The connectivity of graphs of graphs with self-loops and a given degree sequence

JOEL NISHIMURA
School of Mathematical and Natural Sciences
Arizona State University, Glendale, AZ 85306-4908, USA

Abstract

‘Double edge swaps’ transform one graph into another while preserving the graph’s degree sequence, and have thus been used in a number of popular Markov chain Monte Carlo (MCMC) sampling techniques. However, while double edge-swaps can transform, for any fixed degree sequence, any two graphs inside the classes of simple graphs, multigraphs, and pseudographs, this is not true for graphs which allow self-loops but not multiedges (loopy graphs). Indeed, we exactly characterize the degree sequences where double edge swaps cannot reach every valid loopy graph and develop an efficient algorithm to determine such degree sequences. The same classification scheme to characterize degree sequences can be used to prove that, for all degree sequences, loopy graphs are connected by a combination of double and triple edge swaps. Thus, we contribute the first MCMC sampler that uniformly samples loopy graphs with any given sequence.

1 Introduction

Understanding what properties of an empirical graph are noteworthy, as opposed to those which are merely the consequence of the degree sequence, is often addressed by comparing the empirical graph with an ensemble of sampled graphs with the same degree sequence [14, 15]. While uniformly sampling graphs with a fixed degree sequence seems straightforward, it can be surprisingly complex. How one samples and the resulting graph statistics are dependent on the space of graphs considered: e.g. whether self-loops and/or multiedges are considered, and whether graphs with distinct ‘stub-labelings’ are considered unique [10].

Graphs which allow self-loops can arise in many disparate applications. For example, self-loops may represent: an author citing themselves; a protein capable of interacting with itself [12, 19]; gene operon self-regulation [17]; cannibalism in a food web [20]; users on photo sharing site Flickr linking to themselves; a loop road or cul-de-sac in a road network [7]; a repeated word in a word adjacency network; traffic flow inside an autonomous system on the Internet [13], along with many other possible interpretations. Considering networks which may include self-loops can be important both because self-loops are often of interest themselves, and because the inclusion of self-loops effectively reduces the number of edges that aren’t self-loops, potentially affecting many different network statistics, especially in small networks. Moreover, while it is commonly thought that self-loops are asymptotically rare [3], they only are for particular assumptions on degree sequences, and are more rare in ‘stub labeled’ spaces as thoroughly detailed in [10, 5]. In contrast, a so called ‘vertex-labeled’ graph is much more likely to have self-loops, yet techniques for sampling from this
space are largely undeveloped. This paper discusses loopy graphs, graphs where each vertex can have at most a single self-loop and edges are either present or absent (i.e. no multiedges).

For many different types of graphs, one of the most popular sampling techniques is Markov chain Monte Carlo sampling via ‘double edge swaps’. Guarantees about the uniformity of double edge swap MCMC sampling (along with a related family MCMC techniques [4, 6]) are founded on several properties, the most difficult of which is whether an MCMC sampler can sample every possible graph, or equivalently, whether the associated Markov chain is irreducible (equivalently, the associated graph of the Markov chain is strongly connected). For any degree sequence, the following spaces are connected and thus can be sampled using MCMC techniques: simple graphs [21, 2, 1, 9, 18], simple connected graphs [18, 2], multigraphs [11] and multigraphs with self-loops [8]. Absent from this list is the space of loopy graphs. Indeed, for some degree sequences, the standard MCMC approach applied to the space of loopy graphs cannot sample all possible such graphs. In this paper, we investigate which degree sequences have disconnected Markov chains, developing an algorithm that can detect this disconnectivity and prove that augmenting the standard MCMC ‘double edge swap’ with ‘triple edge swaps’ guarantees the chain is connected for all degree sequences. These techniques allow the space of loopy graphs to be used in the study of empirical networks.

2 The graph of loopy-graphs

Consider a graph with self-loops $G = (V, E)$, with $n$ vertices in vertex set $V$ and edge set $E$, which may or may not include self-loops: edges of the form $(u, u)$. Notice that loopy-graphs include simple graphs as a special case. As opposed to multigraphs, edges can appear at most once in $E$. For a vertex $u$, we denote the set of adjacent vertices, or ‘neighbors’ of $u$, as $N(u)$, and we refer to $|N(u)|$ as the degree of vertex of $u$. We adopt the convention that each self-loops contributes two to a node’s degree.

$$
(u, v), (x, y) \rightsquigarrow (u, x), (v, y) \quad (u, v), (y, x) \rightsquigarrow (u, y), (v, x)
$$

swaps can create self-loops

‘triangle-loop’ swap

Figure 1: (a, b) For any pair of edges there are two possible double edge swaps. (c) Swapping adjacent edges creates self-loops, and swaps which involve a single self-loop can remove it. (d) In Theorem 6.1 we show that including a triple edge swap in addition to double edge swaps leads to a connected graph of loopy graphs $G_{\Delta}$.

Transforming one graph into another with the same degree sequence is possible through a double edge swap [16], where, as in figure 2, swapping edges $(u, v)$ and $(x, y)$ replaces those edges with $(u, x)$ and $(v, y)$, a process we denote as $(u, v), (x, y) \rightsquigarrow (u, x), (v, y)$. Repeatedly performing double edge swaps (resampling the current graph whenever a proposed swap would create a multiedge) is the basis of MCMC samplers of loopy graphs. Conceptually, repeatedly performing double edge swaps is a random walk on a graph whose vertices are loopy graphs, with the same prescribed degree sequence. Specifically, for a given degree sequence $\{k_i\}$ let $G(\{k_i\})$ be the graph of loopy
graphs under double edge-swaps where each vertex is a loopy graph and edge \((G_i, G_j)\) exists if and only if there is a single double edge swap that takes \(G_i\) to \(G_j\). Showing that a MCMC sampler can sample from graphs with degree sequence \(\{k_i\}\) requires showing that \(\mathcal{G}(\{k_i\})\) is connected, otherwise random walks will not be able to reach all possible loopy-graphs.

In fact though, the space of loopy-graphs is not connected under double edge-swaps for every possible degree sequence. In section 3, we introduce two classes of graphs, \(Q_1\) and \(Q_2\) such that if \(G\) contains a loopy-graph \(G \in Q_1 \cup Q_2\), then \(G\) is disconnected. Both classes \(Q_1\) and \(Q_2\) require high degree nodes, and in section 5, we discuss tests to determine whether a given degree sequence can create a graph in \(Q_1\) or \(Q_2\).

Moreover, \(Q_1\) and \(Q_2\) exactly characterize the graphs which cause \(G\) to be disconnected, as shown in the first main theorem, Theorem 4.20 in section 4. In contrast, any two graphs not in \(Q_1\) or \(Q_2\) are connected with each other, and this will be established by studying special maximal elements of \(G\). The general outline is as follows: from any graph \(G_i\), let \(\hat{G}_i\) be the graph connected to \(G_i\) in \(G\) with the maximum number of self-loops (along with a few other technical considerations), as in Figure 2. Next, inside a graph \(\hat{G}_i\), let \(V_0^i\) be the subset of vertices that do not have self-loops, let \(V_k^i\) be the vertices that have a shortest path of length \(k\) to a node in \(V_0^i\), and let \(V^\infty\) be the nodes disconnected to \(V_0\). Based on the largest clique \(K^0 \subseteq V^0\), we classify the structure of \(\hat{G}_i\) as one of five different types, (four types are displayed in Figure 4), two of which (\(\hat{G}_3\) and \(\hat{G}_d\), \(d > 3\)) belong to \(Q_1\) and \(Q_2\).

