DIGRAPHS WHOSE NODES ARE MULTIGRAPHS HAVING EXACTLY TWO DEGREES f AND 2.

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ABSTRACT. An $(f,2)$-*graph* is a multigraph G such that each vertex of G has degree either f or 2. Let $S(n,f)$ denote the simple graph whose vertex set is the set of unlabeled $(f,2)$-graphs of order no greater than n and such that $\{G,H\}$ is an edge in $S(n,f)$ if and only if H can be obtained from G by either an insertion or a suppression of a vertex of degree 2. We also consider digraphs whose nodes are labeled or unlabeled $(f,2)$-multigraphs and with arcs (G,H) defined as for $\{G,H\}$.

We study the structure of these graphs and digraphs. In particular, the diameter of a given component is determined. We conclude by defining a random proccess on these digraphs and derive some properties. Chemistry applications are suggested.

1. INTRODUCTION

By an $(f,2)$-*graph* we mean a multigraph G (with loops and multiple edges allowed) such that each vertex of G has degree either f or 2. By the *insertion* of a vertex of degree 2 in a graph we mean the replacement of an edge with a path of length 2 and the *suppression* of a vertex of degree 2 we mean replacing, with an edge, a pair of adjacent edges that meet at a vertex of degree 2. These operations will simply be called *insertions* and *suppressions.*

Let $S(n,f)$ denote the simple graph whose vertex set is the set of unlabeled $(f,2)$-graphs of order no greater than n and such that $\{G,H\}$ is an edge in $S(n,f)$ if and only if H can be obtained from G by either an insertion or a suppression. We are interested in the properties of $S(n,f)$ and relations between $(f,2)$-graphs, the latter being viewed as vertices of $S(n,f)$.

Let G^* be the $(f,2)$-graph obtained from an $(f,2)$-graph G after all possible suppressions of its vertices of degree 2. Note that G^* may have vertices of degree 2. For example, the vertex of degree 2 in a 1-cycle (also called a *loop*) cannot be suppressed, since a 1-cycle does not contain a pair

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of adjacent edges that meet at a vertex of degree 2. The multigraph G^* is called the *suppressed graph associated with* G. The suppressed graph associated with G is unique up to isomorphism. Two $(f,2)$-graphs G and H are called *equivalent,* denoted by $G \equiv H$, if their suppressed graphs are isomorphic. A graph G is called *irreducible* if it is isomorphic to its suppressed graph (that is $G \sim G^*$), otherwise G is *reducible.*

A connected $(1,2)$-graph G is either a path or a cycle. It follows that the suppressed graph of G is either an edge or a loop, respectively. A connected $(2,2)$-graph is a cycle and its suppressed graph is a loop. Thus, our interest is in $(f,2)$-graphs with $f \geq 3$.

If G and H are equivalent $(f,2)$-graphs, the *distance* $d(G,H)$ between G and H is defined as the least number of insertions and/or suppressions in G such that G is transformed into a graph isomorphic to H. If G and H are not equivalent, $d(G,H) = \infty$. Notice that the distance is equivalent to the graph theoretical distance in the $S(n,f)$ graph.

The process considered above may be of interest in chemistry studies if an appropriate molecular graph interpretation of the vertex graphs of $S(n,f)$ is introduced. That is, the vertices of degree f can correspond to chemical species of the same type and all vertices of degree 2 can correspond to species of a second type. For example, when $f = 4$, these types can be thought of as quaternary and secondary carbons, respectively, or the vertices of degree 2 as oxygen atoms. The insertions/suppressions of vertices of degree 2 represent transformations of these molecular graphs into other molecular graphs in which their number of quaternary types remains constant and the secondary species vary. For a model of this kind to be applicable it may be necessary to consider certain of these graphs as not being physically feasible and appropriate adjustments made to handle such a situation. The distance between molecular graphs can be defined as their graph theoretic distance and viewed as a measure of similarity. For a given component of molecular graphs one may be interested in, as in coding theory, finding graphs that are at a maximum distance apart. Such graphs are maximally dissimilar. Other graph theoretic invariants of $S(n,f)$ and the probabilistic/statistical properties of the process when defined as a random process provide topics for further study and possible application.

