Graver basis for an undirected graph and its application to testing the beta model of random graphs

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Abstract   In this paper, we give an explicit and algorithmic description of Graver basis for the toric ideal associated with a simple undirected graph and apply the basis for testing the beta model of random graphs by Markov chain Monte Carlo method.

1 Introduction

Random graphs and their applications to the statistical modeling of complex networks have been attracting much interest in many fields, including statistical mechanics, ecology, biology and sociology (e.g. Newman 2003; Goldenberg et al. 2009). Statistical models for random graphs have been studied since Solomonoff and Rapoport (1951) and Erdős and Rényi (1960) introduced the Bernoulli random graph model. The beta model generalizes the Bernoulli model to a discrete exponential family with vertex degrees as sufficient statistics. The beta model was discussed by Holland and Leinhardt (1981) in the directed case and by Park and Newman (2004), Blitzstein and Diaconis (2010) and Chatterjee et al. (2011) in the undirected case. The

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Rasch model (Rasch 1980), which is a standard model in the item response theory, is also interpreted as a beta model for undirected complete bipartite graphs. In this article, we discuss the random sampling of graphs from the conditional distribution in the beta model when the vertex degrees are fixed.

In the context of social network, the vertices of the graph represent individuals and their edges represent relationships between individuals. In the undirected case, the graphs are sometimes restricted to be simple, i.e., no loops or multiple edges exist. The sample size for such cases is at most the number of edges of the graph and is often small. The goodness of fit of the model is usually assessed by large sample approximation of the distribution of a test statistic. When the sample size is not large enough, however, it is desirable to use a conditional test based on the exact distribution of a test statistic. For the general background on conditional tests and Markov bases, see Drton et al. (2009).

Random sampling of graphs with a given vertex degree sequence enables us to numerically evaluate the exact distribution of a test statistics for the beta model. Blitzstein and Diaconis (2010) developed a sequential importance sampling algorithm for simple graphs which generates graphs through operations on vertex degree sequence. In this article, we construct a Markov chain Monte Carlo algorithm for sampling graphs by using the Graver basis for the toric ideal arising from the underlying graph of the beta model.

A Markov basis (Diaconis and Sturmfels 1998) is often used for sampling from discrete exponential families. Algebraically, a Markov basis for the underlying graph of the beta model is defined as a set of generators of the toric ideal arising from the underlying graph of the beta model. A set of graphs with a given vertex degree sequence is called a fiber for the underlying graph of the beta model. A Markov basis for the underlying graph of the beta model is also considered as a set of Markov transition operators connecting all elements of every fiber. Petrović et al. (2010) discussed some properties of the toric ideal arising from the model of Holland and Leinhardt (1981) and provided Markov bases of the model for small directed graphs. Properties of toric ideals arising from a graph have been studied in a series of papers by Ohsugi and Hibi (1999a,b, 2005).

The Graver basis is the set of primitive binomials of the toric ideal. Applications of the Graver basis to integer programming are discussed in Onn (2010). Since the Graver basis is a superset of any minimal Markov basis, the Graver basis is also a Markov basis, and therefore, connects every fiber. When the graph is restricted to be simple, however, a Markov basis does not necessarily connect all elements of every fiber. A recent result by Hara and Takemura (2010) implies that the set of square-free elements of the Graver basis connects all elements of every fiber of simple graphs with a given vertex degree sequence. Thus, if we have the Graver basis, we can sample graphs from any fiber, with or without the restriction that graphs are simple, in such a way that every graph in the fiber is generated with positive probability.

In the sequential importance sampling algorithm of Blitzstein and Diaconis (2010), the underlying graph for the model was assumed to be complete, i.e., all the edges have positive probability. In our approach, we can allow that some edges are absent from the beginning (structural zero edges in the terminology of contingency table analysis), such as the bipartite graph for the case of the Rasch model. In fact, the Graver basis for an arbitrary graph is obtained by restriction of the Graver basis for the complete graph

to the existing edges of G (cf. Proposition 4.13 of Sturmfels 1996). Moreover our algorithm can be applied not only for sampling simple graphs but also for sampling general undirected graphs without substantial adjustment. These are the advantages of the Graver basis.

The Graver basis for small graphs can be computed by a computer algebra system such as 4ti2 (4ti2 team). For even moderate-sized graphs, however, it is difficult to compute the Graver basis via 4ti2 in a practical amount of time. In this article, we first provide a complete description of the Graver basis for an undirected graph. In general, the number of elements of the Graver basis is too large. Therefore, we construct an adaptive algorithm for sampling elements from the Graver basis, which is enough for constructing a connected Markov chain over any fiber. The recent paper of Reyes et al. (2012) discusses the Graver basis for an undirected graph and gives a characterization of the Graver basis. We give a new description of the Graver basis, which is more suitable for sampling elements from the Graver basis.

The organization of this paper is as follows. In Sect. 2, we give a brief review on some statistical models for random graphs and clarify the connection between the models and toric ideals arising from graphs. In Sect. 3, we provide an explicit description of the Graver basis for the toric ideal associated with an undirected graph. Section 4 gives an algorithm for random sampling of square-free elements of the Graver basis. In Sect. 5, we apply the proposed algorithm to some data sets and confirm that it works well in practice. We conclude the paper with some remarks in Sect. 6.

2 The beta model of random graphs

In this section, we give a brief review of the beta model for undirected graphs according to Chatterjee et al. (2011).

Let G be an undirected graph with n vertices $V(G) = \{1, 2, \ldots, n\}$. Here, we assume that G has no loop. Let $E = E(G)$ be the set of edges. For each edge $\{i, j\} \in E$, let a non-negative integer x_{ij} be the weight for $\{i, j\}$ and denote $\boldsymbol{x} = \{x_{ij} \mid \{i, j\} \in E\}$. $\boldsymbol{x}$ is considered as an $|E|$ dimensional integer vector. We assume that an observed graph H is generated by independent binomial distribution $B(n_{ij}, p_{ij})$ for each edge $\{i, j\} \in E$, i.e., $x_{ij} \sim B(n_{ij}, p_{ij})$ with

$$p_{ij} := \frac{e^{\beta_i + \beta_j}}{1 + e^{\beta_i + \beta_j}} = \frac{\alpha_i \alpha_j}{1 + \alpha_i \alpha_j}, \qquad \alpha_i = e^{\beta_i}.$$

Then the probability of H is described as

$$
\begin{aligned}
P(H) &\propto \prod_{\{i,j\} \in E} p_{ij}^{x_{ij}} (1 - p_{ij})^{n_{ij} - x_{ij}} \\
&= \frac{1}{\prod_{\{i,j\} \in E} (1 + \alpha_i \alpha_j)^{n_{ij}}} \prod_{\{i,j\} \in E} (\alpha_i \alpha_j)^{x_{ij}} \\
&= \frac{\prod_{i \in V} \alpha_i^{\sum_{j:\{i,j\} \in E} x_{ij}}}{\prod_{\{i,j\} \in E} (1 + \alpha_i \alpha_j)^{n_{ij}}}.
\end{aligned}
\tag{1}
$$

The model (1) is called the beta model (Chatterjee et al. 2011). Note that if $x_{ij} = 0$ then the observed graph H does not have an edge $\{i, j\}$ even if $\{i, j\} \in E(G)$ for the underlying graph G.

This model was considered by many authors (e.g. Park and Newman 2004; Blitzstein and Diaconis 2010; Chatterjee et al. 2011). The p_1 model for random directed graphs by Holland and Leinhardt (1981) can be interpreted as a generalization of the beta model. When G is a complete bipartite graph, the beta model coincides with the Rasch model (Rasch 1980). The many-facet Rasch model by Linacre (1994), which is a multivariate version of the Rasch model, can be interpreted as a generalization of the beta model such that G is a complete k-partite graph.

