Constructing bounded degree graphs with prescribed degree and neighbor degree sequences

Uroš Čibej¹ and Aaron Li² and István Miklós³,⁴ and Sohaib Nasir⁵ and Varun Srikanth⁶

¹University of Ljubljana, Faculty of Computer and Information Science, Večna pot 113, 1000 Ljubljana, Slovenia
²University of Minnesota, 206 Church St. SE, Minneapolis, MN, USA, 55455
³Rényi Institute, ELKH, 1053 Budapest, Reáltanoda u. 13-15, Hungary
⁴SZTAKI, ELKH, 1111 Budapest, Lágymányosi u. 11, Hungary
⁵Vassar College, 124 Raymond Avenue, Poughkeepsie, New York 12604
⁶Georgia Institute of Technology North Avenue, Atlanta, GA 30332

Abstract

Let $D = d_1, d_2, \ldots, d_n$ and $F = f_1, f_2, \ldots, f_n$ be two sequences of positive integers. We consider the following decision problems: is there a i) multigraph, ii) loopless multigraph, iii) simple graph, iv) connected simple graph, v) tree, vi) caterpillar $G = (V, E)$ such that for all $k$, $d(v_k) = d_k$ and $\sum_{w \in N(v_k)} d(w) = f_k$ $(d(v)$ is the degree of $v$ and $N(v)$ is the set of neighbors of $v)$. Here we show that all these decision problems can be solved in polynomial time if $\max_k d_k$ is bounded.

The problem is motivated by NMR spectroscopy of hydrocarbons.

Keywords: Degree sequences, Neighbor degree constraint, NMR spectroscopy

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1. Introduction

In statistical testing of networks, a network from real life must be compared with a background distribution of random graphs. In such null models of random graphs, the degree sequence of the graphs is typically fixed. However, there are structural properties that are not preserved by the degree sequence. One example for such a property is the assortativity [16]. A network is called assortative if vertices tend to be connected to vertices with similar degrees, and it is called dissortative if low degree vertices tend to connect to high degree vertices. The observation that real life networks with similar degree sequences might have different assortativity urged research to develop null models that preserve structural properties above the degree sequence. Such models are, for example, the joint degree matrix model [16, 4] that prescribes the number of edges between vertex classes with given degrees and the $dk$-random graphs that considers the distribution of induced sub-graphs up to a given size [14]. While there are polynomial algorithms to construct a realization of a joint degree matrix [4], constructing a graph with prescribed small sub-graph distribution appears to be a hard problem. This motivated the question: “What kind of local properties make the graph construction hard?” Erdős and Miklós showed that it is already NP-complete to ask if there exists a graph with given degree and neighbor degree sequence [2].

In this paper, we show that there exists a polynomial algorithm to construct graphs with prescribed degree and neighbor degree sequence if there is a bound on the maximum
degree. We consider several variants of the problem: we might require that the graph be a simple graph, connected simple graph, tree, or caterpillar. Particular emphases are on the cases when the graph is connected as it also has an application of obtaining the chemical structure of hydrocarbons by NMR spectroscopy data.

Hydrocarbons are the simplest organic molecules consisting of only hydrogen and carbon atoms. A carbon atom makes four covalent bonds, while a hydrogen atom makes only one covalent bond. What follows is that hydrogen atoms can bond only to carbon atoms in hydrocarbons. Therefore, the information on the covalent bonds between carbon atoms completely describes the chemical structure of a hydrocarbon molecule. Indeed, if a carbon atom makes $k$ covalent bonds to other carbon atoms, then it must make $4 - k$ bonds to hydrogen atoms. The diagram representing only the covalent bonds between the carbon atoms is a connected graph with maximum degree 4. This graph is called the skeletal structure. A hydrocarbon might contain multiple bonds between two carbon atoms. Such a hydrocarbon is called unsaturated, and the skeletal structure is a connected, loopless multigraph in that case. When there are only single bonds between carbon atoms, the hydrocarbon is called saturated, and then the skeletal structure is a connected simple graph.

The chemical formula $C_n H_m$ means that there are $n$ carbon atoms and $m$ hydrogen atoms in a molecule. There are simple chemical measurements to obtain $n$ and $m$. When $m = 2n + 2$, the skeletal structure is a tree. Indeed, in that case, there are $n - 1$ covalent bonds between carbon atoms, and any connected graph with $n$ vertices and $n - 1$ edges is a tree. As $m$ decreases, the number of covalent bonds between carbon atoms increases. This might be obtained by multiple bonds between carbon atoms (that is, we are talking about unsaturated hydrocarbons) or making cycles in the skeletal structure. Unsaturated hydrocarbons react with halogens while saturated hydrocarbons do not react, and that simple chemical reaction helps separate unsaturated hydrocarbons from saturated hydrocarbons with cycles in their skeletal structure. In conclusion, the chemical formula $C_n H_m$ is easy to obtain and it is easy to decide if the hydrocarbon is saturated or not as well.

More information on the chemical structure of a hydrocarbon can be attained from NMR spectroscopy. Roughly speaking, the position (frequency) of a peak in the NMR spectroscopy depends on the number of hydrogen atoms bonding to a particular carbon atom causing the peak, and the size of the peak tells the number of such carbon atoms. Further-
more, a peak (roughly, a Gaussian bell-shaped curve) is split depending on the number of hydrogen atoms bonding to neighbor carbon atoms. A peak is split into $l + 1$ parts when there are altogether $l$ hydrogen atoms on the neighbor carbon atoms. From this information, the degree of a carbon atom as well as the sum of the degrees of the neighbor carbon atoms in the skeletal structure can be obtained. Indeed, if a peak related to $k$ hydrogen-carbon bonds is split into $l + 1$ parts, then the degree of the carbon atom is $4 - k$, and the sum of the degrees of the neighbor carbon atoms is $4 \times (4 - k) - l$.

This raises the following graph theoretical question: given degree sequences $D = d_1, d_2, \ldots, d_n$ and $F = f_1, f_2, \ldots, f_n$, is there a graph $G = (V, E)$, such that for all $k$, $d(v_k) = d_k$ and $\sum_{w \in \mathcal{N}(v_k)} d(w) = f_k$, where $d(v)$ is the degree of vertex $v$ and $\mathcal{N}(v)$ is the set of the neighbors of $v$? Erdős and Miklós showed that this decision problem is NP-complete in general [7]. Here we consider a specific case: the maximum degree is 4, and we are looking for connected realizations. We show that this specific case can be solved in polynomial time.

There is typically more than one graph with a given degree and neighbor degree sequence. Some of the solutions are chemically not stable due to spherical constraints. For example, it is known that the hydrocarbon whose skeletal structure would be the balanced unrooted ternary tree with 17 (= 1 + 4 + 12) vertices is chemically not stable. In principle, molecules that have skeletal structure with larger diameter tend to be more stable. Among trees with given degree sequence, caterpillars have the maximum diameter. This motivates us to ask when a caterpillar with given degree and neighbor degree sequence exists.

