Degree sequence realizations with neighbor constraints

Research proposal, 2020 Summer

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Prerequisites: Basic combinatorics, graph theory, algorithm theory. Background in chemistry is not required!
Best for: Students who are interested in algorithms and discrete mathematics

Problem description

A degree sequence $D = d_1, d_2, \ldots d_n$ is a sequence of non-negative integers. A vertex-labelled simple graph $G = (V, E)$ is a *realization* of if $|V| = n$, and for each i, degree of v_i is d_i. If D has a realization, then D is called *graphical*.

Deciding whether or not a degree sequence is graphical is an easy problem. The Erdős-Gallai inequalities are necessary and sufficient, furthermore, easy to verify [3]. The Havel-Hakimi algorithm provides a realization of D whenever it is graphical [6, 7].

The constrained degree sequence problem consideres a degree sequence D and a list of constraints $C_1, C_2, \ldots, C_k$ and asks if there is a realization of D that satisfies $C_1, C_2, \ldots, C_k$. One specific case is when the input is $D = d_1, d_2, \ldots, d_n$ and $F = f_1, f_2, \ldots, f_n$ and asks if there is a realization $G = (V, E)$ of D such that for all i,

$$\sum_{u \in N(v_i)} d(u) = f_i,$$

where $N(v_i)$ is the neighbor set of v_i, and $d(u)$ is the degree of vertex u. Surprisingly, this problem turns to be NP-complete [4]. However, in an ongoing work, we proved that the problem is tractable if the degrees are bounded.

Specifically, we considered the following problem: Given a degree sequence $D = d_1, d_2, \ldots, d_n$ such that for all i, $d_i \leq 4$ and the list of sum of neighbor degrees $F = f_1, f_2, \ldots, f_n$. Is there a tree which is a realization of D and for all i, the sum of the degrees of the neighbors of v_i is f_i? This problem has motivation in combinatorial chemistry. The realization we are looking for is the carbon backbone of a saturated, acyclic hydrocarbon. The mathematical chemistry problem is the following. We are given a hydrocarbon with known formula, C_nH_{2n+2}, so we know that we are looking for some saturated, acyclic hydrocarbon (alkane). We are also given infrared spectroscopy data, from which we know the number of hydrogen atoms on each carbon atom as well as the number of hydrogen atoms on the neighbor carbon atoms for each carbon atom. From this input, we would like to figure out the molecular geometry of the alkane.

We are interested in a bunch of variations of the basic problem. Some of the names of these problems indicate the motivation in mathematical chemistry, however, the description is understandable without any background in chemistry.

1. Geometry of unsaturated and/or cyclic hydrocarbons The input is $D = d_1, d_2, \ldots, d_n$ and $F = f_1, f_2, \ldots, f_n$. For all i, $d_i \leq 4$, and $\sum_{i=1}^{n} d_i > 2n - 2$. We are looking for a connected graph $G = (V, E)$ such that $|V| = n$, for each i, $d(v_i) = d_i$ and $\sum_{u \in N(v_i)} d(u) = f_i$. The graph is not necessary simple, there might be multipe edges between two vertices, but no loops.

2. Isomers The input is $D = d_1, d_2, \ldots, d_n$ and $F = f_1, f_2, \ldots, f_n$. For all i, $d_i \leq 4$, and $\sum_{i=1}^n d_i = 2n-2$. We are looking for the number of solutions.

3. Haloalkanes The input is $D = d_1, d_2, \ldots, d_n$, for all i, $d_i \leq 4$ and $\sum_{i=1}^n d_i = 2n-2$, $H = h_1, h_2, \ldots h_n$ such that for all i $d_i + h_i \leq 4$, $F = f_1, f_2, \ldots, f_n$ and $G = g_1, g_2, \ldots, g_n$. We are looking for a tree $G = (V, E)$ and a labelling $l : V \to \{0, 1, 2, 3\}$ such that

   (a) for all i, $l(v_i) = h_i$,

   (b) for all i, $\sum_{u \in N(v_i)} d(u) = f_i$,

   (c) for all i, $\sum_{u \in N(v_i) l(u) = g_i}$.

We expect to use theorems on degree sequences (Havel-Hakimi, Erdős-Gallai), edge packing theorems as well as some linear/integer programming. The proposed research is related to previous research topics that were quite successfull, see the previous BSM publications [1, 2, 5, 8].

Assignment for the first week

Please, solve the following exercises:

1. Prove the following: if $\sum_{i=1}^n d_i = 2n - 2$ and for each i $d_i > 0$, then the degree sequence $D = d_1, d_2, \ldots, d_n$ always have a tree realization.

2. Prove the following: if $G = (V, E)$ is a realization of $D = d_1, d_2, \ldots, d_n$ such that for all i, $\sum_{u \in N(v_i)} d(u) = f_i$, then

$$\sum_{i=1}^n d_i^2 = \sum_{i=1}^n f_i. \tag{1}$$

3. Prove that the condition in Equation (1) is only necessary but not sufficient. That is, construct D and F satisfying the equality in Equation (1) without any realization. Give a counterexample where D has a tree realization, however, there is no realization satisfying $\sum_{u \in N(v_i)} d(u) = f_i$ for all i.

4. Give a D and F such that $\sum_{i=1}^n d_i = 2n - 2$, D has a realization satisfying $\sum_{u \in N(v_i)} d(u) = f_i$ for all i, however, in all such realization, the realization is not a tree.

5. Give D and F such that D has two, non-isomorphic tree realizations satisfying $\sum_{u \in N(v_i)} d(u) = f_i$ for all i.

References

[1] Aksen, M. Miklós, I., Zhou, K. (2017) Half-regular factorizations of the complete bipartite graph Discrete Applied Mathematics, 230:21-33.

[2] Bérczi, K., Király, Z., Liu, C. Miklós, I. (2019) Packing tree degree sequences. Informatica, 43(1):11-17.

[3] Erdős, P., Gallai, T. (1960) Graphs with vertices of prescribed degrees (in Hungarian) Matematikai Lapok, 11: 264–274.

[4] Erdős, E.L., Miklós, I. (2018) Not all simple looking degree sequence problems are easy, Journal of Combinatorics, 9(3):553-566.

[5] Gollakota, A., Hardt, W., Mikls, I. (2020) Packing tree degree sequences Graphs and Combinatorics, DOI : 10.1007/s00373-020-02153-0

[6] Havel, V.: A remark on the existence of finite graphs. (in Czech), *Časopis Pěst. Mat.* **80** (1955), 477–480.

[7] Hakimi, S.L.: On the realizability of a set of integers as degrees of the vertices of a simple graph. *J. SIAM Appl. Math.* **10** (1962), 496–506.

[8] Miklós, I., Schlafly, G., Wang, Y., Wei, Z. (2020) Edge Disjoint Caterpillar Realizations, Discrete Applied Mathematics, accepted. `https://arxiv.org/abs/1905.05986`