Let $d_1, \ldots, d_n$ be a degree sequence, i.e., $d_i := \sum_{j:\{i,j\}\in E} x_{ij}$ for each vertex i. Denote $\boldsymbol{d} := (d_1, \ldots, d_n)$. The sufficient statistic for (1) is $\boldsymbol{d}$. Let $\boldsymbol{A} : |V| \times |E|$ denote the incidence matrix between vertices and edges of G. Then it is easily seen that $\boldsymbol{x}$ and $\boldsymbol{d}$ are related as

$$\boldsymbol{Ax} = \boldsymbol{d}.$$

A set of graphs (without restriction to be simple) $\mathcal{F}_{\boldsymbol{d}} = \{\boldsymbol{x} \geq 0 \mid \boldsymbol{Ax} = \boldsymbol{d}\}$ with a given degree sequence $\boldsymbol{d}$ is called a fiber for $\boldsymbol{A}$ (or for the underlying graph G). An integer array $\boldsymbol{z}$ of the same dimension as $\boldsymbol{x}$ is called a move if $\boldsymbol{Az} = 0$. A move $\boldsymbol{z}$ is written as the difference of its positive part and negative part as $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$. Since $\boldsymbol{Az} = \boldsymbol{Az}^+ - \boldsymbol{Az}^-$, every move is written as the difference of two graphs in the same fiber. A finite set of moves is called a Markov basis for the incidence matrix $\boldsymbol{A}$ if for every fiber any two graphs are mutually accessible by the moves in the set (Diaconis and Sturmfels 1998). By adding or subtracting moves in a Markov basis, we can sample graphs from any fiber in such a way that every graph in the fiber is generated with positive probability. Note that x_{ij} in the beta model (1) is restricted as $0 \leq x_{ij} \leq n_{ij}$. We denote the subset of the fiber $\mathcal{F}_{\boldsymbol{d}}$ with this restriction as $\mathcal{F}_{\boldsymbol{d},\boldsymbol{n}} = \{\boldsymbol{x} \mid \boldsymbol{Ax} = \boldsymbol{d}, 0 \leq x_{ij} \leq n_{ij}, \{i, j\} \in E\}$.

To assess the goodness of fit of the beta model we usually utilize a large sample approximation of the distribution of a test statistics. However, when n_{ij}'s are not large enough, it is not appropriate to use the large sample approximation. Especially, as mentioned in Sect. 1, graphs are restricted to be simple ($n_{ij} \equiv 1$) in some practical problems. For a simple graph, $x_{ij}, \{i, j\} \in E$, is either zero or one. A Markov basis for the incidence matrix $\boldsymbol{A}$ guarantees the connectivity of every fiber $\mathcal{F}_{\boldsymbol{d}}$ if the restriction that graphs are simple is not imposed. Under the restriction, however, a Markov basis does not necessarily connect the subset $\mathcal{F}_{\boldsymbol{d},\boldsymbol{1}}$ of the fiber $\mathcal{F}_{\boldsymbol{d}}$. For example, consider the beta model with the underlying graph G in Fig. 1 and $n_{ij} = 1$ for each edge $\{i, j\} \in E$. It can be shown that a set of all 4-cycles in G is a Markov basis for the incidence matrix of G. However $\boldsymbol{x}$ and $\boldsymbol{y}$ in Fig. 1 are not mutually accessible by 4-cycles under the restriction that graphs are simple.

For a given $\boldsymbol{x}$, $\text{supp}(\boldsymbol{x}) = \{e \mid x_e > 0\}$ denotes the set of observed edges of $\boldsymbol{x}$. For two moves $\boldsymbol{z}_1, \boldsymbol{z}_2$, the sum $\boldsymbol{z}_1 + \boldsymbol{z}_2$ is called conformal if there is no cancellation of signs in $\boldsymbol{z}_1 + \boldsymbol{z}_2$, i.e., $\emptyset = \text{supp}(\boldsymbol{z}_1^+) \cap \text{supp}(\boldsymbol{z}_2^-) = \text{supp}(\boldsymbol{z}_1^-) \cap \text{supp}(\boldsymbol{z}_2^+)$. The set of moves which can not be written as a conformal sum of two nonzero moves is called the Graver basis. The Graver basis is known to be a Markov basis (e.g. Drton et al. 2009).
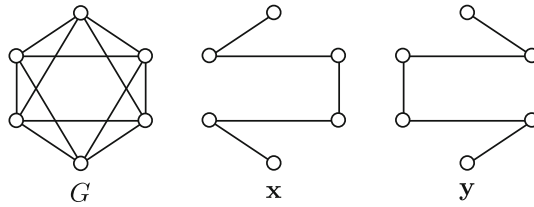
Fig. 1 Example graphs

A move is square-free if the absolute values of its elements are 0 or 1. By the same augment of Proposition 2.1 of Hara and Takemura (2010), we can obtain the following proposition.

Proposition 1 *The Graver basis for the underlying graph of the beta model connects all elements of every fiber. Furthermore, the set of square-free moves of the Graver basis connects all elements of every fiber with the restriction of simple graphs.*

Proof Let x, y be two elements of the same fiber. The difference $y - x$ is written as a conformal sum of primitive moves:

$$y - x = z_1 + \cdots + z_r \tag{2}$$

where z_i, $1 \leq i \leq r$, are elements of the Graver basis. Since there is no cancellation of signs on the right hand side, $x + z_1 + \cdots + z_k$ belongs to the same fiber for $k = 1, \ldots, r$. Therefore the Graver basis connects all elements of every fiber.

Suppose $n_{ij} = 1$ for every $\{i, j\} \in E$ in the setting of the beta model. It is easy to see that each z_i is square-free in (2). It means that the set of square-free moves of the Graver basis connects all elements of every fiber with the restriction of simple graphs.
□

Therefore, it suffices to have the Graver basis to sample graphs from any fiber with or without the restriction that graphs are simple. In the next section, we derive the Graver basis for the underlying graph of the beta model

3 Graver basis for an undirected graph

In this section, we will give two characterizations of the Graver basis for an undirected graph. Theorem 1 in Sect. 3.2 is the main result of this paper which gives a necessary and sufficient condition for a element of the Graver basis as a sequence of vertices. Proposition 3, which is used for the proof of Theorem 1, gives a characterization of the Graver basis through recursive operations on the graph, which is of some independent interests.

3.1 Preliminaries

Let $G = (V(G), E(G))$ be a simple connected graph with $V(G) = \{1, 2, \ldots, n\}$ and $E(G) = \{e_1, e_2, \ldots, e_m\}$. A *walk* connecting $i \in V(G)$ and $j \in V(G)$ is a finite sequence of edges of the form

$$w = (\{i_1, i_2\}, \{i_2, i_3\}, \ldots, \{i_q, i_{q+1}\})$$

with $i_1 = i$, $i_{q+1} = j$. The *length* of the walk w is the number of edges q of the walk. An *even* (respectively, *odd*) walk is a walk of even (respectively, *odd*) length. A walk w is *closed* if $i = j$. A *cycle* is a closed walk $w = (\{i_1, i_2\}, \{i_2, i_3\}, \ldots, \{i_q, i_1\})$ with $i_l \neq i_{l'}$ for every $1 \leq l < l' \leq q$.