The paper is structured as follows. In the Preliminaries, we give some definitions on graphs and also introduce the concept of labeled stub-stars. When each edge in a graph is cut into two half-edges (stubs), we get stub-stars. If each stub is labeled by the degree of the neighbor vertex incident to the edge whose cut resulted in the stub, the sum of these labels is the sum of the neighbor degrees. In the next section, we give necessary and sufficient conditions when an ensemble of labeled stub-stars has graph realizations with certain properties. Our main interest is in the cases when the graph is a connected, simple graph or a tree or a caterpillar. However, for the sake of completeness, we also discuss the cases when the graph is a multigraph, a loopless multigraph, or a simple graph. After this, we show that for each of the six cases (multigraph, loopless multigraph, simple graph, simple connected graph, tree, caterpillar) a polynomial time solvable integer programming
feasibility problem exists to find an ensemble of stub-stars that is consistent with a given degree and neighbor degree sequence and also satisfies the necessary conditions to have a graph realization with the given properties.

2. Preliminaries

First, we give some graph-theoretical definitions.

**Definition 1.** A graph $G = (V, E)$ is a multigraph if $E$ is a multiset of $V \times V$. $G$ is a loopless multigraph if $E$ is a multiset of $\binom{V}{2}$. $G$ is a simple graph if $E$ is a subset of $\binom{V}{2}$.

A caterpillar is a tree in which the non-leaf vertices form a path.

**Definition 2.** A degree sequence $\{d_1, d_2, \ldots, d_n\}$ is graphical if there exists a vertex labeled graph $G = (V, E)$ such that for each $v_i$, $d(v_i) = d_i$.

A pair of degree sequences (or bipartite degree sequence) $\{\{d_{1,1}, d_{1,2}, \ldots, d_{1,n}\}\{d_{2,1}, d_{2,2}, \ldots, d_{2,m}\}$ is graphical if there exists a simple bipartite graph $G = (U, V, E)$, such that for each $u_i$, $d_{u_i} = d_{1,i}$, and for each $v_j$, $d(v_j) = d_{2,j}$.

A degree sequence is forest realizable if it has a forest realization.

**Definition 3.** Let $D = d_1, d_2, \ldots, d_n$ and $F = f_1, f_2, \ldots, f_n$ be a pair of degree and neighbor degree sequences. We say that $G = (V, E)$ is a realization of $(D, F)$ if for all $k$, $d(v_k) = d_k$ and $\sum_{w \in N(v_k)} d(w) = f_k$, where $N(v)$ denotes the set of neighbors of $v$.

We now introduce the main technical concept used in this paper: the labeled stub-stars.

**Definition 4.** A labeled stub-star is a vertex with $d$ stubs (half edges). Each stub $s_k$ is labeled with $d_k$. Let $S = \{S_1, S_2, \ldots, S_n\}$ be a multiset (we will also call it ensemble) of labeled stub-stars. A vertex labeled graph $G = (V, E)$ is a realization of $S$ if for each $v_i$, the neighbors of $v_i$ have degrees $d_{i,1}, d_{i,2}, \ldots, d_{i,k}$, where $d_{i,1}, d_{i,2}, \ldots, d_{i,k}$ are the labels of the stub-star $S_i$. We say that $S$ is multigraph, loopless multigraph, simple graph, connected simple graph, tree, caterpillar realizable, respectively, if it has a realization which is a multigraph, loopless multigraph, simple graph, connected simple graph, tree, caterpillar, respectively.

**Definition 5.** The chromatic degree $d_{(i,j)}$ of a labeled stub-star $S$ is 0 if the degree of $S$ is neither $i$ nor $j$. If its degree is $i$, then $d_{(i,j)}(S)$ is the number of times $S$ contains label $j$. Finally, if the degree of $S$ is $j$, then $d_{(i,j)}(S)$ is the number of times $S$ contains label $i$. For an ensemble of labeled stub-stars $S\{S_1, S_2, \ldots, S_n\}$, we define a degree sequence

$$D_{i,j}(S) := d_{(i,j)}(S_1), d_{(i,j)}(S_2), \ldots, d_{(i,j)}(S_n).$$

We define the bipartite degree sequence $D_{i,j}(S)$ for all $i \neq j$ similarly. The chromatic degrees $d_{(i,j)}(S_k)$ are naturally arranged into the two degree sequences according to the
degree of $S_k$ if it is either $i$ or $j$. For other degrees of $S_k$, the corresponding chromatic degree is 0, and it can be arbitrarily added to any degree sequence in $D_{i,j}(S)$. We can also talk about the monochromatic sub-graphs in a realization of an ensemble of labeled stub-stars: the monochromatic sub-graph with color $(i,j)$ contains the edges that connects vertices with degree $i$ and $j$.

The labels of a labeled stub-star form a partition. Below we give the necessary definitions and notations for partitions used in this paper.

**Definition 6.** We will denote by $\lambda \vdash n$ that $\lambda = \{\lambda_1, \lambda_2, \ldots, \lambda_k\}$ is a partition of a positive integer $n$. That is, each $\lambda_i$ is a positive integer, and it holds that

$$\sum_{i=1}^{k} \lambda_i = n.$$ 

The height of $\lambda = \{\lambda_1, \lambda_2, \ldots, \lambda_k\}$ is $k$, and is denoted by $h(\lambda)$. The size of $\lambda$ is $n$, and is denoted by $|\lambda|$. Finally, $N(\lambda, j)$ denotes how many times $j$ appear in $\lambda$, that is

$$N(\lambda, j) := |\{\lambda_i \in \lambda | \lambda_i = j\}|.$$ 

If $\lambda$ comes from the labels of a stub-star, then $h(\lambda)$ corresponds to the degree of the stub-star while $|\lambda|$ corresponds to the neighbor degree sum.

We are going to solve the graph realization problems defined above via integer programming feasibility problems that we are going to introduce now.

**Definition 7.** The integer programming feasibility problem $(\mathcal{X}, \mathcal{L})$ consists of a set of indeterminates, $\mathcal{X}$ and a linear inequality system $\mathcal{L}$ whose indeterminates are from $\mathcal{X}$ and asks if there is an integer assignment to $\mathcal{X}$ that satisfies $\mathcal{L}$.

Some of the inequalities we are going to use contain the function $\min\{x, y\}$ or $\max\{x, y\}$. These can be expressed as linear inequality systems if an upper bound for $|x - y|$ is available. The following lemma is well-known in operational research, but for the sake of completeness, we give a proof here.