2. Properties of $S(n,f)$

Let $\mathcal{E}_n(G)$ be the subgraph of $S(n,f)$ induced by the $(f,2)$-graphs H equivalent to G and having order $v(H)$ no greater than n. If G is an $(f,2)$-graph and G^* is the suppressed graph associated with G, then G is said to be on *level* $l(G) = v(G) - v(G^*)$ in $\mathcal{E}_n(G)$.

The *insertion outdegree* $d^+_{\mathcal{E}_n(G)}(G)$ of an $(f,2)$-graph G is the number of isomorphically distinct $(f,2)$-graphs of order not greater then n that can be obtained from G by the insertion of one vertex of degree 2.

The *suppression indegree* $d^-_{\mathcal{E}_n(G)}(G)$ of an $(f,2)$-graph G is the number of isomorphically distinct $(f,2)$-graphs that can be obtained from G by the suppression of one vertex of degree 2.

Given the $(3,2)$-graph G^*, an edge with a loop at each endvertex (i.e., G^* = ), the graph $\mathcal{E}_4(G^*)$ in $S(4,3)$ is shown in Figure 2.1.

Let G^* be an irreducible $(f,2)$-graph of order no greater than n. Then, $\mathcal{E}_n(G^*)$ can be generated from G^*, at level 0, to level $n - v(G^*)$ through successive levels using insertions.

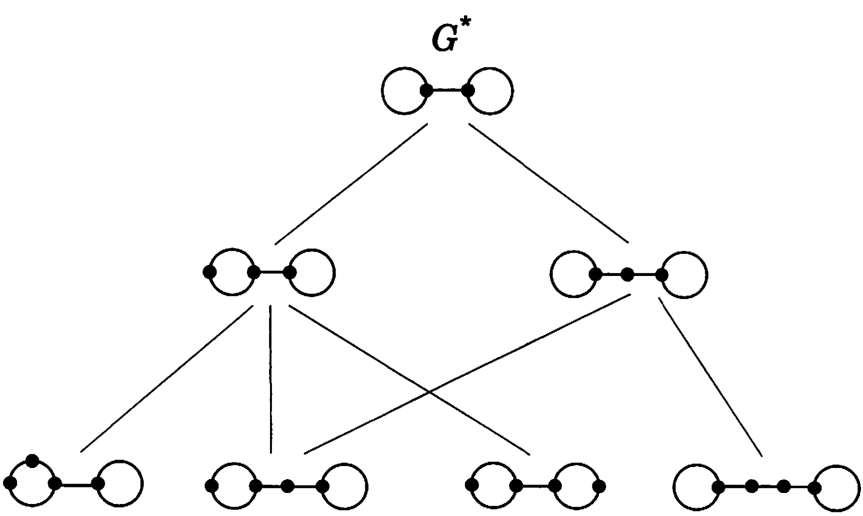
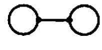


Figure 2.1. The graph $\mathcal{E}_4(G^*) \subset S(4,3)$, with G^* =  .

Observations (*Properties of* $\mathcal{E}_n(G)$)

(1) $\mathcal{E}_n(G)$ is a connected bipartite simple graph.
(2) $\mathcal{E}_n(G)$ can be generated by any graph H in (that is, any vertex H in) $\mathcal{E}_n(G)$ using insertions/suppressions.
(3) $\mathcal{E}_n(\text{cycle})$ is a path of order n in $S(n,f)$ with vertices corresponding to the k-cycles, $k = 1$ to n.
(4) The number of vertices of degree f in each vertex of $\mathcal{E}_n(G)$ is the same.
(5) The number of cycles in each vertex of $\mathcal{E}_n(G)$ is the same.
(6) For any vertex H of $\mathcal{E}_n(G)$, the level of H is $v(H) - v(H^*) = e(H) - e(H^*)$ (note, that $H^* = G^*$).

(7) Let H be a vertex in $\mathcal{E}_n(G^*)$ at a maximum distance from G^*, then $d(G, H)$ is defined to be the *height of* $\mathcal{E}_n(G^*)$ and is denoted $h(\mathcal{E}_n(G^*))$. It follows that $h(\mathcal{E}_n(G^*)) = v(H) - v(G^*) = n - v(G^*)$.