For a walk w, let $V(w) = \{i_1, \ldots, i_{q+1}\}$ denote the set of vertices appearing in w and let $E(w) = \{\{i_1, i_2\}, \{i_2, i_3\}, \ldots, \{i_q, i_{q+1}\}\}$ denote the set of edges appearing in w. Furthermore, let $G_w = (V(w), E(w))$ be the subgraph of G, whose vertices and edges appear in the walk w.

In order to describe known results on the toric ideal I_G arising from an undirected graph G, we give an algebraic definition of I_G. Let $K[\mathbf{t}] = K[t_1, \ldots, t_n]$ be a polynomial ring in n variables over K. We will associate each edge $e_r = \{i, j\} \in E(G)$ with the monomial $\mathbf{t}_r = t_i t_j \in K[\mathbf{t}]$. Let $K[\mathbf{s}] = K[s_1, \ldots, s_m]$ be a polynomial ring in $m = |E(G)|$ variables over K and let π be a homomorphism from $K[\mathbf{s}]$ to $K[\mathbf{t}]$ defined by $\pi : s_r \mapsto \mathbf{t}_r$. Then the *toric ideal* I_G of the graph G is defined as

$$I_G = \ker(\pi) = \{f \in K[\mathbf{s}] \mid \pi(f) = 0\}.$$

A binomial $f = u - v \in I_G$ is called *primitive*, if there is no binomial $g = u' - v' \in I_G$, $g \neq 0$, f, such that $u'|u$ and $v'|v$. The *Graver basis* of I_G is the set of all primitive binomials belonging to I_G and we denote it by $\mathcal{G}(I_G)$. If we write the monomials u, v as $u = s^{\mathbf{x}}$, $v = s^{\mathbf{y}}$, then $u - v \in I_G$ if and only if $\mathbf{x} - \mathbf{y}$ is a move. Furthermore, $u - v \in I_G$ is primitive if and only if $\mathrm{supp}(\mathbf{x}) \cap \mathrm{supp}(\mathbf{y}) = \emptyset$ and $\mathbf{x} - \mathbf{y}$ cannot be written as a conformal sum of two nonzero moves.

For a given even closed walk $w = (e_{j_1}, e_{j_2}, \ldots, e_{j_{2p}})$, we define a binomial $f_w \in I_G$ as

$$f_w = f_w^+ - f_w^-, \quad \text{where } f_w^+ = \prod_{k=1}^{p} s_{j_{2k-1}}, \quad f_w^- = \prod_{k=1}^{p} s_{j_{2k}}.$$

An even closed walk w' is a *proper subwalk* of w, if $g_{w'}^+ \mid f_w^+$ and $g_{w'}^- \mid f_w^-$ hold for the binomial $g = g_{w'}^+ - g_{w'}^- (\neq f_w)$. Note that even if there is a proper subwalk w' of an even closed walk w, w' does not necessarily go along with w, i.e., the edges of w' may not appear as consecutive edges of w. An even closed walk w is called *primitive*, if its binomial f_w is primitive. Then the primitiveness of w is equivalent to non-existence of a proper subwalk of w.

A characterization of the primitive walks of graph G, which gives a necessary condition for a binomial to be primitive, was given by Ohsugi and Hibi (1999b).

Proposition 2 (Ohsugi and Hibi 1999b) *Let G be a finite connected graph. If $f \in I_G$ is primitive, then we have $f = f_w$ where w is one of the following even closed walks:*

  (i)   *w is an even cycle of G.*
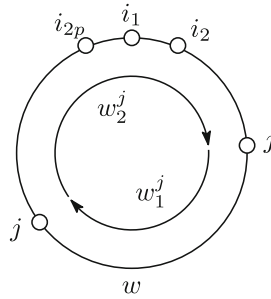 (ii) *$w = (c_1, c_2)$, where c_1 and c_2 are odd cycles of G having exactly one common vertex.*

Fig. 2 Even closed walk w

(iii) $w = (c_1, w_1, c_2, w_2)$, *where c_1 and c_2 are odd cycles of G having no common vertex and where w_1 and w_2 are walks of G both of which contain a vertex v_1 of c_1 and a vertex v_2 of c_2.*

Every binomial in the first two cases is primitive but a binomial in the third case is not necessarily primitive.

3.2 Characterization of primitive walks

In this section, we give a simple characterization of the primitive walks of a graph G as sequences of vertices. Express an even closed walk w as a sequence of vertices: $(i_1, i_2, \ldots, i_{2p}, i_1)$, where $i_1 \equiv i_{2p+1}$. Let $\#_w(i) = \#\{1 \leq l \leq 2p \mid i_l = i\}$ denote the number of times i is visited in the walk w before it returns to the vertex i_1. Consider the following condition for the even closed walk w.

Condition 1 (i) $\#_w(i) \in \{1, 2\}$ for every vertex $i \in V(w)$. (ii) For every vertex $j \in V(w)$ with $\#_w(j) = 2$ and $j = i_l = i_{l'}$, $1 \leq l < l' \leq 2p$, the closed walks $w_1^j = (i_l, \ldots, i_{l'})$ and $w_2^j = (i_{l'}, \ldots, i_{2p}, i_1, \ldots, i_{l-1}, i_l)$ are odd walks with $V(w_1^j) \cap V(w_2^j) = \{j\}$. (cf. Fig. 2).

Remark 1 The equation $V(w_1^j) \cap V(w_2^j) = \{j\}$ in Condition 1 means that there are no crossing chords in Fig. 2 when adding a chord $\{j, j\}$ to the figure for every vertex $j \in V(w)$ with $\#_w(j) = 2$.

Using Condition 1, we can characterize the Graver basis for a graph G as follows.

Theorem 1 *A binomial $f \in I_G$ is primitive if and only if there exists an even closed walk w with $f_w = f$ satisfying Condition 1.*

Remark 2 It follows from the definition of primitive walks and Theorem 1 that if an even closed walk w is primitive, every even closed walk w' with $f_{w'} = f_w$ is primitive and satisfies Condition 1.

Remark 3 As mentioned in Sect. 1, there is another characterization of Graver basis in Theorem 3.1 of Reyes et al. (2012). It also gives a necessary and sufficient condition for the primitiveness of even closed walks, by using some new graphical concepts such
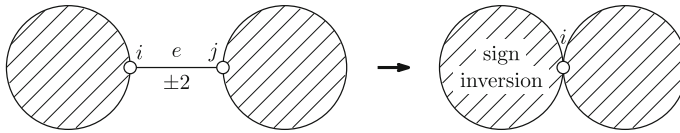
Fig. 3 Contraction

as *"block"* and *"sink"*. Our characterization in Theorem 1 gives a simpler description of Graver basis, because it does not need any new graphical concepts. Furthermore, it is more convenient in the algorithmic viewpoint: when an even closed w is given as a sequence of vertices or edges, we can easily determine if w is primitive by checking directly Condition 1 without distinguishing any graphical objects.

Before proving Theorem 1, we state another characterization of primitive walks given in Proposition 3 below. In order to that, we need some more definitions on graphs. For a walk $w = (e_{j_1}, e_{j_2}, \ldots, e_{j_q})$, let $W = W(w)$ denote the weighted subgraph $(V(w), E(w), \rho)$ of G where $\rho : E(w) \to \mathbb{Z}$ is the weight function defined by $\rho(e) := \#\{l \mid e_{j_{2l+1}} = e\} - \#\{l \mid e_{j_{2l}} = e\}$ for each edge $e \in E(w)$. For simplicity, we denote a weight $+1$ (respectively, -1) by $+$ (respectively $-$) in our figures. For a vertex $i \in V(w)$, we define two kinds of degrees of vertex i:

$$\deg_{G_w}(i) = \#\{e \in E(w) \mid i \in e\},$$
$$\deg_W(i) = \sum_{e \in E(w): i \in e} |\rho(e)|.$$

$\deg_{G_w}(i)$ is the usual degree of i in G_w. Note that the same weighted graph W might correspond to two different even closed walks w, w', i.e. $W(w) = W(w')$. Given a weighted graph W, we say that w *spans* W if $W = W(w)$ and $\{e_{j_l} \mid l:\text{odd}\} \cap \{e_{j_l} \mid l:\text{even}\} = \emptyset$.

