(4)



$$s.t. \sum_{i>i} x_{ij} + \sum_{i$$

$$\sum_{i \in q} \left\{ \sum_{j>i} \sum_{k>j} tr_{ijk} + \sum_{j>i} \sum_{kj}} tr_{jki} \right\} \ge T_d^L - st_q^- \quad \forall q \qquad (6)$$

$$\sum_{i \in q} \left\{ \sum_{j>i} \sum_{k>j} tr_{ijk} + \sum_{j>i} \sum_{kj}} tr_{jki} \right\} \le T_d^U + st_q^+ \quad \forall q \qquad (7)$$

$$tr_{ijk} \le x_{ij} \; ; \; tr_{ijk} \le x_{jk} \; ; \; tr_{ijk} \le x_{ik} \\ tr_{ijk} \ge x_{ij} + x_{jk} + x_{ik} - 2 \end{cases} \; \forall i < j < k$$
 (8)

In addition to the binary variables x_{ij} introduced in (1), the formulation uses two sets of non-negative slack variables, sd_i^+ and sd_i^- , to express the deviation of node i's actual degree $(\sum_{j>i} x_{ij} + \sum_{j<i} x_{ji})$ from the prescribed degree d_i (Eq. 5). Two additional sets of slack variables, st_q^+ and st_q^- , are used to penalize the deviation from the prescribed bounds of the number of triangles formed by the members of each degree class (Eqs. 6,7). We also use continuous variables $tr_{ijk} \in [0, 1]$, $\forall i < j < k$, to denote the existence or not of a triangle between nodes i, j and k. We define these through products of variables, $tr_{ijk} = x_{ij}x_{jk}x_{ik}$, and use their convex/concave envelopes [33,2] in the formulation (Eq. 8). Since at optimality the x_{ij} variables attain only binary values, the envelopes are exact representations of the products. The objective (Eq. 4) calls for minimizing the sum of all slack variables so as to reduce the total deviation of the solution from the prescription.

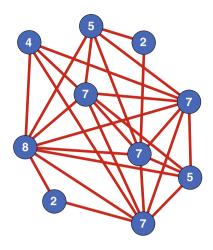
Note that if the optimal objective value of this formulation is $z^* > 0$, then the desired prescription is not attainable; this could be the result of the degree sequence being not $graphic^1$ or the triangle requirement being too restrictive. However, if the prescription is indeed attainable, the above formulation ought to have an optimal solution $z^* = 0$ and will yield at optimality a solution set of arcs x_{ij} that correspond to a network with the desired properties.

Note that a given prescription often admits multiple $z^*=0$ solutions and this is true even for very small problem sizes (e.g., the 10-node instance of Ex. 1). It should be noted, though, that not all of the solutions will be truly unique solutions. This is due to the inherent isomorphism of the problem; the indices of two or more nodes in the same degree class can be interchanged without changing the structure of the network. Typically, two remedies can be applied: (i) differentiation between the nodes in each degree class by adding a few explicit constraints that relate to a property beyond the degree or (ii) designation of some solution features as "nominal" and dynamic rejection during branch-and-cut of other symmetric solutions that do not possess those features.

¹ In the case of degree sequence it is easy to infer a priori, through application of the "Handshake Theorem" and the "Erdös–Gallai Criterion" [22,44], whether the prescription will be graphic or not. However, this is not the case when additional requirements, beyond the degree sequence are imposed.



Fig. 1 Representative solution for a network that satisfies the prescription of Example 1. The node labels correspond to their degree



Example 1 Let N=10 nodes, and let $d_i=\{2,2,4,5,5,7,7,7,7,8\}$ be a prescription for the degree sequence. The set of degree classes is then $q=\{2,4,5,7,8\}$. Let also $T_q^L=\{0,2,4,20,6\}$ and $T_q^U=\{2,6,20,84,26\}$ be a prescription in regards to the allowable intervals for the cumulative number of triangles of each class. Despite the small size of this problem, there exist 72 different (that is, non-isomorphic) solutions. Fig. 1 illustratively depicts one of them.