(8) For any G^*, $\operatorname{diam} \mathcal{E}_n(G^*) \geq h(\mathcal{E}_n(G^*))$. Moreover, there exist graphs H^* and K^* such that $\operatorname{diam} \mathcal{E}_n(H^*) = h(\mathcal{E}_n(H^*))$ and $\operatorname{diam} \mathcal{E}_n(K^*) > h(\mathcal{E}_n(K^*))$.

Proof.

(1) Observe, that in $\mathcal{E}_n(G)$ edges can be only between vertices corresponding to two multigraphs H_1 and H_2 such that one of them has odd order and the second has even order.

(2) If H and F are two vertices in $\mathcal{E}_n(G^*)$, then G^* can be obtained from H by successive suppressions and then F can be obtained from G^* by insertions.

(3) Any insertion/suppression in a cycle generates a new cycle with the number of vertices increased/decreased by one.

(4) Any vertex H in $\mathcal{E}_n(G^*)$ can be obtained from G^* by successive insertions. Each insertion does not change the number of vertices of degree f (but increases by one the number of vertices of degree 2).

(5) Similary as in the previous observation, insertion does not change the number of cycles.

(6) Notice, that multigraph H can be obtained from its suppressed graph H^* by the insertion of $v(H) - v(H^*)$ vertices and that each insertion increases the number of vertices and the number of edges by one.

(7) The height $h(\mathcal{E}_n(G))$ is the level of any vertex in $\mathcal{E}_n(G^*)$ corresponding to a multigraph with n vertices. Thus, from (6) it follows that $h(\mathcal{E}_n(G)) = n - v(G^*)$.

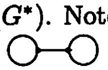
(8) Let G be a vertex in $\mathcal{E}_n(G)$ corresponding to a graph with n vertices. Then, from (7) $h(\mathcal{E}_n(G^*)) = d(G, G^*) \leq \operatorname{diam} \mathcal{E}_n(G^*)$. Let H^* be a loop and K^* the $G^* \subset \mathcal{E}(G)$ in Figure 2.1 with $n \geq 4$.

□

Theorem 2.1. *Let G and H be equivalent $(f, 2)$-graphs ($G \equiv H$), then*

$$|v(G) - v(H)| \leq d(G, H) \leq v(G) + v(H) - 2v(G^*)$$

and that bounds are sharp.

Proof. Let G^* be the suppressed graph of G (G^* is also the suppressed graph of H). Then H can be obtained from G by $v(G) - v(G^*)$ suppressions (resulting in the graph G^*) followed by $v(H) - v(G^*)$ insertions. Thus, H is obtained from G in $v(G) + v(H) - 2v(G^*)$ steps. So, $d(G, H) \leq v(G) + v(H) - 2v(G^*)$. Note that this bound is sharp. Consider, for example, the graph G^* =  in Figure 2.1. Let G be the graph obtained by inserting vertices on the loops and H the graph obtained by only inserting vertices on the edge joining the loops. Then the equality holds.

Assume for simplicity, that $v(G) > v(H)$. Then at least $v(G) - v(H)$ vertices have to be supressed in G to obtain H. This bound is also sharp. For the above example, let both G and H be graphs obtained from G^* by insertions on the edge joining the loops. □

Edges e_1 and e_2 in any suppressed graph G^* are *equivalent* if the insertion of a vertex of degree two in either e_1 or e_2 results in isomorphic multigraphs.

Theorem 2.2. *For $f \geq 3$ the diameter of $\mathcal{E}_n(G)$ equals*

$$\operatorname{diam}\mathcal{E}_n(G) = \begin{cases} 2\,(n - v(G^*)) & \textit{if nonequivalent edges in } G^* \textit{ exist,} \\ 2\left(n - e(G^*) - \left\lfloor \frac{n}{e(G^*)} \right\rfloor + 1\right) & \textit{otherwise.} \end{cases}$$

Proof. Let H_1 and H_2 be two vertices of $\mathcal{E}_n(G)$. Then from Theorem 2.1

$$d(H_1, H_2) \leq v(H_1) + v(H_2) - 2v(G^*) \leq 2n - 2v(G^*).$$

So,

$$\operatorname{diam}\mathcal{E}_n(G) \leq 2n - 2v(G^*).$$

If two nonequivalent edges in G^* exist (say, e_1 and e_2) then let H_1 (H_2) be a graph obtained from G^* by inserting $n - v(G^*)$ vertices in the edge e_1 (e_2). Then

$$\operatorname{diam}\mathcal{E}_n(G) \geq d(H_1, H_2) = 2n - 2v(G^*).$$

This complete the proof in the case of nonequivalent edges.