Now we define two operations, *contraction* and *separation*, on a weighted graph W.

– Let $e = \{i, j\} \in E(w)$ be an edge with $|\rho(e)| = 2$, whose removal from G_w increases the number of connected components of the remaining subgraph. *Contraction* of e is an operation as shown in Fig. 3. That is, it first replaces W by $W' = (V(w)\backslash\{j\}, E', \rho')$ where E' consists of all edges of W contained in $V(w)\backslash\{j\}$, together with all edges $\{\alpha, i\}$, where $\{\alpha, j\}$ is an edge of W different from e. Then, it defines ρ' by inversion of the signs of weights of edges belonging to the i-side of W.

– Let $i \in V(w)$ be a vertex with $\deg_{G_w}(i) = \deg_W(i) = 4$, such that the removal of i increases the number of connected components of the remaining subgraph and the positive side as well as the negative side of i fit to one of three cases (a)–(c) (respectively, to the sign reverse cases) in Fig. 4. *Separation* of i is an operation as shown in Fig. 4. That is, it first deletes the vertex i and all edges connected to i on W. Then, in the case of (a), it adds a new edge $\{k_1, k_2\}$ with weight $+1$. In the case of (b), it redefines $\rho(\{k_1, k_2\}) := +2$ and then contracts $\{k_1, k_2\}$, where we assume that the contraction of $\{k_1, k_2\}$ is possible. In the case of (c), it redefines
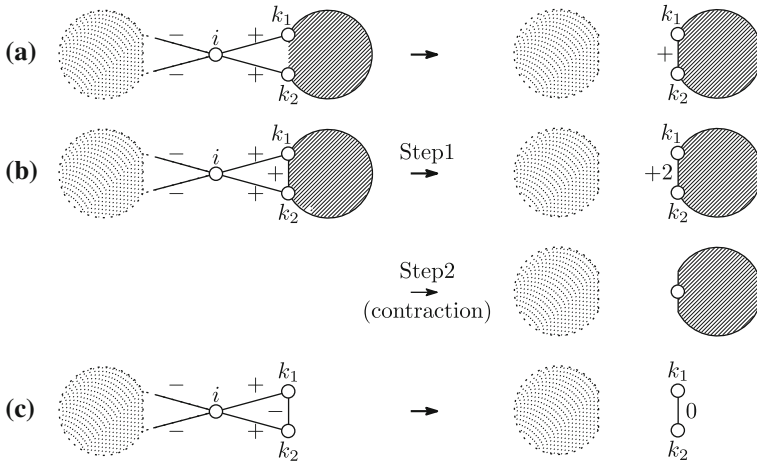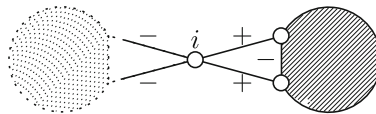
Fig. 4 Separation

Fig. 5 A vertex i whose separation is not defined

$\rho(\{k_1, k_2\}) := 0$. We call this $\{k_1, k_2\}$ an edge with weight 0. The sign reverse cases are defined in the same way.

Note that the separation is not defined for any vertex i with $\deg_{G_w}(i) = \deg_W(i) = 4$, if i fits to none of three cases (a)–(c) in Fig. 4. The vertex i in Fig. 5 is such an example, because its positive side fits to none of three cases (a)–(c) in Fig. 4.

Let *insertion* and *binding* be the reverse operations of contraction and separation, respectively. With these operations, consider the following condition for an even closed walk $w = (e_{j_1}, e_{j_2}, \ldots, e_{j_{2p}})$.

Condition 2   (i) $\{e_{j_l} \mid l\text{:odd}\} \cap \{e_{j_l} \mid l\text{:even}\} = \emptyset$. Every vertex $i \in V(w)$ satisfies $\deg_W(i) \in \{2, 4\}$. For every vertex i with $\deg_W(i) = 4$, its removal from G_w increases the number of connected components of the remaining subgraph.
(ii) Let $\tilde{W}$ be a graph obtained by recursively applying contraction and separation of all possible edges and vertices in W. Then each connected component of $\tilde{W}$ is an even cycle or an edge with weight 0.

Proposition 3 *For an even closed walk w, the binomial f_w is primitive if and only if w satisfies Condition 2.*

We establish some lemmas to prove Proposition 3. Our proof also shows that $\tilde{W}$ in Condition 2 does not depend on the order of application of contractions and separations excepting the sign inversion of weights of edges of each connected component in $\tilde{W}$.
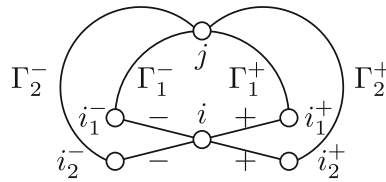
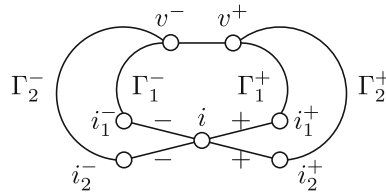**Fig. 6** Case that there exists a vertex $j \in V^+ \cap V^-$

Fig. 7 Case that there exists an edge $\{v^+, v^-\}$

Lemma 1 *If w is a primitive walk, w satisfies (i) in Condition 2.*

Proof Consider a vertex $i \in V(w)$. Since w is closed, $\deg_W(i)$ is even. Furthermore, since w is primitive, $\{e_{j_l} \mid l:\text{odd}\} \cap \{e_{j_l} \mid l:\text{even}\} = \emptyset$ holds which implies that there is no cancellation in the calculation of weight on any edge. Then, a half of the weight $\deg_W(i)/2$ is assigned as positive weights and other half $\deg_W(i)/2$ is assigned as negative weights to the edges connected to i on W. Therefore, $\deg_W(i) \in \{2, 4, 6, \ldots\}$. Now suppose $\deg_W(i) \geq 6$. Consider that we start from a vertex i along an edge with positive weight and go along the walk w or its reverse until returning back to i again for the first time. Since w is primitive, we have to come back to i along an edge with positive weight for the first time. Let us continue along w or its reverse until returning back to i. By the same reasoning, the last edge of this closed walk has a negative weight. This implies that this even closed walk becomes a proper subwalk of w, a contradiction to the primitiveness of w. Therefore, $\deg_W(i)$ is 2 or 4.