![Figure 2: Each of the above graphs has the maximal number of self-loops accessible through double edge swaps. Vertices are categorized by their distance to a vertex without a self-loop and graphs are labeled by the size of the largest clique in \(V^0\). Graphs with cliques of size 3 or greater in \(V^0\) are of class \(Q_1\) or \(Q_2\), as shown by theorem 4.19.](image-url)

The categorization of possible structures of \(\hat{G}\) suggests Algorithm 1 which determines whether a degree sequence has a connected or disconnected \(\mathcal{G}\). Another consequence of Theorem 4.20 is that any degree sequence \(\{k_i\}\) that is disconnected, is disconnected because there are graphs with triangles which cannot be changed into self-loops, which naturally suggests Theorem 6.1, which states that the space of graphs with self-loops is connected under the combination of double and triple edge swaps. Based on this theorem we suggest a MCMC approach that uniformly samples graphs with self-loops and a fixed degree sequence.
3 Degree sequences with disconnected $\mathcal{G}$

First we consider a simple disconnected case, which establishes that for some degree sequences $\mathcal{G}$ is not connected.

3.1 Cycles and cliques

The simplest example of a degree sequence that is not connected is $\{2, 2, 2\}$, which can be wired either as a triangle, or as 3 self-loops. Since there are no valid double edge swaps of either the triangle graph or 3 self-loops (all swaps would create multiedges) the space is disconnected. The disconnectivity of $\{2, 2, 2\}$ can be extended in two ways, to larger cycles with and to larger cliques. The degree sequence of a cycle, $\{2, 2, ..., 2\}$ clearly has a disconnected space, since a graph composed only of nodes with self-loops has no valid double edge swaps. Similarly a clique with additional self-loops at up $n - 3$ vertices has alternate configurations, but lacks any valid double edge swaps, implying that the degree sequence: $\{n + 1, ..., n + 1, n - 1, ..., n - 1, n - 1\}$ is also disconnected.

As a useful exercise, we consider the structure of $\mathcal{G}(\{2, 2, ..., 2\})$ in more detail. Any graph with degree sequence $\{2, 2, ..., 2\}$ is composed of isolated self-loops and cycles of length at least 3. Further, any valid double edge swap either:

1. creates a self-loop and reduces a $k$ cycle, $k \geq 4$, to a $k - 1$ cycle (swapping adjacent edges);
2. combines a self-loop with a $k$ cycle to create a $k + 1$ cycle (swapping a self-loop and an edge in a cycle);
3. merges two cycles into a larger cycle (swapping edges in separate cycles);
4. cuts a cycle into two smaller cycles, each with length at least 3 (non-adjacent edges in the same cycle);
5. swaps two edges in the same cycle without changing its length (non-adjacent edges in the same cycle).

If double edge swaps are augmented with a triple edge swap that takes a triangle to three self-loops (and another triple edge swap that does the reverse), then it is clear that every graph in the space can be taken to the graph made entirely of self-loops (and thus $\mathcal{G}$ is connected) via the following procedure:

1. by swapping edges in different cycles, combine all cycles into a single long cycle;
2. from the graph’s one cycle, swap adjacent edges to create self-loops until the single cycle has length 3;
3. use a triple edge swap to replace the only length 3 cycle with 3 self-loops.

3.2 Other disconnected graphs

These disconnected examples will be generalized into two classes of graphs $Q_1$ and $Q_2$, displayed in Figure 3, which generalize the problems with the clique and the cycle respectively. In section 4 we show that $Q_1$ and $Q_2$ describe all disconnected graphs.

**Definition 3.1** ($Q_1$). A graph $G$ is of class $Q_1$ when the following conditions are true of $G$:

1. There exists a clique $K^0$ in $V^0$ with $|K^0| \geq 4$ (recall: $V^0$ is the set of nodes without self-loops)
Both the degree sequence \( \{n + 1, \ldots, n + 1, n - 1, \ldots, n - 1\} \) and \( \{2, 2, \ldots, 2\} \) have a disconnected graph whose disconnectivity can be generalized to classes \( Q_1 \) and \( Q_2 \). The schematic for \( Q_2 \) includes \( \{2, 2, \ldots, 2\} \) as a special case if when \( V^1 \) is empty, \( V^2 \) is relabeled as \( V^\infty \).

Figure 3: Both the degree sequence \( \{n + 1, \ldots, n + 1, n - 1, \ldots, n - 1\} \) and \( \{2, 2, \ldots, 2\} \) have a disconnected graph whose disconnectivity can be generalized to classes \( Q_1 \) and \( Q_2 \). The schematic for \( Q_2 \) includes \( \{2, 2, \ldots, 2\} \) as a special case if when \( V^1 \) is empty, \( V^2 \) is relabeled as \( V^\infty \).
2. For any $u \in V^0$, either $u$ has no neighbors in $V^0$ or $u$ is in the clique $K^0$.

3. $V^1 \cup K^0$ is a clique,

4. $V^2 = V^\infty = \emptyset$.

We will later show that all $\hat{G}^d$, $d > 3$ are of class $Q_1$. The important feature of $Q_1$ is that it is closed under any double edge swap.

**Lemma 3.2.** For any two graphs $G_1$ and $G_2$ connected via a double edge swap, if $G_1 \in Q_1$ then $G_2 \in Q_1$.

**Proof.** The structure of $Q_1$ implies that all edges have at least one endpoint in $V^1 \cup K^0$. Since $V^1 \cup K^0$ is a clique, there are thus no valid swaps involving any edge in $V^1 \cup K^0$ as any such swap would create a multiedge. Similarly, a swap between a self-loop in $V^1$ and an edge from $V^0$ to $V^1$ would also create a multiedge. The only possible swaps are between two edges $(u, v)$ and $(x, y)$ where $u, x \in V^0 \setminus K^0$ and $v, y \in V^1$. Notice that swap $(u, v)(y, x) \rightsquigarrow (u, x), (y, v)$ is precluded by the presence of edge $(v, y) \in V^1$, while swap $(u, v)(x, y) \rightsquigarrow (u, y), (x, v)$ does not create a new edge in $V^0$, alter the fact that $V^1 \cup K^0$ is a clique or create a vertex in $V^2$ or $V^\infty$. Thus $Q_1$ is closed under edge swaps.

While $Q_1$ includes cliques as a special case, a similar structure, $Q_2$ generalizes the problems associated with cycles and degree sequences $\{2, 2, 2, ..., 2\}$. We will later show that all $\hat{G}^3$ are of class $Q_1$.

**Definition 3.3 (Q2).** A graph $G$ is of class $Q_2$ when the following conditions are true of $G$:

1. There are at least three nodes in $V^0$, each of node in $V^0$ has exactly two neighbors in $V^0$ (i.e. $|N(u) \cap V^0| = 2$ for $u \in V^0$).