If all $e(G^*)$ edges of G^* are equivalent let H_1 be a graph obtained from G^* by inserting $n - e(G^*)$ vertices on one edge of G^*, while H_2 is a graph obtained by inserting $\left\lfloor \frac{n-e(G^*)}{e(G^*)} \right\rfloor$ or $\left\lceil \frac{n-e(G^*)}{e(G^*)} \right\rceil$ on each edge of G^*, such that the number of inserted vertices is $n - e(G^*)$. Then

$$\begin{aligned} d(H_1, H_2) &= 2\left(n - \left(e(G^*) + \left\lfloor \frac{n - e(G^*)}{e(G^*)} \right\rfloor\right)\right) \\ &= 2\left(n - e(G^*) - \left\lfloor \frac{n}{e(G^*)} \right\rfloor + 1\right). \end{aligned}$$

So,

$$\operatorname{diam}\mathcal{E}_n(G) \geq 2\left(n - e(G^*) - \left\lfloor \frac{n}{e(G^*)} \right\rfloor + 1\right).$$

It is easy to see that this is the maximal distance between vertices of $\mathcal{E}_n(G^*)$ in this case. □

Let $d^{-}_{\mathcal{E}_n(G^*)}(G)$ and $d^{+}_{\mathcal{E}_n(G^*)}(G)$ denote the suppression indegree and insertion outdegree of vertex G in the graph $\mathcal{E}_n(G^*)$, respectively.

Theorem 2.3. *For any $(f,2)$-graph G which is a vertex of $\mathcal{E}_n(G)$*

$$d^{+}_{\mathcal{E}_n(G^*)}(G) \le e(G^*)$$

and

$$d^{-}_{\mathcal{E}_n(G^*)}(G) \le e(G^*)$$

where G^* is the suppressed graph of G.

Proof. Note, that the insertion of a new vertex on any edge in a path corresponding to a single edge of G^* results in isomorphic graphs. So, only insertions in paths corresponding to different edges of G^* can give different graphs. Thus, $d^{+}_{\mathcal{E}_n(G^*)}(G) \le e(G^*)$.

Similarly, any vertex H in $\mathcal{E}_n(G)$ has a predecessor obtained by the suppression of a vertex of degree 2 in H. However, suppression of any vertex in a path corresponding to an edge in G^* will yield isomorphic graphs. Thus, $d^{-}_{\mathcal{E}_n(G^*)}(G) \le e(G^*)$. □

Let $\rho(G) = e(G)/v(G)$ denote the *density* of the graph G.

Theorem 2.4. *For any $(f,2)$-graph G which is a vertex of $\mathcal{E}_n(G)$*

$$\rho(G) = \frac{l(G) + e(G^*)}{l(G) + v(G^*)}$$

where $l(G)$ is the level of G in $\mathcal{E}_n(G)$. Moreover, if $l(G) \to \infty$ then $\rho(G) \to 1$.

Proof. From observation (6) it follows that $v(G) = l(G) + v(G^*)$ and $e(G) = l(G) + e(G^*)$. □

Notice, that any $(f,2)$-graph can be uniquely transformed into a $(3,2)$-graph by replacing all vertices of degree f by an f-cycle. Insertion and suppression operations can be done on the $(3,2)$-graph except for insertion in the edges of f-cycles corresponding to the initial vertices of degree f. Then the reverse process (that is, contractions of the f-cycles corresponding to the initial vertices of degree f) can be used to obtain an, equivalent to the original, $(f,2)$-graph. So, $(3,2)$-graphs are basic, in the sense that some properties of $(f,2)$-graphs ($f \ge 3$) can be viewed as properties of $(3,2)$-graphs. An example of $(5,2)$-graph G and corresponding $(3,2)$-graph H is shown in Figure 2.2.