To prove the remaining part, let $i \in V(w)$ be a vertex with $\deg_W(i) = 4$ and consider all closed walks on W, where the edge starting from i and the edge coming back to i have positive weights. Let V^+ be the set of vertices other than i which appear in one of these walks and V^- is defined in the same way. Then $V^+ \cup V^- \cup \{i\} = V(w)$ holds. First, we show $V^+ \cap V^- = \emptyset$. Suppose that there exists a vertex $j \in V^+ \cap V^-$. Then, as shown in Fig. 6, there are two closed walks $(\{i, i_1^+\}, \Gamma_1^+, \Gamma_2^+, \{i_2^+, i\})$ and $(\{i, i_1^-\}, \Gamma_1^-, \Gamma_2^-, \{i_2^-, i\})$. This implies that we can construct a proper subwalk of w by the combination of $\{i, i_k^+\}, \Gamma_k^+ (k = 1, 2)$, and $\Gamma_l^-, \{i_l^-, i\}(l = 1, 2)$, a contradiction to the primitiveness of w. Therefore $V^+ \cap V^- = \emptyset$. Second, suppose that the removal of the vertex i from G_w does not increase the number of connected components of the remaining subgraph. Then, there are vertices $v^+ \in V^+, v^- \in V^-$ such that $\{v^+, v^-\} \in E(w)$, because $V^+ \cap V^- = \emptyset$ holds as shown above. Hence, as shown in Fig. 7, an even closed walk $(\{i, i_k^+\}, \Gamma_k^+, \{v^+, v^-\}, \Gamma_l^-, \{i_l^-, i\})$ is a proper subwalk of w for appropriate $k, l \in \{1, 2\}, k \neq l$, which contradicts to the primitiveness of w. Therefore the removal of i from G_w increases the number of connected components of the remaining subgraph. $\square$

In the following four lemmas, we show that contraction, separation, and these inverse operations preserve the primitiveness of an even closed walk. The proofs of lemmas are postponed to Appendix.

Lemma 2 (Preservation of the primitiveness under contraction) *Let an even closed walk w be primitive and $\tilde{W}$ be the weighted graph which is obtained by a contraction for an edge with its weight ± 2 on W. Then any even closed walk $\tilde{w}$ spanning $\tilde{W}$ is primitive.*

Lemma 3 (Preservation of the primitiveness under separation) *Let an even closed walk w be primitive and W_1, W_2 be the weighted graphs obtained by the separation of a vertex i. Then any even closed walks $w_l(l = 1, 2)$ spanning $W_l(l = 1, 2)$ are primitive or of length two with $f_{w_l} = 0$.*

Lemma 4 (Preservation of the primitiveness under insertion) *Let w be a primitive walk and let $\tilde{W}$ be the weighted graph obtained by the insertion to i with $deg_W(i) = 4$ on W. Then any even closed walk $\tilde{w}$ spanning $\tilde{W}$ is primitive.*

Lemma 5 (Preservation of the primitiveness under binding) *Let each w_l $(l = 1, 2)$ be a primitive walk or a closed walk with length two, and W be the weighted subgraph obtained by binding of W_1 and W_2. Then any even closed walk w spanning W is primitive.*

We now give proofs of Proposition 3 and Theorem 1.

Proof (Proof of Proposition 3) Let w be a primitive walk. From Lemma 1 w satisfies (i) in Condition 2 and every edge e with $|\rho(e)| = 2$ can be contracted. Furthermore, it is easy to see that every vertex i with $deg_W(i) = 4$ can be separated after recursively applying contractions of all possible edges. Therefore $deg_W(i) = 2$ holds for every vertex i on $\tilde{W}$. From Lemmas 2 and 3, each even closed walk corresponding to the connected component of $\tilde{W}$ is primitive or of length two. Then, every connected component of $\tilde{W}$ is an even cycle or an edge with weight 0, because from Proposition 2 every primitive walk includes a vertex i with $deg_W(i) = 4$ if it is not an even cycle. Therefore, a primitive walk w satisfies Condition 2. Conversely, suppose an even closed walk w satisfies Condition 2. From Proposition 2 and Lemmas 4 and 5, w is primitive.   □

Proof (Proof of Theorem 1) Let w be a primitive walk. From Lemma 1, $\#_w(i) \in \{1, 2\}$ holds for each vertex $i \in V(w)$ and $V(w_1^j) \cap V(w_2^j) = \{j\}$ holds for each vertex $j \in V(w)$ with $\#_w(j) = 2$. By the primitiveness of w, the closed walks $w_1^j = (j, \ldots, j)$ and $w_2^j = (j, \ldots, i_1, \ldots, j)$ along w are odd closed walks. Therefore, w satisfies Condition 1.

Conversely, let w be an even closed walk with Condition 1. From Proposition 3, it suffices to show that w satisfies Condition 2. The condition (i) in Condition 2 follows from Condition 1. Then, it is enough to confirm that w satisfies the condition (ii) in Condition 2.

First, we claim that every edge $e \in E(w)$ with $|\rho(e)| = 2$ can be contracted and every vertex j with $\#_w(j) = 2$ and $deg_{G_w}(j) = 4$, i.e. $deg_{G_w}(j) = deg_W(j) = 4$, can be separated. The case of contraction is obvious from Condition 1. We confirm

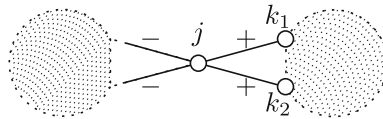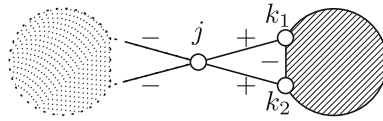**Fig. 8** A vertex j with $\deg_{G_w}(j) = \deg_W(j) = 4$

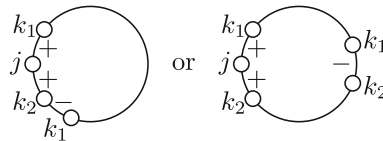**Fig. 9** A vertex j which does not exist in w with Condition 1

Fig. 10 Case that there exists a vertex j in Fig. 9

the case of separation. Consider the vertex j in Fig. 8. If an edge $\{k_1, k_2\}$ dose not exist or exists with weight $+1$, it belongs to the case (a) or (b) in Fig. 4, respectively. Let us consider the case that there exists an edge $\{k_1, k_2\}$ with weight -1 and suppose that the vertex k_1 connects to more than three edges as shown in Fig. 9. Then, j, k_1 and k_2 appear in w like $(j, k_1, \ldots, k_1, k_2, j)$ or $(j, k_1, \ldots, k_1, k_2, \ldots, k_2, j)$, because $V(w_1^j) \cap V(w_2^j) = \{j\}$ holds. This implies that $(k_1, \ldots, k_1)$ is even as shown in Fig. 10, which contradicts Condition 1. Hence the case with $\{k_1, k_2\}$ with weight -1 belongs to (c) in Fig. 4. Therefore, the claim is confirmed.

Second, we verify that contraction and separation on W preserve Condition 1. Consider the case of contraction of an edge $\{i, j\} \in E(W)$. From Condition 1, such i, j appear in w as $w = (i_1, \ldots, i_{l_1}, i, j, i_{l_2}, \ldots, i_{l_3}, j, i, i_{l_4}, \ldots, i_1)$. The contraction of $\{i, j\}$ is equivalent to replacing w by $(i_1, \ldots, i_{l_1}, i, i_{l_2}, \ldots, i_{l_3}, i, i_{l_4}, \ldots, i_1)$. This change causes the decrease of two edges from w, and preserves Condition 1. The case of separation is checked in the same way.

Finally, consider the weighted graph W' obtained by all possible contractions and separations on W. From the claims above, every connected component of W' satisfies Condition 1 and has no vertex j with $\#_w(j) = 2$, i.e. an even cycle or an edge with weight 0. Therefore, w satisfies Condition 2.   □

Remark 4 We proved Theorem 1 using an alternative characterization of a primitive binomial in Proposition 3. However, as suggested by a referee, there may exist a shorter direct proof of Theorem 1. It is of interest to consider such a direct proof.

4 Algorithm for generating elements of Graver basis

In this section, we present an algorithm for generating elements randomly from the Graver basis for a simple undirected graph. As shown in Proposition 1, for testing the beta model of random graphs with $n_{ij} = 1$, we only need square-free elements of the

Graver basis. Therefore, the restriction to square-free elements of our algorithm will be discussed in Remark 5. Theorem 1 guarantees the correctness of our algorithm.