**Lemma 8.** Let $x$, $y$ and $M$ be integer numbers satisfying

$$M \geq |x - y|,$$
and let $z$ and $b$ be indeterminates. Then the following inequality system

\begin{align*}
z &\leq x \quad (1) \\
z &\leq y \quad (2) \\
z &\geq x - Mb \quad (3) \\
z &\geq y - M(1 - b) \quad (4) \\
0 &\leq b \quad (5) \\
b &\leq 1 \quad (6)
\end{align*}

has at most two integer solutions, and in every case $z = \min\{x, y\}$.

Similarly, the following inequality system

\begin{align*}
z &\geq x \quad (7) \\
z &\geq y \quad (8) \\
z &\leq x + Mb \quad (9) \\
z &\leq y + M(1 - b) \quad (10) \\
0 &\leq b \quad (11) \\
b &\leq 1 \quad (12)
\end{align*}

has at most two integer solutions, and in every case $z = \max\{x, y\}$.

**Proof.** We prove the $\min\{x, y\}$ case. Observe that $b$ is either 0 or 1. If $x < y$, then there is no solution with $b = 1$ since the inequalities in equations (1) and (4) would contradict to each other. On the other hand, $b = 0$ and $z = x$ is a solution, and the only solution since $x \leq z \leq x$ must hold.

Similarly, when $y < x$, the only solution is $z = y, b = 1$. Finally, if $x = y$, then $z = x(= y)$ and $b \in \{0, 1\}$.

The proof for $\max\{x, y\}$ goes analogously. \qed

3. Realizations of a set of labeled stub-stars

In this section, we state and prove theorems on realizations of labeled stub-stars. We need the well-known Erdős-Gallai and Gale-Ryser inequalities.

**Theorem 9** (Erdős-Gallai, [6]). Let $D = d_1 \geq d_2 \geq \ldots \geq d_n$ be a degree sequence. Then $D$ is simple graph realizable if and only if the sum of the degrees is even, and for all $k$, the inequality

$$
\sum_{g=1}^{k} d_g \leq k(k - 1) + \sum_{h=k+1}^{n} \min\{k, d_h\}
$$

holds.
Theorem 10 (Gale-Ryser, [8, 15]). Let $D = (\{d_{1,1} \leq d_{1,2} \leq \ldots \leq d_{1,n}\}, \{d_{2,1}, d_{2,2}, \ldots, d_{2,m}\})$ be a bipartite degree sequence. Then $D$ is bipartite graph realizable if and only if

$$\sum_{g=1}^{n} d_{1,g} = \sum_{h=1}^{m} d_{2,h}$$

and for each $k$, the inequality

$$\sum_{i=g}^{k} d_{1,i} \leq \sum_{h=1}^{m} \min\{k, d_{2,h}\}$$

(14)

holds.

When the degree sequences have a maximum degree $\Delta$, then only the first $\Delta$ Erdős-Gallai and the first $\Delta - 1$ Gale-Ryser inequalities have to be checked as the following lemma states.

Lemma 11. Let $D = d_1 \geq d_2 \geq \ldots \geq d_n$ be a degree sequence. Then for each $k > d_1$, the inequality in equation (13) holds. Similarly, let $D = (\{d_{1,1} \geq d_{1,2} \geq \ldots \geq d_{1,n}\}, \{d_{2,1}, d_{2,2}, \ldots, d_{2,m}\})$ be a bipartite degree sequence. Then for all $k \geq \max_j\{d_{2,j}\}$, the inequality in equation (14) holds.

Proof. First we consider the Erdős-Gallai inequalities. If $k > d_1$, then it holds that

$$\sum_{i=1}^{k} d_i \leq k \times d_1 \leq k(k-1) \leq k(k-1) + \sum_{j=k+1}^{n} \min\{k, d_j\}.$$  

Regarding the Gale-Ryser inequalities, if $k \geq \max_j\{d_{2,j}\}$, then it holds that

$$\sum_{i=1}^{k} d_{1,i} \leq \sum_{j=1}^{n} d_{2,j} \leq \sum_{j=1}^{m} \min\{k, d_{2,j}\}.$$ 

\[ \square \]

Theorem 12. Let $S = S_1, S_2, \ldots, S_n$ be an ensemble of labeled stub-stars with maximum degree $\Delta$. Let $x_\lambda$ denote the number of labeled stub-stars in $S$ whose labels form the partition $\lambda$. Then $S$ is

(a) multigraph

(b) loopless multigraph

(c) simple graph

realizable if and only if
(a) for each $i$,
\[ \sum_{\lambda|h(\lambda)=i} x_\lambda N(\lambda, i) \equiv 0 \pmod{2} \quad \text{(15)} \]
and for each $i \neq j$,
\[ \sum_{\lambda|h(\lambda)=i} x_\lambda N(\lambda, j) = \sum_{\lambda'|h(\lambda')=j} x_{\lambda'} N(\lambda', i). \quad \text{(16)} \]

(b) the conditions in case (a) holds and for each $i$,
\[ 2 \max_{\lambda|h(\lambda)=i} \{\min\{1, x_\lambda\} N(\lambda, i)\} \leq \sum_{\lambda'|h(\lambda')=i} x_{\lambda'} N(\lambda, i). \quad \text{(17)} \]

(c) the conditions in case (a) holds, for each $i$, the first $\Delta$ Erdős-Gallai inequalities hold for $D_{i,i}(S)$, and for each $i \neq j$, the first $\Delta - 1$ Gale-Ryser inequalities hold for the bipartite degree sequence $D_{i,j}(S)$.

Proof.

(a) It is well known that a degree sequence $\{d_1, d_2, \ldots, d_n\}$ has a multigraph realization if and only if $\sum_{i=1}^{n} d_i$ is even. Similarly, the bipartite degree sequence $\{(d_{1,1}, d_{1,2}, \ldots, d_{1,n}), (d_{2,1}, d_{2,2}, \ldots, d_{2,m})\}$ has a bipartite multigraph realization if and only if $\sum_{i=1}^{m} d_{1,i} = \sum_{j=1}^{m} d_{2,j}$. Observe that equation (15) says that the sum of the degrees in $D_{i,i}(S)$ is even, furthermore, equation (16) says that the sum of the degrees in the two vertex classes are the same in $D_{i,j}(S)$.

Let $G$ be a multigraph realization of $S$. Then for each $i$, the monochromatic subgraph with color $(i, i)$ is a multigraph, and for each $i \neq j$, the monochromatic subgraph with color $(i, j)$ is a bipartite multigraph. That is, equations (15) and (16) hold.

On the other hand, if equations (15) and (16) hold, then there are multigraph realizations for each $D_{i,i}(S)$ and there are bipartite multigraph realizations for each $D_{i,j}(S)$. The union of them is a multigraph realization of $S$.

(b) It is also well known that a degree sequence $\{d_1, d_2, \ldots, d_n\}$ has a loopless multigraph realization if and only if the sum of the degrees is even and
\[ \max_{i} \{d_i\} \leq \sum_{i=1}^{n} d_i - \max_{i} \{d_i\} \]

Observe that equation (17) describes this condition for the degree sequence $D_{i,i}(S)$.