3.2 Preprocessing algorithm

Overall, the degree-dependent clustering formulation cannot be addressed efficiently with uncustomized commercial MILP software. For reference, we attempted to solve for multiple test prescriptions and for network sizes of as low as 20 nodes. CPLEX v11.0 [18] with various parameter configurations² had not been able to attain a feasible solution after 10 hours.³ In order to address this limitation, we need to somehow reduce the combinatorial complexity of the problem and, to that end, we have developed a customized preprocessing algorithm. The basic idea behind this algorithm is to rank-order the set of possible network arcs in terms of their likelihood to participate in feasible solutions, and enforce the existence of the most likely arcs as part of the solution (through fixing the corresponding variables x_{ij}).

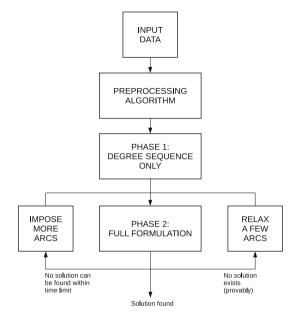
The preprocessing algorithm works in an iterative greedy fashion. At each step, we select—out of the pool of non-fixed arcs—the one that appears at the given moment to be the most attractive to be appended to the set of fixed arcs, that is, the one that (i) addresses the triangle prescription the most, i.e., forms new triangles that involve the degree-classes q that deviate the most from their upper allowable limit, T_q^U , and at the

³ All computational experiments in this paper were performed on an Intel Core2 Quad 2.83 GHz (single-processor runs).



 $^{^2}$ We attempted various options in regards to upper bounding heuristics, LP solver, search emphasis, and application of cuts.

Fig. 2 High-level algorithm flowsheet for solving the Network Generation Problem with prescribed degree-dependent clustering



same time (ii) does not over-constrain the remaining problem, rendering it infeasible. Such a preprocessing step can significantly reduce the combinatorial complexity of the problem and, as presented later in Sect. 4, allow us to address instances with 100 nodes in as little as a few seconds.

After the preprocessing step has been applied and a possible model reduction has occured, the overall algorithm for the Network Generation Problem with degree-dependent clustering prescriptions proceeds through a number of phases, as depicted in Fig. 2. The first phase corresponds to imposing the degree sequence prescription by itself, that is, minimizing the sum of degree slack variables, $\sum_i (sd_i^+ + sd_i^-)$, subject only to Eq. (5). Due to the near-total-unimodularity of this problem, solving it is a fast⁴ operation and can be used to obtain a good initialization for the full problem. The algorithm then moves to the second phase, which is the application of Formulation (4–8). If no solution has been found within some predefined time limit, we augment the set of imposed arcs with some additional selections and rerun this phase (which now corresponds to a more resticted formulation and should, thus, be easier to solve). On the other hand, if no solution with objective value $z^* = 0$ exists, 5 we relax some of the imposed arcs before attempting to rerun the second phase (which now corresponds to a less restricted formulation).

⁵ This can be inferred when the overall lower bound during the search process rises to a value above $z^{LB} = 0$.



 $^{^4}$ 1,000-node instances can be solved in 5 s by CPLEX v11.0 (default options). Available machine memory was the limiting factor to solving larger instances.

4 Computational experiments

We illustrate our MILP framework with prescriptions resulting from the acquaintance network formation model proposed by Davidsen et al. [19]. The model demonstrates the emergence of small world behavior in social networks, where the nodes represent people and the edges represent some sort of relationship between them. We first initialize the simulation with a random Erdös–Rènyi graph (0.1 edge probability). The model evolves at each time step according to the dynamics presented in detail in [19]. For reference, we used a p=0.04 removal probability. In each experiment, we evolve 100 different 100-node networks. After a given number of steps, we stop the simulations and obtain a degree-dependent clustering prescription by averaging over the 100 resulting networks. We then use the approach presented in this paper to construct a single 100-node network that possesses this prescription. The actual prescriptions used as input data to our framework are presented in the Appendix.