We need some tools in order to construct an algorithm. Let T be a weighted tree $(V(T), E(T), \mu)$ where $\mu : V(T) \to \mathbb{Z}_{\geq 2} = \{2, 3, \dots\}$ is a weight function. For this weighted tree T, let us consider the following condition.

Condition 3 For each vertex $v_T \in V(T)$, $\deg(v_T) \leq \mu(v_T)$ and $\deg(v_T) \equiv \mu(v_T)$ mod 2.

With these tools, let us consider generating an element of the Graver basis for a simple undirected graph $G = (V(G), E(G))$. For simplicity, first consider the case that that G is complete. We call an edge e with $|\rho(e)| = 2$ a cycle in G_w for an even closed walk w in this section. We will discuss later the case that G is not complete. Let $T = (V(T), E(T), \mu)$ be a weighted tree satisfying Condition 3 and the following equation:

$$\sum_{v_T \in V(T)} \mu(v_T) - |E(T)| \leq |V(G)|. \tag{3}$$

Then, we can construct a primitive walk in G using T as follows. First, we assign the set of vertices $V_{v_T} \subseteq V(G)$ with $|V_{v_T}| = \mu(v_T)$ for each vertex $v_T \in V(T)$ under the equation

$$|V_{v_T} \cap V_{v'_T}| = \begin{cases} 1, & \text{if } \{v_T, v'_T\} \in E(T), \\ 0, & \text{if } \{v_T, v'_T\} \notin E(T), \end{cases} \quad (v'_T \in V(T))$$

and every vertex $v \in V(G)$ is assigned at most twice. Equation (3) guarantees that this assignment is possible. Second, we make cycles in G by arbitrarily ordering the vertices V_{v_T}. Then we make a subgraph of G by taking the union of these cycles. Finally, we obtain a closed walk by choosing a root vertex from this subgraph and going around it. It is easy to see that this closed walk is primitive by Theorem 1.

Conversely we can construct a weighted tree with Condition 3 and (3) from each primitive walk. Let w be a primitive walk. First, the vertex set $V(T)$ is constructed by creating a vertex v_c of T for each cycle c in G_w. Second, the edge set $E(T)$ is obtained by adding edge $\{v_c, v_{c'}\}$ to $E(T)$ for each pair of cycles c, c' in G_w with $V(c) \cap V(c') \neq \emptyset$. Then, we assign weight $\mu(v_c) := |V(c)|$ to each vertex $v_c \in V(T)$.

Therefore, once we have a weighted tree T with Condition 3 and (3), we can construct an element of the Graver basis for G. Such a tree T is constructed by the following algorithm.

Algorithm 1 (Algorithm for constructing an weighted tree)
 Input : A complete graph $G = (V(G), E(G))$.
Output : A weighted tree $T = (V(T), E(T), \mu)$ with Condition 3 and (3).

1. Let $V(T), E(T)$ be empty sets and $n := |V(G)|$.
2. Add a root vertex r to $V(T)$.
3. Assign $\mu(r)$ a weight from $\{2, 3, \dots, n\}$ randomly.
4. Grow T by the following loop.

(a) For each vertex $v_T \in V(T)$ which is deepest from r, add edges $\{v_T, v_T^i\}$ to $E(T)$ and the endpoints v_T^i ($i = 0, 1, \ldots, I_{v_T}$) to $V(T)$, where the number I_{v_T} is randomly decided under the following two conditions:

  – $I_{v_T} + 1 \le \mu(v_T)$.
  – $I_{v_T} + 1 \equiv \mu(v_T) \mod 2$.

(b) For each new vertex v_T^i, assign $\mu(v_T^i)$ a weight from $\{2, 3, \ldots, n - \alpha\}$ randomly, where $\alpha := \sum_{v_T \in V(T)} \mu(v_T) - |E(T)|$.

(c) Recompute α and if $\alpha > n$, delete all new vertices and edges in the above (a) and break the loop.

(d) If the total number of new edges is equal to 0, break the loop.

(e) Return to (a).

5. If $|V(T)| = 1$ and $\mu(r)$ is odd, change $\mu(r)$ to $\mu(r) - 1$ or $\mu(r) + 1$.

6. If $|V(T)| > 1$ and T has a leaf with even weight, subtract or add 1 to the weight.

7. Output T.

Algorithm 1 provides a simple algorithm for generating an element of Graver basis as follows.

Algorithm 2 (Algorithm for generating an element of Graver basis)

Input : A complete graph $G = (V(G), E(G))$.
Output : A primitive walk w.

1. Construct a weighted tree T with Condition 3 and (3) by Algorithm 1.
2. Construct a primitive walk by assigning vertices of G and ordering them randomly.
3. Output w.

Since there is no restarts in Algorithm 2, it has a fixed worst case running time for a complete graph G. In each step, the algorithm performs $O(|V(G)|)$ operations. Then it generates one element of the Graver basis for G in $O(|V(G)|)$ time. A demonstration for the case of a complete graph G with $|V(G)| = 25$ is shown in Figs. 11 and 12. The output of this demonstration is a primitive walk w with $|V(G_w)| = 21$ in Fig. 12.

Remark 5 For the case that an input graph G is not complete, the elements of the Graver basis for G can be generated by throwing away elements with supports not contained in G (Proposition 4.13 of Sturmfels 1996). In fact this is the advantage of considering the Graver basis. The restriction for generation of square-free elements of the Graver basis can be realized by a slight modification in Algorithm 1. In fact, it suffices to change merely $\{2, 3, 4, \ldots\}$ to $\{3, 4, \ldots\}$ in Step *3* and in *(b)* of Step *4* in Algorithm 1.

Remark 6 The output of Algorithm 2 is not uniformly distributed over all elements of Graver basis. The distribution depends on how to implement the randomness in Step *3* and in *(b)* of Step *4* in Algorithm 1.

Algorithm 2 allows us to uniformly sample graphs with the common degree sequence via Metropolis–Hastings algorithm with the Graver basis, with or without the restriction that graphs are simple. It is done by constructing a connected Markov chain of graphs with the common degree sequence. In each iteration, a primitive walk is randomly generated by Algorithm 2. If the primitive walk is applicable, a new sample graph with the same degree sequence is obtained by adding the primitive walk,
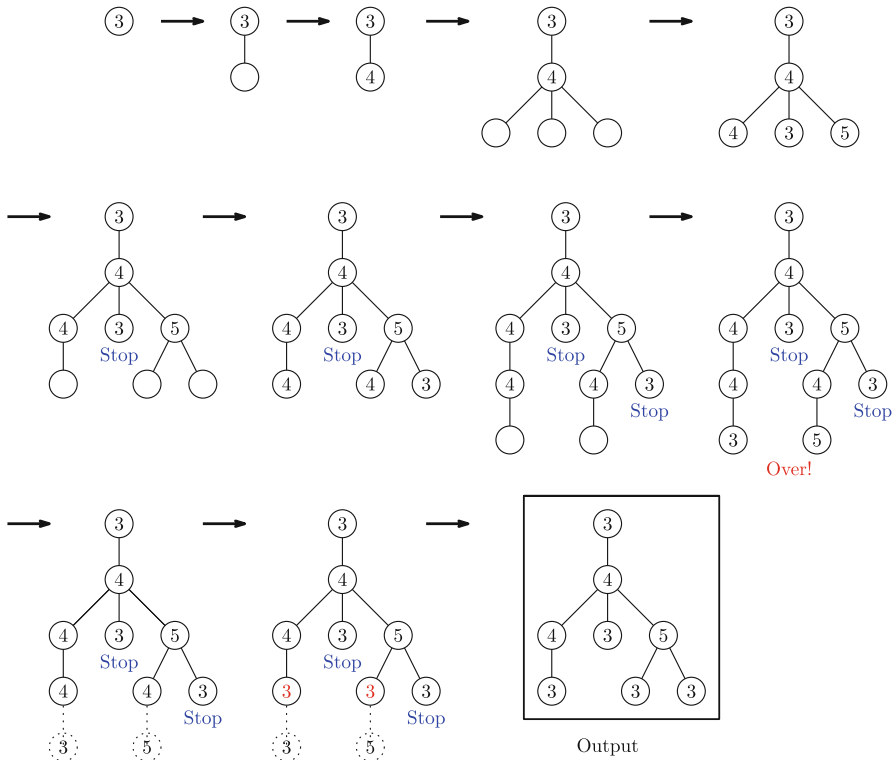
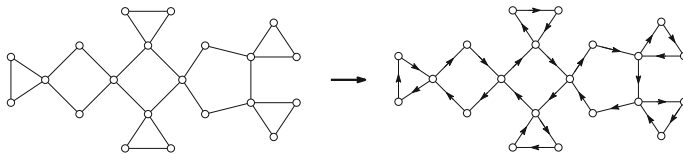**Fig. 11** Demonstration of Algorithm 1