Let $G$ be a loopless multigraph realization of $S$. Then for each $i$, the monochromatic subgraph with color $(i, i)$ is a loopless multigraph, and for each $i \neq j$, the monochro-
matic subgraph with color \((i, j)\) is a bipartite (loopless) multigraph. (Observe that bipartite graphs cannot contain a loop.) That is, equations (15), (16) and (17) hold.

On the other hand, if equations (15), (16) and (17) hold, then there are loopless multigraph realizations for each \(D_{i,i}(S)\) and there are bipartite multigraph realizations for each \(D_{i,j}(S)\). The union of them is a loopless multigraph realization of \(S\).

(c) Let \(G\) be a simple graph realization of \(S\). Then for each color \((i, i)\), the monochromatic subgraph is a simple realization of the degree sequence \(D_{i,i}(S)\), and for each color \((i, j), i \neq j\), the monochromatic subgraph is a simple bipartite realization of the bipartite degree sequence \(D_{i,j}(S)\). Therefore the conditions in case (a) as well as the first \(\Delta\) Erdős-Gallai and the first \(\Delta - 1\) Gale-Ryser inequalities hold.

On the other hand, if the conditions in case (a) as well as the first \(\Delta\) Erdős-Gallai and the first \(\Delta - 1\) Gale-Ryser inequalities hold, then there are monochromatic simple graph realizations of each color \((i, i)\), and there are monochromatic simple bipartite graph realizations for each color \((i, j), i \neq j\). Observe that the union of them is a simple graph realization of \(S\). Indeed, no parallel edges are possible in the union of these monochromatic graphs.

We now consider when an ensemble of labeled stub-stars has a forest realization. Given the previous theorem, we might hope that a sufficient condition is if for each \(i \leq j\), \(D_{i,j}\) is a forest realizable degree sequence. However, this is not the case, as the following example demonstrates.

The example ensemble of labeled stub-stars \(S\) consists of four labeled stub-stars, \(S_1, S_2, S_3, S_4\), respectively, with labels forming partitions \((3, 2), (3, 2), (3), (2, 2, 1)\), respectively.

In this case, each \(D_{i,i}(S)\) and \(D_{i,j}(S)\) is forest realizable, but \(S\) has only one realization, shown below.

```
(2, 2)   (2, 3)
(2, 3)   (1, 3)
```

The issue is that unlike loops and parallel edges, cycles can occur among multiple colors, so checking each individual degree sequence is not sufficient. This motivates the next
definition.

**Definition 13.** Let \( S = S_1, S_2, \ldots, S_n \) be an ensemble of labeled stub-stars with maximum degree \( \Delta \). For any subset \( I \subseteq \{(i, i)|1 \leq i \leq \Delta \} \cup \binom{\Delta}{2} \), we define the multichromatic degree of \( S_i \) to be \( d_I(S_i) := \sum_{(i,j) \in I} d_{(i,j)}(S_i) \) and the multichromatic degree sequence to be \( D_I := d_I(S_1), d_I(S_2), \ldots, d_I(S_n) \).

For example, let \( I = \{(2, 2), (2, 3)\} \) for the previous example \( S \). Then \( d_I(S_1) = 2, d_I(S_2) = 2, d_I(S_3) = 0, \) and \( d_I(S_4) = 2 \).

**Theorem 14.** Let \( S = S_1, S_2, \ldots, S_n \) be an ensemble of labeled stub-stars with maximum degree \( \Delta \). \( S \) is forest realizable if and only if it is multigraph realizable and for any subset \( I \subseteq \{(i, i)|1 \leq i \leq \Delta \} \cup \binom{\Delta}{2} \), the multichromatic degree sequence \( (d_I(S_1), d_I(S_2), \ldots, d_I(S_n)) \) is forest realizable.

**Proof.** We first show the conditions are necessary. Let \( G \) be a forest realization of \( S \). Then \( G \) is also a multigraph realization, so \( S \) is multigraph realizable. For any subset of colors \( I \), we define the color-induced subgraph of \( G \), denoted \( G[I] \), to be the subgraph consisting of all vertices of \( G \) along with all edges labeled with some element of \( I \). Since \( G \) is a forest, then \( G[I] \) is also a forest. The degree sequence of \( G[I] \) is \((m_{I, 1}, m_{I, 2}, \ldots, m_{I, n})\), so this sequence must be forest realizable.

To show the conditions are sufficient, we consider a graph realization \( G \) which is minimal among all realizations of \( S \) in the number of components. It is easy to see that such realization exists. Indeed, since for each color the corresponding degree sequence is forest realizable, it is multigraph realizable (actually, simple graph realizable, too). Any union of monochromatic simple graphs is a simple graph. As multigraph realizations exist, and there are a finite number of them, there exists a realization with minimal number of components.

Assume for contradiction that \( G \) has a cycle. Then we will produce another realization \( G' \) with one fewer components. First we construct a subgraph \( H_k \), then we will find a series of swap operations that lead to \( G' \) with one fewer components.

Let \( C = C_0 \) be a cycle, and let \( I_0 \) be the set of colors of its edges. Let \( H_0 = G[I_0] \). \( H_0 \) cannot be one component as it would contradict that \( D_{I_0} \) is forest realizable. However, it can happen that \( H_0 \) is in one component of \( G \). Therefore while \( H_i \) is in one component of \( G \), we construct an \( H_{i+1} \) in the following way:

1. For all pair of edges \((e_1, e_2)\) such that \( e_1 \) and \( e_2 \) have the same color, \( e_1 \) is in \( C_i \) and \( e_2 \) is in another component of \( H_i \), construct a path from \( e_1 \) to \( e_2 \). For each edge \( f \) in that path whose color is not in \( I_i \), add its color to \( I_{i+1} \), and label \( f \) by \((e_1, e_2)\). An edge might be in several paths for several \((e_1, e_2)\) pairs, in that case take any of these labels.

2. Add all the colors in \( I_i \) to \( I_{i+1} \). Then \( H_{i+1} \) is defined as \( G[I_{i+1}] \) and \( C_{i+1} \) is defined as the component of \( H_{i+1} \) that contains \( C_i \).
In finite number of steps, this procedure will create an $H_k$ which spans in more than one component of $G$. Indeed, for all $i = 0, 1, \ldots, k-1$, $I_i \subset I_{i+1}$, and $G$ cannot be a connected graph as it contains a cycle and is forest realizable.

Now we are going to construct a $G'$ that has one fewer components than $G$. Let $f_{1,k}$ and $f_{2,k}$ be two edges with the same color in $I_k \setminus I_{k-1}$ such that $f_{1,k}$ is in $C_k$ and $f_{2,k}$ is not in the same component in $G$ than $f_{1,k}$. Assume that $f_{1,k} = (v_1, v_2)$, $f_{2} = (v_3, v_4)$, and $v_1$ and $v_4$ have the same degree. Furthermore, let us call the two components containing $f_{1,k}$ and $f_{2,k}$ by $G_1$ and $G_2$.