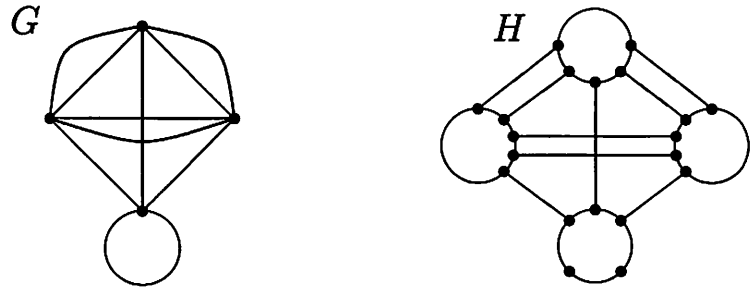


Figure 2.2. An example of (5, 2)-graph G and its corresponding (3, 2)-graph H.

3. Random Processes Based on $S(n, f)$

We shall now define a random process with the vertices of $\mathcal{E}_n(G)$ as the states of this process. Let G^* have order $v(G^*)$, size $e(G^*)$, k vertices of degree f and for technical reasons that follow, let the $e(G^*)$ edges of G^* be labeled.

If G is a vertex of $\mathcal{E}_n(G^*)$, there is a one-to-one correspondence between the labeled edges of G^* and the paths in G that start at a vertex of degree f, end at a vertex of degree f, and have no intermediate vertices of degree f. Let these paths be labeled with the same labels as the edges they correspond to in G^*. If G^* has an edge that is a loop, we shall consider this edge in correspondence with the closed path in G that starts and ends with the same vertex of degree f on which the original loop was based.

The transition digraph $D\mathcal{E}_n(G^*)$ for the random process on $\mathcal{E}_n(G^*)$ is defined as follows. An arc (G, H) is in $D\mathcal{E}_n(G^*)$ if and only if a path-labeled copy of H can be obtained from a path-labeled copy of G either by the insertion of a vertex of degree 2 into one of its labeled paths or by the suppression of a vertex of degree 2 in one of its x_G labeled paths that contain at least one vertex of degree 2 ($0 \leq x_G \leq e(G^*)$). Such a transition from G to H is called an *admissible move*.

For each G there are $e(G^*) + x_G$ possible admissible moves. Assuming each of these are selected with uniform probability $1/(e(G^*) + x_G)$ completes the definition of this random process on the vertices of $\mathcal{E}_n(G^*)$. Note that $x_{G^*} = 0$. If G has order n, no vertex of degree 2 can be inserted into G. Thus, an admissible move is a suppression that only involves paths with vertices of degree 2 and these are selected uniformly with probability $1/x_G$.

Since $D\mathcal{E}_n(G^*)$ is strongly connected, $D\mathcal{E}_n(G^*)$ is the transition digraph for an ergodic Markov chain (see [3]).

For any ergodic Markov chain two fundamental things to determine are:

(a) the *equilibrium vector*, defined as the unique probability vector $\mathbf{w} = [w_G]$ such that $\mathbf{wT} = \mathbf{w}$, where $\mathbf{T} = [p_{GH}]$ is the transition matrix for the chain, and
(b) whether the chain is *time-reversible*, for which a necessary and sufficient condition is $w_G p_{GH} = w_H p_{HG}$, for all states G and H in the chain. For interpretations of the equilibrium vector $\mathbf{w}$ and time-reversibility see [4].

Starting with G^*, we shall now define a random process with the path-labeled $(f,2)$-graphs homeomorphic to G^* as the states of this process. The path-labeled $(f,2)$-graphs are as defined in the definition of the random process $D\mathcal{E}_n(G^*)$, but remain labeled and distinct as path-labeled graphs not as graphs as is done in $D\mathcal{E}_n(G^*)$.

The transition digraph $d\mathcal{E}_n(G^*)$ for this random process is defined analogously to that for $D\mathcal{E}_n(G^*)$ as follows. An arc (G,H) is in $d\mathcal{E}_n(G^*)$ if and only if (a path-labeled copy of) H can be obtained from (a path-labeled copy of) G either by the insertion of a vertex of degree 2 into one of its labeled paths or by the suppression of a vertex of degree 2 in one of its x_G labeled paths that contain at least one vertex of degree 2. Here too we call such a transition from G to H an *admissible move.*

For each G there are $e(G^*) + x_G$ possible admissible moves. Assuming each of these moves is selected with uniform probability $1/(\ e(G^*) + x_G)$ completes the definition of the random process on the path-labeled $(f,2)$-graphs homeomorphic to G^*. As in the Markov chain $D\mathcal{E}_n(G^*)$ we have $x_{G^*} = 0$ and if G has order n, no vertex of degree 2 can be inserted into G so that as before an admissible move can only be a suppression and only involves paths with vertices of degree 2 selected uniformly with probability $1/x_G$.