2. For any $u \in V^0$, either, $u$ has no neighbors in $V^0$ or $u$ has exactly two neighbors in $V^0$ and is adjacent to all of $V^1$.

3. $V^1$ is a clique

4. For any $u \in V^2$, $N(u) = V^1$,

5. $V^3 = \emptyset$,

6. Either $V^\infty$ is empty or both $V^1$ is empty and $k_u = 2$ for $u \in V^\infty$.

Implicit in the definition of $Q_2$ is that there is a cycle in $V^0$ of length at least 3. Similarly to $Q_1$, $Q_2$ is also closed under double edge swaps.

**Lemma 3.4.** For any two graphs $G_1$ and $G_2$ connected via a double edge swap, if $G_1 \in Q_2$ then $G_2 \in Q_2$.

**Proof.** If $V^\infty$ is non-empty then properties 1 and 6 of $Q_2$ immediately imply that the degree sequence of non-isolated nodes is $\{2, 2, ..., 2\}$, and this scenario was fully described earlier.

If $V^1 \neq \emptyset$, a quick check reveals that the only edge swaps that are possible (all others would require multiedges) involve swaps between two edges in $V^0$, swaps between an edge in $V^0$ and a self-loop in $V^2$, and swaps between two edges joining $V^0$ to $V^1$. However, each of these three swaps preserves the properties of $Q_2$: swaps between the two edges in $V^0$ rearrange the cycle structure of $V^0$ and potentially move a node from $V^0$ to $V^2$, but this preserves the properties of
Q_2$: swaps between a self-loop in \( V^2 \) and an edge in \( V^0 \) move a node from \( V^2 \) to \( V^0 \), reversing the previous swap; For edges \((u,v) \) and \((x,y)\), \( u, x \in V^0 \) and \( v, y \in V^1 \) swap \((u,v)(y,x) \sim (u,x),(y,v)\) is precluded by the presence of edge \((v,y) \in V^1\), while swap \((u,v)(x,y) \sim (u,y),(x,v)\) is only possible if both \(|N(u) \cap V^0| = |N(x) \cap V^0| = 0\) and such a swap does not affect the properties of \( Q_2 \).

This implies the first half of Theorem 4.20.

**Corollary 3.5.** Any \( G \) which contains a graph in \( Q_1 \) or \( Q_2 \) is disconnected.

**Proof.** All graphs in \( Q_1 \) and \( Q_2 \) contain a closed cycle of length at least 3 in \( V^0 \). For a graph \( G \in \mathcal{G} \) and \( G \in Q_1 \cup Q_2 \) let \( C \) be all the cycles in \( V^0 \). Deleting each edge in \( C \) and placing a self-loop at each node in \( C \) preserves the degree sequence and thus creates a graph \( H \in \mathcal{G} \), but \( H \) does not satisfy the first criterion of either \( Q_1 \) or \( Q_2 \). By lemmas 3.2 and 3.4 \( Q_1 \) and \( Q_2 \) are not simple-graphical degree sequences (i.e. \( \bar{k}_i \) denote the ‘simplified degree sequence’, the degree sequence of a graph if all self-loops were deleted, \( k_i = k_i \) for all \( i \in V^0 \) and \( k_i = k_i - 2 \) for all \( i \not\in V^0 \)). Assuming a degree sequence \( \{k_i\} \) is in an unique decreasing order let a degree sequence be \( m \)-simple-graphical if there are self-loops on the \( m \) largest degree vertices. A degree sequence being \( m \)-simple-graphical is equivalent to the condition that the following degree sequence is simple-graphical: \( k_i^* = k_i - 2 \) for \( i \leq m \) and \( k_i^* = k_i \) for \( i > m \). For a degree sequence, let \( m^* \) be the maximum value of \( m \) for which the degree sequence is \( m \)-simple-graphical. We call graphs with \( m^* \) self-loops on the \( m^* \) highest degree vertices:

**Definition 4.1** \((m^*\)-loopy graphs\). A graph \( G \) is \( m^* \)-loopy if \( G \) has \( m^* \) self-loops on vertices \( i \leq m^* \).

Determining the cases where \( \hat{G} \) is \( m^* \)-loopy will be critical in the categorization of different possible \( \hat{G} \) for the following reason.

**Lemma 4.2.** For \( G_1, G_2 \in \mathcal{V} \), if both \( G_1 \) and \( G_2 \) are \( m^* \)-loopy then \( G_1 \) is connected to \( G_2 \).

**Proof.** Since both \( G_1 \) and \( G_2 \) are \( m^* \)-loopy they have self-loops at the same vertices and the same simplified degree sequences and thus, by the connectivity of simple graphs, \( G_1 \) and \( G_2 \) are connected.

In some degree sequences, a graph is obviously \( m^* \)-loopy because all nodes with degree at least two have self-loops. It is not always as straightforward though. For example, the degree sequences \( \{4,4,2\} \) and \( \{6,6,5,3,3,3,2\} \) have no configurations where all vertices have self-loops, as \( \{2,2,0\} \) and \( \{4,4,3,1,1,1,0\} \) are not simple-graphical degree sequences (i.e. there is not a simple graph

4 Categorizing the components of \( \mathcal{G} \)

For any graph \( G_i \in \mathcal{G} \), let \( \mathcal{V}(G_i) \) be the graphs connected to \( G_i \) with the maximum number of self-loops. Of the graphs in \( \mathcal{V}(G_i) \), let \( \hat{G}_i \) be a graph with the maximum number of edges contained in \( V^0 \). While \( \hat{G}_i \) has at least as many self-loops as any other graph connected to \( G_i \), if \( \mathcal{G} \) is not connected, \( \hat{G}_i \) may not have the maximum number of self-loops possible.

In order to formalize the meaning of a graph with the maximum number of self-loops, let \( \{k_i\} \) denote the ‘simplified degree sequence’, the degree sequence of a graph if all self-loops were deleted, (i.e. \( k_i = k_i \) for all \( i \in V^0 \) and \( k_i = k_i - 2 \) for all \( i \not\in V^0 \)). Assuming a degree sequence \( \{k_i\} \) is in an unique decreasing order let a degree sequence be \( m \)-simple-graphical if there are self-loops on the \( m \) largest degree vertices. A degree sequence being \( m \)-simple-graphical is equivalent to the condition that the following degree sequence is simple-graphical: \( k_i^* = k_i - 2 \) for \( i \leq m \) and \( k_i^* = k_i \) for \( i > m \). For a degree sequence, let \( m^* \) be the maximum value of \( m \) for which the degree sequence is \( m \)-simple-graphical. We call graphs with \( m^* \) self-loops on the \( m^* \) highest degree vertices:

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In some degree sequences, a graph is obviously \( m^* \)-loopy because all nodes with degree at least two have self-loops. It is not always as straightforward though. For example, the degree sequences \( \{4,4,2\} \) and \( \{6,6,5,3,3,3,2\} \) have no configurations where all vertices have self-loops, as \( \{2,2,0\} \) and \( \{4,4,3,1,1,1,0\} \) are not simple-graphical degree sequences (i.e. there is not a simple graph

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with those degree sequences). Instead, these graphs have valid configurations where all but the vertex with degree 2 has self-loops.