Now we remove $f_{1,k}$ and $f_{2,k}$ from $G$ and add edges $f_1' = (v_1, v_3)$ and $f_2' = (v_2, v_4)$. This swap operation creates another simple graph realization of $S$ from $G$. If $f_{1,k}$ or $f_{2,k}$ is in a cycle in $G$, then the swap operation merges the two components of $G$ into one component, thus, we arrive to a $G'$ realization with one less component. Otherwise the swap operation does not change the number of components. Indeed, in that case, both removing $f_{1,k}$ and $f_{2,k}$ splits their components in $G$ into two, however, the two new edges connects two pairs.

On the other hand, consider the label $(f_{1,k-1}, f_{2,k-1})$ of $f_{1,k}$ if the swap operation does not decrease the number of components. We claim the following: if the swap operation does not decrease the number of components in $G$ then $f_{1,k-1}$ and $f_{2,k-1}$ are in different components of $G$ after the swap operation. Indeed, we know that there was a path between $f_{1,k-1}$ and $f_{2,k-1}$ before the swap operation that contained $f_{1,k}$. If there is a path between $f_{1,k-1}$ and $f_{2,k-1}$ after the swap operation, then either this path is in $G_1$, and in that case $f_{1,k}$ was in a cycle, a contradiction, or this path contains edges in $G_2$, but in that case $f_{2,k}$ was in a cycle, also a contradiction (or both).

Now we can also perform a swap operation using edges $f_{1,k-1}$ and $f_{2,k-1}$. This operation either decreases the number of components, and then we arrive to $G'$ with one fewer components, or separates $f_{1,k-2}$ and $f_{2,k-2}$, the two edges in the label of $f_{1,k-1}$. We can iterate this process since all the swap operations separating $f_{1,i}$ and $f_{2,i}$ use edges with color in $I_k \setminus I_i$, and thus do not change any edge in the paths between $f_{j,1}$ and $f_{j,2}$ for any $j < i$.

Eventually, one of the swap operations will merge two components in $G$ since $f_{0,1}$ is in the cycle $C$.

We arrived to a contradiction that $G$ had the minimum number of components. Therefore, $G$ does not have a cycle, thus it is a forest realization. 

Observe that the proof also provides an algorithmic construction. Take any union of monochromatic forest realizations and if it contains a loop, then the construction in the proof provides a series of swap operation decreasing the number of components in the realization. Eventually, after a finite number of swap operations, a forest realization is constructed.
Finally, we give the necessary and sufficient conditions when an ensemble of labelled
stub-stars are caterpillar realizable.

**Theorem 15.** Let \( S = S_1, S_2, \ldots, S_n \) be an ensemble of labeled stub-stars. Then \( S \) has a
caterpillar realization if it is forest realizable, the sum of the degrees is \( 2n - 2 \), and there
is no labelled stub-star in \( S \) with more than two labels larger than 1.

**Proof.** First we show that the conditions are necessary. Let \( G \) be a caterpillar realization
of \( S \). Then \( S \) is clearly forest-realizable, and the sum of the degrees of the labelled stub-
stars is \( 2n - 2 \). Also, in a caterpillar realization, any vertex has at most two neighbors
with degree larger than 1.

Now we show that the conditions are sufficient. If \( S \) is forest realizable, take any forest
realization of it, \( G \). We show that \( G \) is a caterpillar. First, \( G \) is a tree since the sum of
the degrees is \( 2n - 2 \). Furthermore, it is a caterpillar since there is no vertex with more
than two neighbors whose degrees are larger than 1.

4. Degree and neighbor degree constraint realizations

In the previous section, we gave necessary and sufficient conditions when an ensemble
of labeled stub-stars have realizations with given properties. In this section, we show
how those results fit into an integer programming feasibility problem. Recall that an
integer programming feasibility problem asks if a bunch of linear inequalities have an
integer solution. Although the integer programming feasibility problem in general is NP-
complete, here we will have constant number of variables and equations.

First, we give the equation system that defines the possible ensembles of labeled stub-stars
whose realizations are realizations of a given degree and neighbor degree sequence.

**Lemma 16.** Let \( D = d_1, d_2, \ldots, d_n \) and \( F = f_1, f_2, \ldots, f_n \) be a pair of degree and neighbor
degree sequences. Then \( G = (V,E) \) is a realization of \( (D,F) \) if and only if \( G \) is a
realization of \( S = S_1, S_2, \ldots, S_n \) satisfying the following inequality system:

\[
\sum_{\lambda \vdash f \land h(\lambda) = d} x_\lambda = y_{d,f} \quad (18)
\]

\[
x_\lambda \geq 0 \quad (19)
\]

where \( x_\lambda \) is the number of labeled stub-stars in \( S \) with labels \( \lambda \) and \( y_{d,f} \) is the number of
cases when \( d_i = d \) and \( f_i = f \).

**Proof.** Assume that \( G = (V,E) \) is a realization of \( (D,F) \). Then cutting each edge in \( E \)
and labeling the stubs of the so-emerging stub-stars by the degree of the neighbor vertices
yields a labeled stub-star \( S \) for each vertex \( v \). The degree of \( S \) is \( d(v) \) and its labels form
a partition of \( f := \sum_{w \in \mathcal{N}(v)} d(w) \). Therefore any realization of \((D, F)\) is also a realization of an ensemble of labeled stub-stars that satisfies the equation system summarized in equation (18).

Similarly, if \( G = (V, E) \) is a realization of an ensemble of labeled stub-stars satisfying the equation system presented in equation (18) then the degree sequence of \( G \) is \( D \), and the neighbor degree sum sequence is \( F \).

We can combine the equation system given in equation (18) with appropriate linear inequality systems describing the conditions (a)–(c) in Theorem 12 and the conditions in Theorem 14 and 15.

First, we start with multigraph realizations.

**Theorem 17.** Let \( D = d_1, d_2, \ldots, d_n \) and \( F = f_1, f_2, \ldots, f_n \) be a pair of degree and neighbor degree sequences. Let \( \Delta \) denote the largest degree in \( D \). Then \((D, F)\) is multigraph realizable if and only if the integer programming feasibility problem \( \{\mathcal{X}, \mathcal{L}\} \) has a solution, where \( \mathcal{X} \) consists of all \( x_\lambda \) variables for all partitions \( \lambda = \lambda_1, \lambda_2, \ldots, \lambda_{h(\lambda)} \) such that \( h(\lambda) \leq D \) and for all \( i, \lambda_i \leq \Delta \) and auxiliary variables \( p_1, p_2, \ldots, p_\Delta \), and \( \mathcal{L} \) consists of

- the inequality system given in equations (18) and (19),
- for all \( 0 < i < j \leq \Delta \), the equation
  \[
  \sum_{\lambda : h(\lambda) = i} x_\lambda N(\lambda, j) = \sum_{\lambda' : h(\lambda') = j} x_{\lambda'} N(\lambda', i),
  \]
  \( (20) \)
- and for all \( i \), the equation
  \[
  \sum_{\lambda : h(\lambda) = i} x_\lambda N(\lambda, i) = 2p_i.
  \]
  \( (21) \)

**Proof.** Assume that \((D, F)\) has a multigraph realization \( G \). Decompose \( G \) into labeled stub-stars \( \mathcal{S} \), then \( G \) is a multigraph realization of \( \mathcal{S} \).