Since $d\mathcal{E}_n(G^*)$ is strongly connected, $d\mathcal{E}_n(G^*)$ is the transition digraph for an ergodic Markov chain which we denote $\mathcal{E}_n^d(G^*)$.

We note that the transition digraph $d\mathcal{E}_n(G^*)$ is equivalent to the simple graph with vertex set the same as the nodes of $d\mathcal{E}_n(G^*)$ and transitions from a vertex G to a neighboring vertex H are uniform with probability $p_{HG} = 1/\deg G$, where $\deg G = e(G^*) + x_G$. Thus, the analysis of the chain with transition digraph $d\mathcal{E}_n(G^*)$ can be pursued using the theory of random walks on graphs (see[4]). This observation yields the following theorem.

Theorem 3.1. *The Markov chain $\mathcal{E}_n^d(G^*)$ is time-reversible and has equilibrium vector with components $w_G = \frac{\deg G}{2m}$, where m is the size of $d\mathcal{E}_n(G^*)$.*

Proof. That $w_G = \frac{\deg G}{2m}$ is given in [4]. Since time-reversibility is equivalent to the condition $w_G p_{GH} = w_H p_{HG}$, it is sufficient to show that $w_G p_{GH}$ does not depend on G and H. We have $w_G p_{GH} = \frac{\deg G}{2m} \frac{1}{\deg G} = \frac{1}{2m}$. □

The following, as noted in [4], is an immediate corollary of this theorem.

Corollary 3.1. *If a random walk is at vertex G, then the expected number of steps before it returns to G is $\frac{1}{w_G} = \frac{2m}{\deg G}$.* □

Theorem 3.2. *The order of $\mathcal{E}_n^d(G^*)$ is $\binom{n+e(G^*)-v(G^*)}{n-v(G^*)}$.*

Proof. Let G^* be an f-regular multigraph of order $v = v(G^*)$ and size $e = e(G^*)$. Let the edges of G^* be labeled. Inserting t vertices of degree 2 into G^* yields a graph on level t . Noting that the t vertices can be considered as t indistinguishable objects and the labeled paths of G^* as distinguished boxes implies there are $\binom{e+t-1}{t}$ different path-labeled $(f,2)$-graphs on level t. Let t^* be the number of vertices of degree 2 that have to be inserted into G^* to obtain a graph of order n ($t^* = n - v(G^*)$). Thus the total number of such graphs up to and including those on level t^* is $\sum_{t=0}^{t^*} \binom{e+t-1}{t} = \binom{e+t^*}{t^*}$. □

4. Some Examples

The graph $\mathcal{E}_4(G^*)$ with $G^* = K_2$ with a loop at each vertex is shown in Figure 2.1. The transition digraph $D\mathcal{E}_4(G^*)$ is shown in Figure 4.1.

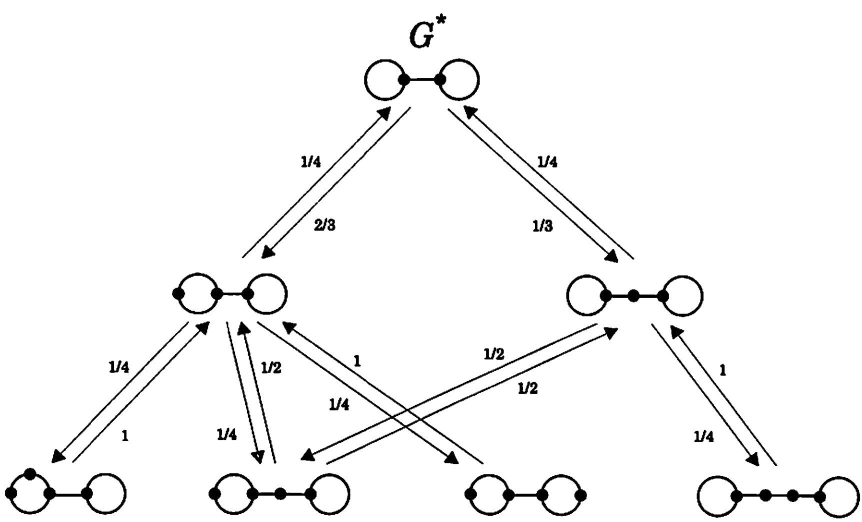
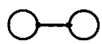


Figure 4.1. The digraph $D\left(\mathcal{E}_4(G^*)\right)$ with $G^* =$  .