For any degree sequence there are thus two possibilities, either all graphs in $\mathcal{G}$ are connected to $m^*$-loopy graphs and $\mathcal{G}$ is connected, or there exists some graph not connected to any $m^*$-loopy graph and $\mathcal{G}$ is not connected.

Understanding the possible forms of $m^*$-loopy graphs will comprise the majority of the remaining effort, but the simplest case may also be the most common case. For any $\hat{G}$ where $V^0$ contains only vertices of degree 0 and 1, $\hat{G}$ is clearly $m^*$-loopy. We now turn our attention to the much more complicated scenarios where there exists some $u \in V^0$ with $k_u \geq 2$.

The classification of the possible $\hat{G}$ is broken up according to the size of the largest clique, $K^0 \subseteq V^0$, where $\hat{G}^d$ has $|K^0| = d$. The critical lemmas to prove will be Lemmas 4.9 and 4.14. Lemma 4.9 states that there exists a sequence of double edge swaps which can exchange any vertex in $V_0$ with any other vertex of equal or lower degree. Thus any $\hat{G}_i$ is connected to a similar graph $\hat{G}_j$ where $V^0_j$ contains only the smallest degrees. Building on this, Lemma 4.14 states that a graph $\hat{G}^d$, $d \leq 2$, is $m^*$-loopy. Thus, by lemma 4.2 only degree sequences that can wire a $\hat{G}^d$, $d \geq 3$ can be disconnected and, as will be shown in theorem 4.20, a graph $\hat{G}^3 \in Q_2$ and $\hat{G}^d \in Q_1$ for $d > 3$.

![Diagram](image)

Figure 4: The size of $K^0$ imposes strict requirements on the possible structure of $\hat{G}^d$. When $K^0$ is a clique larger than 3 vertices ($d > 3$), $\hat{G}^d$ is simply a clique of vertices some with self-loops, some without, and a number of vertices with connections only into members of the clique which have self-loops. Note: in $\hat{G}^3$ either $V^\infty$ or $V^1$ must be empty.

Before proving lemmas 4.9 or 4.14 we first construct some general purpose lemmas. We begin with some investigations into restrictions on the sets $V^k$ for all $\hat{G}^d$. Consider the following definition:
Definition 4.3 (Open Wedge $uvw$). There exists open wedge $uvw$ at $u$ if there exists edges $(u,v)$ and $(u,x)$ and $x \notin N(v)$.

If there exists open wedge $uvw$ for $u \in V^0$ then the swap $(u,x), (u,v) \leadsto (u,u), (x,v)$ is possible and creates a self-loop. Since $\hat{G}$ has the maximum number of self-loops, it must be free of: any open wedges centered at vertices in $V^0$, any rewires that can create such open wedges, or any other sequence of rewires that net create self-loops.

Lemma 4.4. For any $u \in V^0$ and $v \in N(u)$, if $u$ connects to a vertex $x$, so does $v$.

Proof. If not, then there exists open wedge $xuv$.

Lemma 4.4 implies that any subgraph of $V^0$ is a clique plus isolated nodes’, as is the subgraph on vertices $u \cup N(u)$ for $u \in V^0$.

Lemma 4.5. If there exists disjoint $(u,v)$ and $(x,y)$ both in $V^0$, $k_u \geq 2$ then $N(u) \cap V^1 = N(x) \cap V^1$

Proof. Suppose first that $N(u) \cap V^1 \not\subseteq N(x) \cap V^1$, then there exists $w \in N(u) \cap V^1$ such that $w \notin N(x)$. If $(u,x)$ exists, then by lemma 4.4 $x$ must be connected to $w$, a contradiction. Thus $(u,x)$ isn’t present, and similarly, lemma 4.4 also implies that $(u,y), (v,x)$ and $(v,y)$ aren’t present. Swap $(u,v), (x,y) \leadsto (u,x), (v,y)$ is thus possible but creates open wedge $wux$ contradicting that $\hat{G}$ has the maximal number of self-loops.

If instead $N(x) \cap V^1 \not\subseteq N(u) \cap V^1$ then $k_x \geq 2$ and the above argument holds.

Lemma 4.6. If there exists $u \in V^0$, $k_u \geq 2$ then all non self-loops contain a vertex in $V^0$, $V^1$ or $V^2$.

Proof. Suppose to the contrary that there exists $(x,y)$ with neither $x$ nor $y$ in $V^0$, $V^1$ or $V^2$. For $v,w \in N(u)$, notice $(v,w)$ must exist, otherwise there exists an open wedge $vwu$, swap $(v,w), (x,y) \leadsto (x,v), (y,w)$ is thus valid, but creates an open wedge at $u$.

This implies that $V^d$ is empty for all finite $d > 3$, and $V^3$ contains no edges aside from self-loops. This also implies that the set of vertices disconnected from $V^0$ can only contain isolated self-loops.

Lemma 4.7. For $\hat{G}_d$ with $d \geq 3$, $V^1 \subseteq N(u)$ for all $u \in K^0$.

Proof. Suppose not, that there exists $x \in V^1$ independent of $K^0$. Since $x \in V^1$ there exists $y \in V^0 \setminus K^0$ along with edge $(x,y)$. Let $u,v,w \in K^0$. Lemma 4.4 implies that since $y \notin K^0$ then $y$ is independent of $K^0$. Swapping $(u,v), (x,y) \leadsto (u,x), (v,y)$ creates an open wedge $yvw$.

Lemma 4.8. If there exists $u \in V^0$, $k_u \geq 2$ then $V^1$ is a clique.

Proof. If $|V^1| = 1$, then $V^1$ is trivially a clique. If $|V^1| \geq 2$, then suppose to the contrary that there exists $x,y \in V^1$ such that $(x,y) \notin E$. Consider the two possible cases:

1. There exists some $u \in V^0$ such that $x,y \in N(u)$. In this case, if $(x,y) \notin E$ then there is an open wedge $xuy$. Thus $(x,y) \in E$.

2. There exists $u,v \in V^0$, such that $(u,x)$ and $(v,y)$ are in $E$ but $(u,y)$ and $(v,x)$ are not. If $(u,v) \in E$ then there exists an open wedge $xuv$. Thus both $(x,y)$ and $(u,v)$ are not in $E$ and the swap $(u,x), (v,y) \leadsto (x,y), (u,v)$ is valid, but produces a graph with one additional edge in $V^0$, contradicting that $\hat{G}$ has the maximum number of edges in $V^0$.  


Lemma 4.9. For any vertex $x \not\in V^0$, and any vertex $u \in V^0$, if $k_x \geq k_u$ then there exists a sequence of swaps that exchanges $x$ for $u$ in $V^0$.

Proof. First we consider the case where $x \in V^1$. For $d \in \{1, 2\}$, since $V^1$ is a clique, each $x \in V^1$ contains a self-loop and any $u \in V^0$ contains at most a single neighbor not in $V^1$ then $k_x \geq k_u$.