Table 1 presents the results of our methodology for 28 independent experiments. The simulation stoppage time (in terms of simulation steps) is denoted by t_S , while |q| denotes the number of the different degree-classes. The total number of arcs in the required graph is denoted by a_T , while a_P denotes the arcs that were fixed by the preprocessing algorithm. The latter took t_P time and all the optimization phases took cumulatively t_O time, for a total computation time of $t_P + t_O$. We were able to generate a network satisfying the required prescription in all 28 instances, with 20 of those instances requiring less than $1 \, min$ of computation. The preprocessing algorithm, on average, fixed $\sim 90\%$ of the total arcs; yet in the majority (24/28) of the instances, that was not over-restrictive and they were solved at first pass. The remaining 4 instances (denoted with an asterisk) required 1 round of arc removal where 10% of the fixed arcs (a_P) were removed. The total computation time for these 4 problems was significantly larger.

5 Conclusions

A mathematical optimization-based framework was introduced for the solution of the Network Generation Problem with degree-dependent clustering prescriptions. This was the first time in the open literature that a framework with theoretical guarantees of achieving the required prescription, when feasible, was presented for this problem. However, the optimization of the resulting formulation presents computational challenges and is beyond the capabilities of off-the-shelf commercial optimization software. To that end, we developed a preprocessing scheme to judiciously prefix a subset of the optimization variables and reduce the model's complexity. We were then able to address the construction of 100-node networks for test data sets generated through a social network evolution method. We conclude by noting that this approach can be readily generalized to other prescriptions of network collective properties and this will be the subject of a forthcoming publication.

⁶ This is not necessarily equal to the maximum required degree, as some degree levels may be missing from the sequence



Table 1 Computational results for a suite of 100-node test-problems

Prob	t_S	q	Arcs		Time (se	ec)
ID			$\overline{a_T}$	a_P	$\overline{t_P}$	t_O
A	0	29	496	461	10	26
В	0	16	573	328	7	1,144
C	500	33	579	550	12	5
D	1,000	34	713	682	15	2
E	1,000	30	721	691	13	4
F	1,000	30	812	764	15	11
G	1,000	33	703	665	13	7,810*
Н	1,000	31	755	650	14	135
I	2,000	35	832	777	16	17,175*
J	2,000	36	824	803	18	2
K	2,000	37	725	696	13	3
L	2,000	32	655	632	14	2
M	2,000	32	834	636	13	6,499*
N	4,000	31	637	616	13	2
O	4,000	30	572	537	11	4
P	4,000	35	723	700	14	3,101*
Q	4,000	31	605	555	11	27
R	6,000	35	700	675	14	3
S	6,000	31	602	423	11	1,215
T	6,000	33	633	543	12	5
U	6,000	34	622	518	12	15
V	6,000	37	740	607	14	365
W	10,000	33	632	598	12	5
X	10,000	35	650	609	12	4
Y	10,000	34	606	582	12	2
Z	10,000	37	712	674	15	6
AA	10,000	27	749	703	14	9
AB	10,000	32	606	508	14	25

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Appendix: Prescriptions used

Each row represents a different degree class q. The row format is $\{D_q, n_q, T_q^L, T_q^U\}$, where D_q is the degree of the class, n_q is the number of nodes in the class, and (T_q^L, T_q^U) is the allowable range for the number of triangles that can be formed collectively by the nodes in this class.



	0	11	21	42	27	48	16	59	46	31	30	238	120	200	192	132	282	73	516	267	294	104	324	484	128	612	148	318	171	180	189	400	236	
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	0	4	13	16	28	51	4	6	24	19	36	45	45	56	126	141	104	86	51	256	146	317	180	95	270	506	342	246	128	339	157	152	164	300
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D	_	7	\mathcal{E}	4	2	9	7	∞	6	10	=	12	13	4	17	18	19	20	21	22	23	24	25	56	27	28	59	30	31	34	35	36	40	48
	0	0	∞	30	28	81	52	52	100	96	235	48	192	113	195	166	237	196	110	138	274	141	345	703	390	424	227	239	997	987	329	351	404	
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	0	6	30	54	54	120	35	48	128	103	200	112	214	276	137	202	208	136	166	372	764	486	482	258	279	337	635	333	375	395	976			
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