Let \( x_\lambda \) denote the number of labeled stub-stars in \( \mathcal{S} \) whose labels are \( \lambda \). Furthermore, let

\[
p_i := \frac{1}{2} \sum_{\lambda : h(\lambda) = i} x_\lambda N(\lambda, i).
\]

We claim that these assignments form a solution to \((\mathcal{X}, \mathcal{L})\). Indeed, the inequality system in equations (18) and (19) holds due to Lemma 16. Equations (20) and (21) hold due to Theorem 12. Indeed, equation (20) shows that for each \( i \neq j \), the degree sequence \( D_{i,j}(\mathcal{S}) \) has a bipartite graph realization where all edges go between center of stub-stars with degree \( i \) and \( j \). Furthermore, equation (21) shows that for each \( i \), the sum of the degrees in
$D_{i,i}(S)$ is even Therefore, if $(D, F)$ has a multigraph realization, the integer programming feasibility problem $(\mathcal{X}, \mathcal{L})$ has a solution.

Now assume that $(\mathcal{X}, \mathcal{L})$ has a solution. Let $S$ denote the ensemble of labeled stub-stars in which the number of labeled stub-stars with labels $\lambda$ is $x_\lambda$. Since equations 20 and 21 hold, $S$ has a multigraph realization $G$ according to Theorem 12. This realization $G$ is a realization of $(D, F)$ by Lemma 16 since the inequality system given in equations 18 and 19 holds.

For loopless multigraphs, a similar theorem can be proved.

**Theorem 18.** Let $D = d_1, d_2, \ldots, d_n$ and $F = f_1, f_2, \ldots, f_n$ be a pair of degree and neighbor degree sequences. Let $\Delta$ denote the largest degree in $D$. Then $(D, F)$ is loopless multigraph realizable if and only if the integer programming feasibility problem $(\mathcal{X}, \mathcal{L})$ has a solution, where $\mathcal{X}$ consists of all $x_\lambda$ variables for all partitions $\lambda = \lambda_1, \lambda_2, \ldots, \lambda_{h(\lambda)}$ such that $h(\lambda) \leq D$ and for all $i$, $\lambda_i \leq \Delta$ and auxiliary variables $p_1, p_2, \ldots, p_\Delta, z_1, z_2, \ldots, z_r, b_1, b_2, \ldots, b_r$, with $r = \sum_{i=1}^{\Delta} (4i - 2)$ and $\mathcal{L}$ consists of

- the inequality system given in equations 18 and 19,
- for all $0 < i < j \leq \Delta$, the equation
  \[ \sum_{\lambda : h(\lambda) = i} x_\lambda N(\lambda, j) = \sum_{\lambda' : h(\lambda') = j} x_{\lambda'} N(\lambda', i), \]
  (22)
- and for all $i$, the equation
  \[ \sum_{\lambda : h(\lambda) = i} x_\lambda N(\lambda, i) = 2p_i. \]
  (23)

the integer linear programming feasibility problem defining

\[ z_{s(i)} = \max_{k \in \{1, 2, \ldots, i\}} \left\{ \min \left\{ 1, \sum_{\lambda : h(\lambda) = i \land N(\lambda, i) = k} x_\lambda \right\} k \right\}, \]
(24)

where $s(i)$ is the index of the auxiliary variable storing the maximum degree in the $(i, i)^{th}$ row of the special color-degree matrix as well as the inequality

\[ 2z_{s(i)} \leq \sum_{\lambda : h(\lambda) = i} x_\lambda N(\lambda, i) \]
(25)

**Proof.** Similar to the proof of Theorem 17. Observe that the linear programming described in equations 24 and 25 is equivalent with the inequality in equation 17. ■

In case of simple graph realizations, the first few Erdős-Gallai and Gale-Ryser inequalities
should be checked. The challenge is that the degrees in $D_{i,j}(S)$ and $D_{i,i}(S)$ are not ordered so we do not know what the first $k$ highest degrees are. Fortunately, it is possible to give a dynamic programming algorithm that computes the sum of the first $k$ highest degrees.

**Lemma 19.** Let $S$ be an ensemble of labeled stub-stars in which the number of labeled stub-stars with labels $\lambda$ is $x_\lambda$. Fix an $i$ and $j$, and let

$$s_l := \sum_{\lambda | h(\lambda) = i \land N(\lambda, j) = l} x_\lambda$$

Let $t_{l,k}$ denote the largest possible sum of at most $k$ entries in $D_{i,j}(S)$ corresponding to labeled stub-stars with degree $i$ such that each term in the sum is at most $l$. Then the following equations hold:

$$t_{l,0} = 0 \quad (26)$$

$$t_{l,k} = \max_{0 \leq k' \leq k} \{t_{l-1,k-k'} + l \times \min\{k', s_l\}\} \quad \forall \ l > 1 \quad (27)$$

**Proof.** Equation (26) is trivial. We prove equation (27) by proving two inequalities. To prove that the left hand side is smaller than or equal the right hand side, consider the sum that maximizes $t_{l,k}$. Assume that it contains $\tilde{k}$ terms that are smaller than $l$. Then

$$t_{l,k} \leq t_{l-1,k-\tilde{k}} + l \times \min\{\tilde{k}, s_l\}$$

since the sum of the other $k - \tilde{k}$ terms cannot be larger than $t_{l-1,k-\tilde{k}}$. Thus,

$$t_{l,k} \leq t_{l-1,k-\tilde{k}} + l \times \min\{\tilde{k}, s_l\} \leq \max_{0 \leq k' \leq k} \{t_{l-1,k-k'} + l \times \min\{k', s_l\}\}.$$  

To prove that the left hand side is greater than or equal the right hand side, consider the $\tilde{k}$ that maximizes the right hand side, and consider the sum that maximizes $t_{l-1,k-\tilde{k}}$. Add $\min\{\tilde{k}, s_l\}$ times $l$ to this sum, then we get a sum that contains at most $k$ terms, the largest term is at most $l$, and its value is $t_{l-1,k-k'} + l \times \min\{k', s_l\}$. It cannot be larger than $t_{l,k}$, thus we get that

$$t_{l,k} \geq t_{l-1,k-\tilde{k}} + l \times \min\{\tilde{k}, s_l\} = \max_{0 \leq k' \leq k} \{t_{l-1,k-k'} + l \times \min\{k', s_l\}\}. \quad \square$$