For $d \geq 3$, lemmas 4.7 and 4.8 imply that $K^0 \cup V^1$ is a clique, and lemma 4.4 implies that all subgraphs of $V^0$ are cliques, then $k_x \geq k_u + 2$ for any $x \in V^1$ and $u \in V^0$.

For $x \in V^m$, $m \geq 2$ suppose to the contrary that there exists $x$ with degree less than $u$. Consider two cases, first that $N(u) \subseteq V^1$ and second that there exists edge $(u, z) \in V^0$.

1. $N(u) \subseteq V^1$: Since $(x, x)$ contributes 2 to $x$’s degree, $N(u) \subseteq V^1$ and $k_x \leq k_u$ then there exists $v, w \in N(u)$ and $v, w \not\in N(x)$. In such a case, notice that swap $(x, x), (v, w) \sim (x, v), (x, w)$ and subsequent swap $(u, v), (u, w) \sim (u, u), (v, w)$ exchanges $x$ for $u$ in $V^0$.

2. There exists edge $(u, z) \in V^0$: First, $(x, x), (u, z) \sim (x, u), (x, z)$. Since $k_x \leq k_u$ and $x$ is connected to $z$ while $z \not\in N(u)$ then there must be some $y \in N(u)$ but $y \not\in N(x)$. Thus there exists open wedge $xuy$ and $(x, u), (u, y) \sim (u, u), (x, y)$ exchanges $x$ for $u$ in $V^0$ without increasing the number of edges inside $V^0$.

Based on lemma 4.9 we will assume WLOG that $\hat{G}^0$ has $k_u \leq k_x$ for all $u \in V^0$ and $x \not\in V^0$. It thus remains to show that lemma 4.14 is true for $d \in \{1, 2\}$ and to further restrict the possible structures when $d \geq 3$.

4.1 The structure of $\hat{G}^1$

Lemma 4.10. Every $\hat{G}^1$, is $m^*$-loopy.

Proof. Suppose not, that there exists $\hat{G}^1$ which is not $m^*$-loopy. Since $\hat{G}^1$ is not $m^*$-loopy then there exists some simple graph $G^* = \{V^*, E^*\}$ with degree sequence equal to the simplified degree sequence of $\hat{G}^1$, except at vertices in some nonempty set $S \subseteq V^0$, where $k_u^* = k_u - 2$ for $u \in S$, as in Figure 5.

For each $u \in S$ there must be at least two vertices $l_u, r_u \in N(u)$ where $l_u, r_u \not\in N^*(u)$. Let $B = \bigcup_{u \in S}\{l_u \cup r_u\}$ and let $G' = \hat{G}^1$ except without self-loops and edges $(u, l_u)$ and $(u, r_u)$ for each $u \in S$. Notice that $G'$ and $G^*$ have the same degree sequence, except at vertices $B$, where those in $G^*$ have a greater degree.

Let $\Omega' = E' \setminus E^*$ be the edges in $G'$ not in $G^*$ and let $\Omega^* = E^* \setminus E'$ be the edges in $G^*$ not in $G'$. Now consider the edge disjoint cycles and paths that alternate between edges in $\Omega'$ and $\Omega^*$. Since the degrees of all vertices in $V \setminus B$ is the same in $G'$ and $G^*$, there exists a decomposition that consists entirely of alternating cycles and alternating paths beginning and ending with edges in $\Omega^*$ at vertices in $B$. We now consider three cases:

1. There exists an alternating cycle $C$, containing some edge of the form $\{(l_u, r_u)\}$: Let $C' = C \cap E'$ and $C^* = C \cap E^*$. Since the cycle is alternating, removing edges $C'$ from $\hat{G}^1$ and adding edges in $C^*$ to create a new graph $G$ is possible and preserves the degree sequence. Further, since the graph of simple graphs is connected, there exists a sequence of double edge swaps to create $G$ from $\hat{G}^1$. However, $G$ still contains edges $(u, l_u)$ and $(u, r_u)$ as these edges were precluded from set $\Omega'$, but since $(l_u, r_u)$ was in $C'$ it is not in $G$ and thus $(u, l_u)$ and $(u, r_u)$ form an open wedge $l_u ur_u$ contradicting the maximality of $\hat{G}^1$.  

Figure 5: If there exists a graph with more self-loops than a graph $\hat{G}^1$ then an alternating cycle argument can show that there exists a graph $G$, with the same simplified degree sequence as $\hat{G}$ but with an open wedge at $u \in V^0$.

2. There is an alternating path $L$ beginning and ending with edges in $\Omega^*$ at nodes $u, v \in B$ where $u \neq v$: Since $B \subseteq V^1$, lemma 4.8 grants that $(u, v) \in E'$ and thus not also in $\Omega^*$. The union $(u, v) \cup L$ produces a cycle with edges alternatingly in $E'$ and not in $E'$ and, as in the first case, augmenting $\hat{G}^1$ with this cycle produces a graph without an edge $(u, v)$, in violation of lemma 4.8 (Note, by classification $G^1$ cannot contain any edges in $V^0$).

3. There is an alternating path $L_l$ beginning and ending at the same vertex $l_u \in B$ and with edges in $\Omega^*$: Since $r_u$ has a lower degree in $G^1$ than in $G'$, there must be some alternating path $L_r$ beginning at $r_u$. Further, if the second case doesn’t hold, then neither $L_l$ nor $L_r$ can visit any other vertex in $B$ other than $l_u$ and $r_u$ respectively. Let $r_1$ be the first vertex in path $L_r$. Since $(r_1, r_u) \in \Omega^*$, then by lemma 4.8 $r_1 \in V^2$. Next, if $(l_u, r_1) \in E'$, then notice that the union $(l_u, r_1) \cup L_l \cup (l_u, r_u) \cup (r_u, r_1)$ creates an alternating cycle that includes $(l_u, r_u)$, as in the first case. If $(l_u, r_1) \not\in E'$ then the union of $(r_u, u) \cup (u, r_1) \cup L_r \setminus (r_u, r_1)$ creates an alternating cycle, and augmenting $\hat{G}^1$ with this cycle would create open wedge $l_u r_1 r_1$.

4.2 The structure of $\hat{G}^2$

A similar alternating path argument can be applied to $\hat{G}^2$, but in some ways it’s easier to investigate $\hat{G}^2$ directly.

First, notice that $V^1$ is nonempty, since a vertex $u \in V^0$ with $k_u \geq 2$ must have two neighbors but since $V^0$ does not contain a triangle only one of $u$’s neighbors can be in $V^0$. For $u \in V^0$, let $V^1_u = N(u) \cap V^1$, $V^1_K = N(K^0) \cap V^1$ and let $n_k = |V^1_K|$. 

Lemma 4.11. For $\hat{G}^d$, $d \geq 2$, $u \in K^0$ and any $x$ then either $V^1_u \subseteq N(x)$ or $N(x) \subseteq V^1_u$.

Proof. Suppose to the contrary that there exists $y \in N(x)$ and $w \in V^1_u$ but $y \notin V^1_u$ and $w \notin N(x)$. $x$ is not connected to $u$ as otherwise there exists open wedge $xuw$. If $y \in N(u)$, then it must be that $y \in V^0$ (otherwise $y \in V^1_u$) and thus there exists open wedge $xyu$. Thus $y \notin N(u)$.