Fig. 12 Demonstration of Algorithm 2

otherwise the primitive walk is rejected. Note that Metropolis-Hastings algorithm does not require the uniformity of the distribution of generated primitive walks. As long as there is a positive probability of generating every element of the Graver basis, the Metropolis–Hastings algorithm realizes uniform sampling of graphs with the common degree sequence.

5 Numerical experiments

In this section, we present numerical experiments with elements of the Graver basis computed by Algorithm 2 in Sect. 4. The implementation of Metropolis-Hastings algorithm with Algorithm 2 is done by Java 1.6.0 on Windows OS with Intel(R) Core(TM) i7-2829QM CPU@2.30GHz.
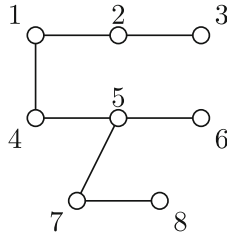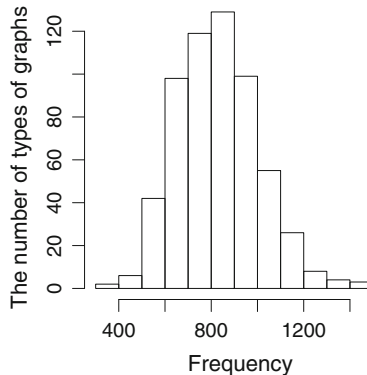
Fig. 13 Small graph H_0

Fig. 14 Histogram from sampling

5.1 A simulation with a small graph

We run a Markov chain over the fiber containing a small graph H_0 in Fig. 13. The under-lying graph $G = K_8$ is assumed to be complete with eight vertices. By the Markov chain we sampled 510,000 graphs in the fiber, including 10,000 burn-in steps. The number of types of obtained graphs in our chain is 591. By enumeration we checked that 591 is actually the number of the elements of the fiber of H_0. The histogram of this experiment is shown in Fig. 14. The horizontal axis expresses the frequency of each type of graph and the vertical axis expresses the number of types. The mean of the number of appearances of each type is 829 and the standard deviation is 179. This experiment shows that the algorithm samples each element of the fiber almost uniformly.

5.2 The beta model for the food web data

We apply Algorithm 2 for testing of the real data, the observed food web of 36 types of organisms in the Chesapeake Bay during the summer. This data is available online at Ulanowicz (2005). Blitzstein and Diaconis (2010) analyzed essentially the same data set.

The graph H of the data is shown in Fig. 15. The vertices represent the types of organisms like blue crab, bacteria etc., and the edges represent the relationship of one preying upon the other. The degree sequence of H is

$$(9, 10, 6, 2, 3, 3, 9, 11, 6, 4, 6, 7, 5, 7, 8, 4, 3, 8,$$
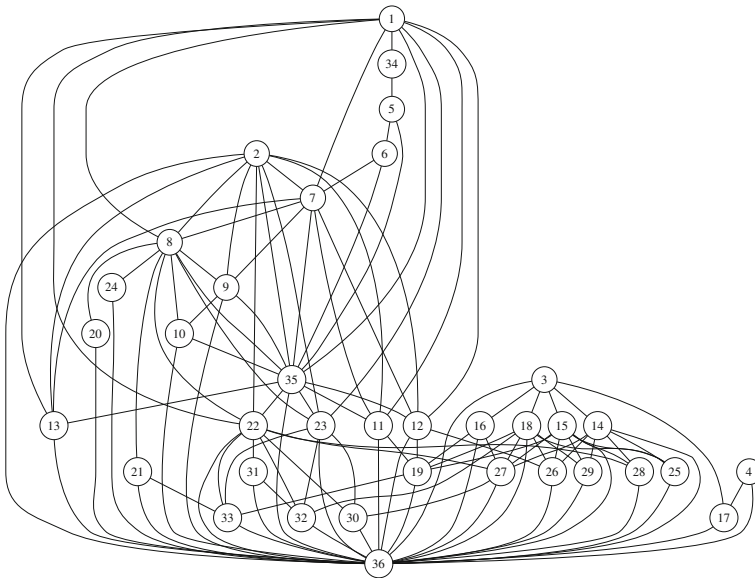$$7, 2, 3, 11, 8, 2, 4, 5, 7, 4, 4, 4, 3, 5, 5, 2, 14, 29).$$

Fig. 15 Food web for the Chesapeake Bay during the summer

Although there is a self loop at the vertex 19 in the observation, we ignored it for simplicity.

We set the beta model (1) in Sect. 2 with $n_{ij} = 1$ for each edge $\{i, j\}$ as the null hypothesis. Then the probability of H is described as

$$P(H) \propto \frac{\prod_{i \in V} \alpha_i^{d_i}}{\prod_{\{i,j\} \in E}(1 + \alpha_i \alpha_j)}. \tag{4}$$

Parameter α_i $(i \in V)$ is interpreted as the value of organism represented by the vertex i as a food to other organisms. Then the beta model (4) implies that a vertex i with large α_i is likely to be connected to many edges. Let $P \in (4)$ mean that P can be expressed by (4) for a set of parameters $\{\alpha_i\}_{i \in V}$. Consider now the statistical hypothesis testing problem

$$H_0 : P \in (4) \text{ versus } H_1 : P \notin (4).$$

Starting from the graph in Fig. 15, we construct a Markov chain of 10,100,000 graphs including 100,000 burn-in steps and compute the chi-square statistic of each graph as a test statistic. The running time of the calculation is 5 min and 4.8 s. Using the maximum likelihood estimator, the chi-square value of observed graph H is 477 and the histogram of the estimated distribution of the chi-square values is shown in Fig. 16. The approximate p-value is 0.286. This value is not so small and there is no evidence against the beta model (4).