For sake of readability, we omitted indexes $i$ and $j$. We need the same dynamic programming algorithm for each $D_{i,j}((S))$, and we will denote the variables in equation (27) by $t_{l,k}^{i,j}$. In the Erdős-Gallai inequalities, we also need to compute $\sum_{h=k+1}^n \min\{k, d_h\}$. We can
define the degree sequence $\tilde{D}$ as $\tilde{d}_h := \min\{k, d_h\}$, and then

$$\sum_{h=1}^{n} \min\{k, d_h\} = \sum_{g=1}^{n} \tilde{d}_g - \tilde{t}_k$$

where $\tilde{t}_k$ is the sum of the at most $k$ largest degrees in $\tilde{D}$. This can be obtained by the dynamic programming recursion

$$\tilde{t}_{l,0} = 0$$

$$\tilde{t}_{l,k} = \max_{0 \leq k' \leq k} \left\{ \tilde{t}_{l-1,k-k'} + \min\{l, k\} \times \min\{k', s_l\} \right\} \quad \forall \ l > 1,$$

and then defining $\tilde{t}_k := \tilde{t}_{l,k}$. The correctness of the equations 28 and 29 can be proved similarly to the proof of Lemma 19. We need the same dynamic programming algorithm for each $D_{i,i}(S)$, and we will denote the variables in the equation 29 by $\tilde{t}_{i,k}$.

Now we are ready to prove the theorem on simple graph realizations.

**Theorem 20.** Let $D = d_1, d_2, \ldots, d_n$ and $F = f_1, f_2, \ldots, f_n$ be a pair of degree and neighbor degree sequences. Let $\Delta$ denote the largest degree in $D$. Then $(D, F)$ is simple graph realizable if and only if the integer programming feasibility problem $\{X, L\}$ has a solution, where $X$ consists of all $x_\lambda$ variables for all partitions $\lambda = \lambda_1, \lambda_2, \ldots, \lambda_{h(\lambda)}$ such that $h(\lambda) \leq D$ and for all $i, \lambda_i \leq \Delta$ and auxiliary variables $p_1, p_2, \ldots, p_\Delta, \tilde{t}_{i,j}$ for all $1 \leq i \leq j \leq \Delta$ and $1 \leq k, l \leq \Delta$, $\tilde{t}_{i,k}$ for all $1 \leq i \leq \Delta$ and $1 \leq k, l \leq \Delta$, $z_1, z_2, \ldots, z_r, b_1, b_2, \ldots, b_r$, with $r = O(\Delta^5)$ and $L$ consists of

- the inequality system given in equations 18 and 19.
- for all $1 \leq i \leq j \leq \Delta$, the integer linear programming feasibility problem defining the dynamic programming recursions in equation 27, and for all $i$, the integer linear programming feasibility problem defining the dynamic programming recursions in equation 29,
- for all $1 \leq i < j \leq \Delta$, the equation

$$\sum_{\lambda: h(\lambda) = i} x_\lambda N(\lambda, j) = \sum_{\lambda': h(\lambda') = j} x_{\lambda'} N(\lambda', i),$$

as well as the linear inequality system for the first $\Delta - 1$ Gale-Ryser inequalities presented as

$$\tilde{t}_{i,j}^{i,j} \leq \sum_{\lambda: h(\lambda) = j} x_\lambda \min\{k, N(\lambda, i)\}$$

17
• and for all \( i \), the equation

\[
\sum_{\lambda | h(\lambda) = i} x_\lambda N(\lambda, i) = 2p_i. \tag{32}
\]

as well as the first \( \Delta \) Erdős-Gallai inequalities expressed as

\[
t_{i,k}^i \leq k(k+1) + \left( \sum_{\lambda | h(\lambda) = i} x_\lambda \min\{k,N(\lambda, i)\} \right) - \tilde{t}_{i,k}^i. \tag{33}
\]

Proof. Similar to the proof of Theorem 17.

The theorem for tree realizations do not need inequalities with minimums and/or maximums.

Theorem 21. Let \( D = d_1, d_2, \ldots d_n \) and \( F = f_1, f_2, \ldots, f_n \) be a pair of degree and neighbor degree sequences. Let \( \Delta \) denote the largest degree in \( D \). Then \((D, F)\) is tree realizable if and only if the integer programming feasibility problem \( \{X, L\} \) has a solution, where \( X \) consists of all \( x_\lambda \) variables for all partitions \( \lambda = \lambda_1, \lambda_2, \ldots, \lambda_{h(\lambda)} \) such that \( h(\lambda) \leq D \) and for all \( i, \lambda_i \leq \Delta \) and auxiliary variables \( p_1, p_2, \ldots, p_{\Delta} \) and \( L \) consists of

• the inequality system given in equations 18 and 19,

• for all \( 1 \leq i < j \leq \Delta \), the equation

\[
\sum_{\lambda | h(\lambda) = i} x_\lambda N(\lambda, j) = \sum_{\lambda' | h(\lambda') = j} x_{\lambda'} N(\lambda', i), \tag{34}
\]

• for all \( i \), the equation

\[
\sum_{\lambda | h(\lambda) = i} x_\lambda N(\lambda, i) = 2p_i. \tag{35}
\]

item and for all subsets \( \mathcal{I} \subseteq \{(i, j)|1 \leq i \leq j \leq \Delta\} \), the inequality

\[
\sum_{(i, j) \in \mathcal{I} | i \neq j} \left( \sum_{\lambda | h(\lambda) = i} x_\lambda N(\lambda, j) + \sum_{\lambda | h(\lambda) = j} x_\lambda N(\lambda, i) \right) + \sum_{(i, j) \in \mathcal{I}} \sum_{\lambda | h(\lambda) = i} x_\lambda N(\lambda, i) \leq

2 \sum_{\lambda} x_\lambda \min\left\{1, \sum_{j | (h(\lambda), j) \in \mathcal{I}} N(\lambda, j) \right\} - 2. \tag{36}
\]

Furthermore, \((D, F)\) has a caterpillar realization if a solution exists with

\[
x_\lambda = 0 \tag{37}
\]
for all $\lambda$ for which $h(\lambda) > 1$ and $\sum_{j>1} N(\lambda, j) \leq 2$.

Proof. Similar to the proof of Theorem 17.

5. Simulation results

In order to demonstrate the practical implications of the presented results, we devised a set of experiments which show the potential of our approach in certain types of applications. Furthermore, we were also able to show where the limitations of this approach were. Since the original motivation for this work comes from chemistry, we considered evaluating the reconstruction of saturated hydrocarbons.