As $d = 2$, there exists $v \in N(u) \cap K^0$. Since $y, x \notin N(u)$ then by lemma 4.4 $y, x \notin N(v)$. Now notice that swap $(x, y), (u, v) \leadsto (u, x), (v, y)$ and creates open wedge $xuw$. \hfill \Box

Notice that this also gives that $V^3 = \emptyset$, that $k_y \geq k_x$ for any $y \in V^1_u$ and any $x$ and, in conjunction with lemma 4.4, that $V^1_u = V^1_K$ for any $u \in K^0$.

Lemma 4.12. For $\hat{G}^d$, $d \geq 2$, for $u \in K^0$ and any $x \in V^0$ then $k_u \geq k_x$.

Proof. Suppose to the contrary that there exists $x \in V^0$ with $k_x > k_u$. Since $u \in K^0$ there exists $v \in N(u) \cap V^0$. Lemma 4.4 implies that $x \notin N(u) \cup N(v)$ (otherwise $k_x = k_u$) and that there exists $y, z \in N(x)$ with $y, z \notin N(u)$. Notice that swap $(x, y), (u, v) \leadsto (x, u), (v, y)$ creates open wedge $zux$, a contradiction. \hfill \Box

Together with lemma 4.11, lemma 4.12 gives that all vertices $u \in V^0$ have at most one neighbor outside of $V^1_K$, which is the key to the following lemma.

Lemma 4.13. Every $\hat{G}^2$, is $m^*$-loopy.

Proof. To show this we will count the total degree inside $V^1_K$, revealing it is tight with the Erdős-Gallai theorem. Consider the edges internal to $V^1_K$, the edges from $V^0$ and the edges from all remaining vertices separately. Since $V^1_K \subseteq V^1$, it is a clique and thus contributes $n_k(n_k - 1)$ to the degrees inside $V^1_K$. Lemma 4.4 implies that for all $u \in K^0$, $u$ connects to all of $N(K^0)$. Further, lemma 4.11 gives that for any remaining vertex $x$, either $N(x) \subseteq V^1_u$, in which case all $k_x$ edges from $x$ connect to $V^1_K$, or $V^1_K \subseteq N(x)$ in which case $x$ connects to all of $V^1_K$. Aggregating these leads to the statement

$$\sum_{u \in V^1_K} k_u = n_k(n_k - 1) + \sum_{u \in K^0} (k_u - 1) + \sum_{u \in V \setminus (K^0 \cup V^1_K)} \min(n_k, k_u) \quad (1)$$

Notice if any subset of vertices $S \in V^0$ have their degree reduced by 2 then each vertex $u \in S$ connects to at least one less vertex in $V^1_K$. Thus, reducing the degree of any vertex in $V^0$ by 2 reduces the right side of equation 1 but not the left side, and thus by the Erdos Gallai theorem, the new degree sequence would not be simple-graphical. \hfill \Box

Thus we have shown:

Lemma 4.14. A graph $\hat{G}^d$, $d \leq 2$, is $m^*$-loopy.

However, as seen in Figure 2 there exists $\hat{G}^d$, $d \geq 3$ which are not $m^*$-loopy.

4.3 Structure of $\hat{G}^d$, $d \geq 3$

Finally we investigate the possible structures of $\hat{G}^d$ for $d \geq 3$, showing that any $\hat{G}^3$ is in the classes $Q_2$, any $\hat{G}^d$ for $d > 3$ is in the class $Q_1$ and thus $\hat{G}^d$, $d \geq 3$ indicates a disconnected $G$. First, we show the following:

Lemma 4.15. For $\hat{G}^d$, when $d \geq 3$ all edges in $V^0$ are contained in $K^0$.  

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Lemma 4.16. For $\hat{G}^d$ with $d > 3$ ($d = 3$), all edges (non self-loop edges) have at least one vertex in either $V^0$ or $V^1$.

Proof. Suppose not, that there exists $(x, y)$ with both $x, y \not\in V^0 \cup V^1$. For $u, v, w \in K^0$ notice that swapping $(u, v)(x, y) \sim (u, x)(v, y)$ creates open wedges $xuw$ and $ywv$. If $x = y$ and there are $u, v, w, z \in K^0$ then closing wedge $xuw$ opens a second wedge at $xwz$.

Lemma 4.17. For $\hat{G}^3$, either $V^\infty$ or $V^1$ is empty.

Proof. Suppose not, that there exists $x \in V^\infty$ and $y \in V^1$. Let $u, v, w \in K^0$. Lemma 4.7 implies that $u, v, w \in N(y)$. Consider the following swaps: $(x, x)(u, w) \sim (u, x)(w, x)$, then $(y, u)(u, x) \sim (u, u)(y, x)$ and $(v, w)(w, x) \sim (w, v)(w, x)$ which net creates a self-loop.

Lemma 4.18. For $\hat{G}^d$, when $d = 3$, all vertices in $V^2$ have degree $|V^1| + 2$, while when $d > 3$, $V^2 = \emptyset$.

Proof. Since $V^3 = \emptyset$ and $V^2$ has no internal edges by lemma 4.16, the maximum degree in $V^2$ is $|V^1| + 2$, while the degree of vertices in $K^0$ is $|V_1| + |K^0| - 1 = |V^1| + d - 1$. Since lemma 4.9 gives that $|V^1| + 2 \geq |V_1| + d - 1$ then when $d = 3$, vertices in $V^2$ have degree $|V^1| + 2$, and when $d > 3$, $V^2$ must be empty.

Taken together, lemmas 4.18 and 4.15 imply that $\hat{G}^d$ for $d \geq 3$ is composed of a single large clique on $K^0 \cup V^1$ along with vertices who solely connect into that clique. Further, all vertices in $V^0$ have less than or equal degree than all other vertices. Meanwhile, the degrees of vertices in $V^2$, and $K^0$ are $|V^1| + 2$ and $|V^1| + d - 2$ respectively while those in $V^1$ and $V^0 \setminus K^0$ have lower and upper bounds $|V^1| + |V^2| + d + 1$ and $|V^1|$ respectively. Taken together, these constraints on the form of $\hat{G}^d$, $d \geq 3$ (as summarized in Figure 4), can be used to detect degree sequences for which $\hat{G}$ is disconnected.

Theorem 4.19. A graph $\hat{G}^3$ is in the classes $Q_2$ while a graph $\hat{G}^d$ for $d > 3$ is in the class $Q_1$.