In Figure 4.2 we show the transition digraph $d\mathcal{E}_4(G^*)$.

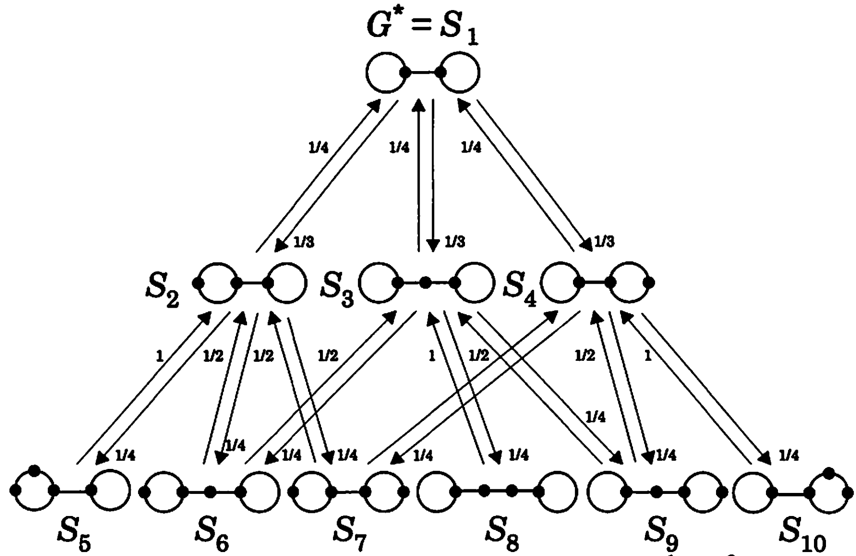


Figure 4.2. The digraph $d\,(\mathcal{E}_4(G^*))$ with $G^* =$ (1, 2, 3) .

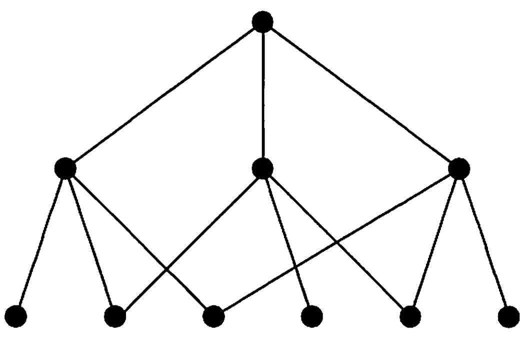


Figure 4.3. The simple graph associated with $d\,(\mathcal{E}_4(G^*))$ with $G^* =$ (1, 2, 3) .

Analysis of these examples yields the following information. By Theorem 3.1 the equilibrium vector for the random process $\mathcal{E}_4^d(G^*)$ is

$$\frac{1}{24}\left[\begin{array}{cccccccccc} 3 & 4 & 4 & 4 & 1 & 2 & 2 & 1 & 2 & 1 \end{array}\right]$$

and $\mathcal{E}_4^d(G^*)$ is time-reversible.

Furthermore, we find that by combining components, that correspond to isomorphic graphs, in the equilibrium vector for $\mathcal{E}_4^d(G^*)$ and summing their values we can obtain the equilibrium vector for $D\mathcal{E}_4(G^*)$. The equilibrium vector for the random process $\mathcal{E}_4(G^*)$ is

$$\frac{1}{24}\left[\begin{array}{ccccccc} 3 & 8 & 4 & 2 & 4 & 2 & 1 \end{array}\right]$$

and $D\mathcal{E}_4(G^*)$ is time-reversible. It is conjectured that a formalization of the above operations for the general case will yield a method for obtaining the equilibrium vector for $D\mathcal{E}_n(G^*)$ for any G^*. See [1] [2] for what was done for an analogous random process.

Problem: For $D\mathcal{E}_n(G^*)$ determine the equilibrium vector and whether time-reversibility holds.

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