We wanted to see two main results 1) how fast we can find one solution (i.e., one tree from a given input sequence) and 2) how fast the number of solutions grows with the size of the input. We constructed two different testsets for each of these two goals. For the first goal we generated trees of sizes 100 to 1000 with a step of 100. For the second goal we generated testsets of sizes only from 10 to 80 with a step of 10 (for reasons that will be obvious from the results). For all sizes we generated 100 trees and the obtained results are all averages (average times and average counts) for these 100 measurements.

Each tree is generated with a simple recursive procedure described below. The procedure generates a random tree with maximal degree $k$ such that for the current vertex,

1. it generates a random degree $d$ from $[1 \ldots k-1]$ (except for the first node where the interval is $[1 \ldots k]$) uniformly at random,

2. it chooses a random partition of $n-1$ into $d$ pieces, i.e., choose how large each of the $d$ subtrees will be,

3. then it recursively repeats the process for all $d$ neighbors until reaching the leaves.

In order to harness the best practices in integer programming, we used a state-of-the-art solver and used it to construct feasible color-degree matrices. Our goal was to use out-of-the-box IP solvers and evaluate its performance by varying the size of the problem. Since in chemical applications the input represents a feasible tree (i.e. we know there exists a feasible solution) we also start with a tree, decompose it into a degree sequence and a sequence of sums of neighbor degrees.

We used an openly accessible SCIP solver [9] and in order to generate a specific integer
program we used the ZIMPL language [10]. The final trees were reconstructed with the custom written program in python.

The main two results are presented in Figure 1 and Figure 2. Figure 1 shows that the time required to find one feasible solution does not increase in the range that we tested it. It is not surprising that neither the number of variables nor the number of inequalities in the integer programming depends on the input size. In the indicated range of input size, most of the time is spent on solving the integer programming problem and only a minor part of the running time of the solver is spent on actually building the tree.

Figure 2 shows the exponential growth of the average number of feasible solutions to the given input. Already with \( n = 30 \) carbon atoms, the average number of solutions to a random input approaches 10 and with \( n = 40 \) carbon atoms, the average number of solutions is about 86. The average number of solutions keeps growing exponentially with the number of carbon atoms, indicating that it is not feasible to reconstruct large hydrocarbons using only NMR data and then testing each potential solution.

In chemistry however, besides the information about the neighborhood, other information could be used. Some of those chemical and physical limitations also infer various structural limitations which need to be further explored. Namely, completely unrestricted trees yield chemically unfeasible compounds so further work needs to be focused on trees with special structures so that the exponential growth of the number of solutions is postponed even further thus making this approach practical for even larger compounds.

6. Discussion

In this paper, we considered the problem of constructing a bounded degree graph with prescribed degree and neighbor degree sequence. The key is to find an appropriate ensemble of labeled stub-stars that can realize the given degree and neighbor degree sequence. We talked about monochromatic subgraphs that considers only stubs with given labels incident to vertices with given degrees. This approach highly resembles to the color-degree matrix problem that is also intensively studied [1, 2, 12, 13].

Indeed, an ensemble of labeled stub-stars, \( S = \{S_1, S_2, \ldots, S_n\} \), can be represented by a special color-degree matrix \( M \). \( M \) has \( \binom{\Delta}{2} + \Delta \) rows and \( n \) columns, where \( \Delta \) is the maximum degree in \( S \). The rows are labeled by \((i, j) \in \binom{\Delta}{2}\) and \((i, i) \in \Delta^2\). When \((i, j)\)
Figure 1: The average time ($t$, measured in milliseconds) needed to generate one feasible solution of a tree with $n$ vertices, maximum degree 4 and prescribed degree and sum of neighbor degree sequences. See text for detail about generating input trees and finding a solution.

Figure 2: The average number of solutions of a (degree, sum of neighbor degree) sequence of length $n$. See text for detail.
is the label of the \( k \)th row, then

\[
m_{k,l} = \begin{cases} 
\text{number of } j \text{ labels of } S_l \text{ if } S_l \text{ has degree } i \\
\text{number of } i \text{ labels of } S_l \text{ if } S_l \text{ has degree } j \\
0 & \text{otherwise}
\end{cases}
\]

We call the \((i, j)\) and \((i, i)\) labels colors. We will index the rows of \( M \) by their color indexes, that is, we will talk about the \((i, j)\)th row and we index entries as \( m_{(i,j),l} \).

Color-degree matrices appeared earlier in the scientific literature, see for example [13]. The color-degree matrices introduced here are special in two ways: first, for any two rows with indexes \((i, j)\) and \((i', j')\) such that \(i \notin \{i', j'\}\) and \(j \notin \{i', j'\}\) and for any column index \(l\), \(m_{(i,j),l} \neq 0\) implies that \(m_{(i',j'),l} = 0\). Second, we consider only special realizations of these special color-degree matrices.

Indeed, observe that not all edge disjoint monochromatic realizations of the degree sequences in the rows of \( M \) are realizations of the corresponding ensemble of stub-stars. For each \(i \neq j\), it is required that the monochromatic realization be a forced bipartite realization, that is, we require that each edge goes between prescribed vertex classes.

![Figure 3: Caterpillar counterexample C1. See text for details.](image)

To see why this is necessary, consider the caterpillar \( C_1 \), shown in Figure 3. Its color-degree matrix will have the form

\[
M = \begin{pmatrix}
(1,2) & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\
(1,3) & 1 & 2 & 1 & 0 & 1 & 1 & 0 \\
(2,3) & 0 & 1 & 0 & 2 & 2 & 0 & 1 \\
(1,1) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(2,2) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(3,3) & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.
\]

Notice that the plain, dashed, dotted subgraphs in Figure 4, respectively, are edge disjoint realizations for the \((1, 2)\)-th, \((1, 3)\)-th, and \((2, 3)\)-th rows of \( M \), respectively. However, their union is \( C_2 \) which is not a realization of \( M \) because \( C_2 \) has \((2, 2)\) and \((3, 3)\) edges. Also
observe that the dotted subgraph in Figure 4 is a bipartite graph, however, it is not a forced bipartite graph.

![Figure 4: Caterpillar counterexample $C_2$.](image)

In general, it is NP-complete to decide if a color-degree matrix has any realization [5, 11]. On the other hand, Carrol and Isaak showed that the problem is easy if each row if the column sums form a degree sequence of a forest [3]. Hillebrand and McDiarmid showed that the problem remains easy if the column sums form a degree sequence that has a realization with at most one cycle [13]. These results cannot be directly applied on our problem since we require special realizations as discussed above.

Nonetheless, it is worth mentioning that the hard part of the degree and neighbor degree realization problem is to find the appropriate ensemble of stub-stars. Indeed, it remains easy to decide if a special color-degree matrix has a simple graph realization even if there is no bound on the maximal degree: due to the speciality of the color-degree matrices obtained from ensemble of stub-stars, it is guaranteed that the union of monochromatic simple graph realizations will remain simple graphs (given that the realizations for $(i, j)$ colors, $i \neq j$ are forced bipartite).

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