Proof. In the definition of the classes $Q_1$ and $Q_2$, the first criterion, the existence of a clique inside $V^0$ or of nodes with degree 2 inside $V^0$ are satisfied by the definitions of $\hat{G}^d$ for $d > 3$ and $\hat{G}^3$ respectively. Lemma 4.15 establishes that there aren’t edges in $V^0$ outside $K^0$, and lemma 4.7 gives that any node in $K^0$ connects to all of $V^1$; together these satisfy the second criterion. Lemma 4.8 shows hat $V^1$ is a clique, the third criterion of $Q_2$ for $\hat{G}^3$, while lemmas 4.8 and 4.7 give that $V^1 \cup K^0$ is a clique for $\hat{G}^d$ for $d > 3$, the third criterion for $Q_1$. Finally, lemmas 4.18 and 4.16 imply that in $\hat{G}^d$ for $d > 3$, $V^2 = V^\infty = \emptyset$, the fourth criterion of $Q_1$. Meanwhile, in $\hat{G}^3$ lemma 4.16 and 4.18 imply that each $u \in V^2$ has $N(u) = V^1$, the fourth criterion of $Q_2$. The last two criteria of $Q_2$ are satisfied by lemmas 4.17 and 4.16. Thus, $\hat{G}^3 \in Q_2$ while $\hat{G}^d \in Q_1$ for $d > 3$.

An immediate consequence of this along, with Lemma 4.14 and Corollary 3.5 is the following.

Theorem 4.20. A degree sequence has a disconnected $\hat{G}$ if and only if there is some graph in $Q_1$ or $Q_2$ in $\hat{G}$.

Corollary 4.21. Aside from the degree sequences associated with the cycle and the clique all simple graphical degree sequences have a connected $\hat{G}$.
\textbf{Proof.} Applying the Erdős-Gallai theorem to the set \(V^1\) in a graph in \(Q_1\) or \(Q_2\) reveals that such a graph’s degree sequence is not simple-graphical, unless \(|V^1| = 0\), in which case the graph is either a clique, or has degree sequence \(\{2, 2, 2, \ldots, 2\}\).

Thus, many of the most commonly examined degree sequences have a connected \(G\). However, in the space of loopy-graphs, there are many possible degree sequences which are loopy-graphical, but not simple-graphical (for example, those in Figure 2). In this next section, we discuss several ways to detect if a loopy-graphical degree sequence has a connected or disconnected space.

## 5 Detecting connectivity in \(G\)

For many applications, detecting if a degree sequence is not at risk of being disconnected can be achieved simply by examining the maximum degree. Let \(n^*\) be the number of nodes with nonzero degree in a degree sequence \(\{k_i\}\).

\textbf{Theorem 5.1.} For degree sequence \(\{k_i\} \neq \{2, 2, 2, \ldots, 2\}\), if \(\max_i k_i < 2\sqrt{n^* - 3} + 1\) then \(G(\{k_i\})\) is connected.

\textbf{Proof.} Since only degree sequences that can wire graphs in \(Q_1\) and \(Q_2\) have a disconnected graph of graph, we need only show that the maximum degree of graphs in \(Q_1\) and \(Q_2\) is never less than \(\sqrt{n^* - 3} + 2\). For a graph \(G \in Q_1 \cup Q_2\), let \(\alpha = |V^1|\). Notice that the highest degree node in \(G\) must be in \(V^1\). Counting the edges into \(V^1\): at least three nodes in \(K^0\) connect to all nodes in \(V^1\) and the remaining \(n^* - 3 - \alpha\) nodes have at least one edge into \(V^1\). Since \(V^1\) is a clique, there are at least \(\alpha(\alpha - 1) + 3\alpha + (n^* - 3 - \alpha)\) edge endpoints into \(V^1\), and thus the maximum degree of a node in \(V^1\) must be at least \(\alpha + 1 + \frac{n^* - 3}{\alpha}\). Minimizing this over \(\alpha\) yields the bound \(2\sqrt{n^* - 3} + 1\). 

When the maximum degree is larger than the bound in theorem 5.1, the following procedure can exactly identify all degree sequences aside from \(\{k_i\} = \{2, 2, 2, \ldots, 2\}\) and \(\{k_i\} = \{n - 1, n - 1, \ldots, n - 1\}\) which can wire a \(Q_1\) or \(Q_2\) are detected by the following procedure:

1. delete the vertex with minimum degree \(k_i\)
2. reduce the largest \(k_i\) degrees by 1
3. if all remaining degrees have two different values \(\{a, b\} \geq 3, n_a \geq 3, b - 2 = n_a + n_b - 1\) and \(a - 2 = n_b\) then it is possible to place nodes with degree \(b\) in \(V^1\), three vertices with degree \(a\) into \(K^0\) and the remaining vertices with degree \(a\) as vertices in \(V^2\), creating a graph \(\hat{G}^3\).
4. if all remaining degrees have two different values \(\{a, b\} \geq 3, a \geq 3, a = b - 2\) and \(a = n_a + n_b - 1\) then it is possible to wire this into a clique with self-loops at each of \(b\), creating a graph \(\hat{G}^d, d \geq 4\).

Stated more formally, this procedure leads to Algorithm 1.

\textbf{Theorem 5.2.} For any degree sequence, Algorithm 1 correctly identifies whether \(G\) is connected or disconnected.

\textbf{Proof.} To see the correctness of Algorithm 1 consider it applied to a graph with the structures \(\hat{G}^d\) for \(d = 3\) and \(d > 3\) in Figure 4 where the structure in Figure 2 is established in the preceding lemmas. First, notice that the algorithm directly tests for \(\{2, 2, 2, \ldots, 2\}\) and \(\{n - 1, n - 1, \ldots, n - 1\}\).

If a degree sequence can construct a \(G^d\) for \(d \geq 3\) then \(V^0 \setminus K^0\) contains only the smallest degrees and these all connect to vertices in \(V^1\) which have the largest degrees. Further, notice that
Algorithm 1 Attempt non \( m^* \)-loopy wiring

**Require:** degree sequence \( \{k_i\} \)

**Ensure:** a non \( m^* \)-loopy graph \( \hat{G} \), otherwise \( False \)

\[ n = |\{k_i|k_i > 0\}| \]

\( G \leftarrow \) graph initialized with vertices from \( \{k_i\} \)  

sort \( \{k_i\} \) in decreasing order  

if \( n \leq 2 \) then  
    return \( False \)

end if  

if \( \min_i k_i = \max_i k_i = 2 \) then  
    return a cycle graph on \( n \) vertices  

end if  

if \( \min_i k_i = \max_i k_i = n - 1 \) then  
    return a clique on \( n \) vertices  

end if  

for \( j \in 0 : n \) do  
    if \( \{k_i\} \) has exactly two unique values then  
        \( a \leftarrow \min_i k_i \)  
        \( b \leftarrow \max_i k_i \)  
        \( n_a \leftarrow \) number of occurrences of \( a \) in \( \{k_i\} \)  
        \( n_b \leftarrow \) number of occurrences of \( b \) in \( \{k_i\} \)  
        \( n_t \leftarrow n_a + n_b \)  
        if \( a \geq 3 \) and \( n_a \geq 3 \) then  
            if \( a = b - 2 \) and \( a = n_t - 1 \) then  
                for \( u \in 0 : n_b \) do  
                    add edge \((u, u)\) to \( G \)  
                end for  
                add clique on vertices \( 0 : n_t \) to \( G \)  
                return \( G \)  
            end if  
            if \( b - 2 = n_t - 1 \) and \( a - 2 = n_b \) then  
                for \( u \in 0 : n_b \) do  
                    for \( v \in 0 : n_t \) do  
                        add edge \((u, v)\) to \( G \)  
                    end for  
                end for  
                for \( u \in 0 : (n_t - 3) \) do  
                    add edge \((u, u)\) to \( G \)  
                end for  
                add clique on vertices \( (n_t - 3) : n_t \) to \( G \)  
                return \( G \)  
            end if  
        end if  
    end if  

MinInd \( \leftarrow n - j - 1 \)  
MinDeg \( \leftarrow k_{\text{MinInd}} \)  
delete\((k_{\text{MinInd}})\)  
if \( \text{MinDeg} > |\{k_i\}| \) then  
    return \( False \)  
end if  

for \( y \in 0 : \text{MinDeg} \) do  
    \( k_y \leftarrow k_y - 1 \)  
    add edge \((\text{MinInd}, y)\) to \( G \)  
end for
for two edges \((u, v)\) and \((x, y)\) with \(u, x \in V^0 \setminus K^0\) and \(v, y \in V^1\), swap \((u, v), (x, y) \sim (u, y), (x, v)\) exchanges \(u\) and \(x\)’s neighbors in \(V^1\). Thus, there is some \(G^d\) for which deleting the smallest degree vertices and subtracting one from the largest remaining degrees, as in Algorithm \(6\) is precisely sequentially deleting actual vertices and edges from \(G^d\).

Once all vertices in \(V^0 \setminus K^0\) have been deleted, the remaining vertices are either in \(K^0\), in \(V^1\) and if \(d = 3\) possibly also in \(V^2\) but with the same degree as vertices in \(K^0\). Thus, the entire remaining degree sequence is composed of just two values, \(a\) and \(b\) with \(a < b\). Let \(n_a\) denote the number of occurrences of degree \(a\) and \(n_b\) the number of occurrences of \(b\). If \(d = 3\) then vertices in \(K^0\) and \(V^2\) connect to themselves or two other vertices and all of \(V^1\), giving that \(a = n_a + 2\); while vertices in \(V^1\) connect to all remaining vertices, implying \(b = n_a + n_b - 1\). If \(d > 3\) then \(V^0\) and \(V^1\) form a clique and so \(b = a + 2\) and \(a = n_a + n_b - 1\). Thus, any degree sequences that produce an \(m^*\)-loopy graph are correctly identified and conversely.

Conversely, when the algorithm returns a graph, analyzing the steps of the algorithm in reverse reveals that it has indeed constructed a valid \(G^d\) graph with the specified degree sequence. Thus, Algorithm \(6\) only returns valid non \(m^*\)-loopy graphs.

6 Sampling loopy-graphs

A small change to \(G\) can connect the space. For distinct \(u, v, w\) consider the following triple edge swap, the ‘triangle-loop’ swap, \((u, v), (v, w), (w, u) \sim (u, v), (w, w)\) along with its reverse \((u, u), (v, v), (w, w) \sim (u, v), (v, w), (w, u)\). Let \(G_\Delta\) be the graph \(G\) but with additional edges connecting graphs which are separated by a single triangle-loop swap.

**Theorem 6.1.** \(G_\Delta\) is connected.

**Proof.** Since every \(G^d\), \(d \geq 3\) contains a triangle in \(V^0\), no such graph has the maximal number of self-loops. Thus for every degree sequence, any graph is connected to a \(G^d\) for \(d \leq 2\), which are \(m^*\)-loopy and since all \(m^*\)-loopy graphs are connected, the space is thus connected.

This allows for an MCMC sampler of the uniform distribution of graphs in \(G_\Delta\). For a given degree sequence, if Algorithm \(6\) indicates that \(G\) is connected then the standard double edge swap MCMC in \([10]\) suffices. On the other hand, if Algorithm \(6\) returns a valid \(G^d\) for \(d \geq 3\) then triangle-loop swaps are required to connected the space, as in the procedure in Algorithm \(2\) Stated succinctly the stub-labeled version does the following:

From any graph \(G\) with probability \(\epsilon > 0\) pick three edges from \(G\), if possible perform a triangle-loop swap, otherwise resample \(G\); with probability \(1 - \epsilon\) pick 2 edges at random, if possible perform a double edge swap, otherwise resample \(G\).

For any \(\epsilon > 0\), theorem \([6, 4]\) gives that this procedure will be able to reach all graphs in \(\mathcal{V}\), however, since the majority of proposed triple swaps will not result in a new graph, the value of \(\epsilon\) that produces the optimal mixing time is likely small. In order to see that triangle-loop swaps preserve the regularity of the \(G_\Delta\), notice that since each triangle-loop swap is reversible, that at any graph \(G\) each of the exactly \(\binom{m}{3}\) sets of three distinct edges corresponds to an incoming edge, either from a self-loop, or a valid triangle-loop swap.

To see that \(G_\Delta\) is aperiodic consider several cases. Notice that for any degree sequence, if \(|\mathcal{V}| \geq 2\), \(G_\Delta\) must contain a graph with at least one of the following: a triangle, an open wedge, two self-loops or two independent edges. Attempting to rewire two sides of a triangle or two self-loops would create a self-loop, and this attempted swap corresponds to a self-loop in \(G_\Delta\), which implies that \(G_\Delta\) is aperiodic. Any graph with an open wedge or two independent edges has a sequence of
Algorithm 2 MCMC step (labeled stubs)

**Require:** loopy-graph \( G \), stubs_labels \( \in \{True, False\} \)

**Ensure:** a loopy-graph adjacent to \( G \) in \( G_\Delta \)

if \( Unif(0, 1) < \epsilon \) then
  choose three edges at random
  if edges create a triangle or are self-loops & triangle-loop wouldn’t create multiedges then
    perform triangle-loop swap
  end if
else
  choose two edges \( e_1 \) and \( e_2 \) at random
  if double edge swap wouldn’t create multiedges then
    if neither \( e_1 \) or \( e_2 \) is a self-loop OR not stubs_labels then
      perform double edge swap
    else
      if \( Unif(0, 1) < \frac{1}{2} \) then
        perform double edge swap
      end if
    end if
  end if
end if
return \( G \)

three double-edge swaps which return to the same graph, this combined with the reversible nature of double-edge swaps implies that \( G_\Delta \) is aperiodic.

This leads to the following theorem, which lets us conclude that Algorithm 2 forms the basis for a MCMC sampler of loopy-graphs.

**Theorem 6.2.** A random walk on \( G_\Delta \) has a uniform stationary distribution.

**Proof.** As an aperiodic, regular, connected graph \( G_\Delta \) has a unique uniform stationary distribution.

\( \square \)

7 Conclusion

By examining the possible structures of graphs with the maximum number of self-loops reachable via double edge swaps we have a complete categorization of the degree sequences where double edge swaps can change any graph into any other valid graph. This understanding is exemplified in Algorithm 1 which can detect whether a degree sequence has a connected space or not. Further, we proved that augmenting double-edge swaps with triangle-loop swaps connects the space of loopy-graphs, creating the first provably correct MCMC technique for sampling loopy-graphs. In addition to filling a gap in the understanding of graph space connectivity, this work builds a tool to allow for the sampling of loopy-graphs and their subsequent use as statistical null-models. As greater emphasis is placed on sampling graphs without labeled-stubs the need for carefully sampling loopy-graphs will likely increase.
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