Next, we consider some other characteristics of the observed graph H and graphs obtained by the above Markov chain. We compute their clustering coefficient defined
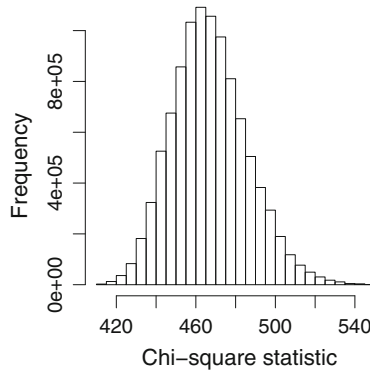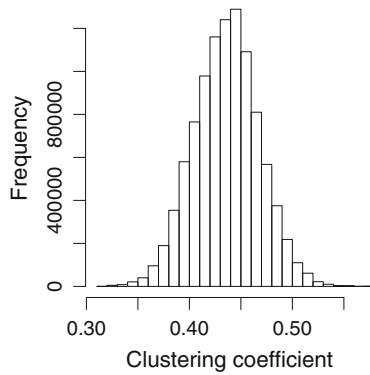
Fig. 16 Histogram of chi-square statistic

Fig. 17 Histogram of clustering coefficient

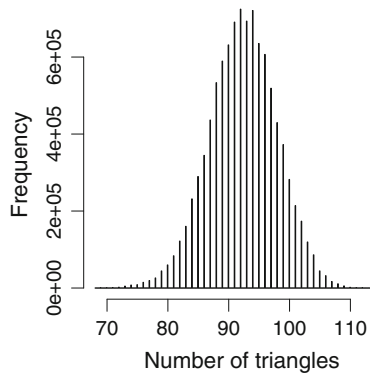**Fig. 18** Histogram of number of triangles

by Wattz and Strogatz (1998) and also count the number of triangles (3-cycles). For the observed graph H, the values of clustering coefficient and the number of triangles are 0.447 and 101, respectively. For the sampled graphs, the histograms are obtained as in Fig. 17 and 18 and their mean values are 0.436 and 92.4, respectively. The differences

between the actual values and the means of sampled graphs are not large. It suggests that these statistics agree with the beta model (4).

As mentioned in Sect. 1 there are computer algebra systems such as 4ti2 (4ti2 team) to compute the Graver basis. However the whole Graver basis is huge and difficult to compute even for a moderate-sized graph like the real data above. Algorithm 2, our adaptive algorithm, enables us to perform the Markov chain Monte Carlo method for such a moderate-sized graph.

6 Concluding remarks

In this paper, we obtained a simple characterization of the Graver basis for toric ideals arising from undirected graphs. This Graver basis allows us to perform the conditional test of the beta model for arbitrary underlying graph. Our characterization allows us to construct an algorithm for sampling elements of the Graver basis, which is sufficient for performing the conditional test.

By numerical experiments, we confirmed that our procedure works well in practice. We should mention that the sequential importance sampling method of Blitzstein and Diaconis (2010) may work faster for the case of complete underlying graph.

If we allow multiple edges, then we do not need the Graver basis. A minimal Markov basis, which is often much smaller than the Graver basis, is sufficient for connectivity of Markov chains. Properties of Markov basis for the p_1-model have been given in Petrović et al. (2010). It is of interest to study properties of minimal Markov bases for undirected graphs, including the case of allowing self loops.

Appendix A: Proofs of Lemmas in Sect. 3.2

A.1 Proof of Lemma 2

The contraction of the edge with its weight ± 2 on W is possible from Lemma 1. We denote this edge by $e = \{i, j\}$ as shown in Fig. 19. Suppose $\tilde{w}$ is not primitive. Then there exists an proper subwalk $\tilde{w}'$ of $\tilde{w}$. If $i \notin V(\tilde{w}')$, $\tilde{w}'$ is also a proper subwalk of w, a contradiction to the primitiveness of w. Then $i \in V(\tilde{w}')$. However, a proper subwalk of w is constructed by embedding e into $\tilde{W}'$. Therefore, $\tilde{w}$ is primitive. □
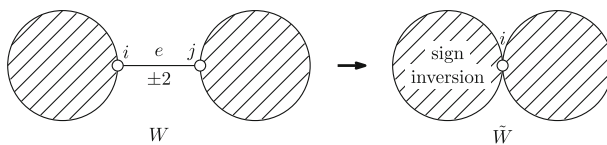

Fig. 19 Contraction of an edge e
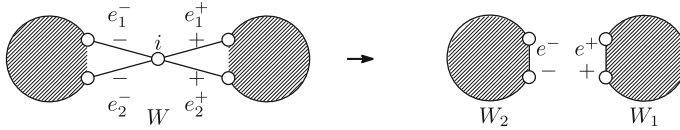
Fig. 20 Separation of a vertex i
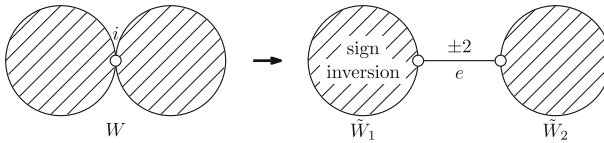

Fig. 21 Insertion to a vertex i

A.2 Proof of Lemma 3

We consider the case that both positive and negative sides of i correspond to (a) in Fig. 4 and relevant edges are labeled as shown in Fig. 20. Suppose w_1 is neither primitive nor of length two. Then there exists a proper subwalk w_1' of w_1 on W_1. If $e^+ \notin E(w_1')$, w_1' is also a proper subwalk of w, a contradiction to the primitiveness of w. Then $e^+ \in E(w_1')$. Now w_1' is expressed as follows:

$$w_1' = (e_{i_1}, e_{i_2}, \ldots, e_{i_k}, e^+, e_{i_{k+1}}, \ldots, e_{i_s}).$$

Then an even closed walk on W

$$(e_{i_1}, e_{i_2}, \ldots, e_{i_k}, e_1^+, e_1^-, \ldots, e_2^-, e_2^+, e_{i_{k+1}}, \ldots, e_{i_s})$$

is a proper subwalk of w. This contradicts the primitiveness of w. Therefore w_1 is primitive or of length two. The cases of (b) and (c) in Fig. 4 are shown in the same way. Note that it is easy to confirm the possibility of contraction after the step 1 in the case (b) from Lemma 1 and then the primitiveness is guaranteed by Lemma 2. By the same argument, the case of w_2 is confirmed.   □

A.3 Proof of Lemma 4

Let e be the new edge appearing through the insertion to i as shown in Fig. 21. Suppose $\tilde{w}$ is not primitive. Then, there exists a proper subwalk $\tilde{w}'$ of $\tilde{w}$. If $e \notin E(\tilde{w}')$, $\tilde{w}'$ is contained in $\tilde{W}_1$ or $\tilde{W}_2$. Then $\tilde{w}'$ or its reverse becomes a proper subwalk of w. This contradicts the primitiveness of w. Hence $e \in E(\tilde{w}')$. Then we can construct a proper subwalk of w by removing e from $\tilde{w}'$ and reversing the weights of edges belonging to $E(w_1)$, a contradiction to the primitiveness of w. Therefore, $\tilde{w}$ is primitive.   □
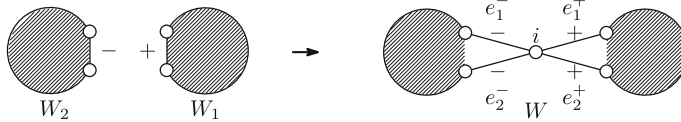
Fig. 22 Binding of W_1 and W_2

A.4 Proof of Lemma 5

Let i be the new vertex appearing through the binding. We consider the case that both positive and negative sides of i correspond to (a) in Fig. 4 and relevant edges are labeled as shown in Fig. 22. Other cases are shown in the same way.

Suppose w is not primitive. Then there exists a proper subwalk w' of w. Here, we choose a primitive walk as w'. If $i \notin V(w')$, w' is also a proper subwalk of w_1 or w_2. Then $i \in V(w')$. This implies that all four edges connected to i appear in w'. Let us consider the separation of i to W'. Then the resulting two weighted graphs W_1', W_2' are primitive from Lemma 3. Furthermore at least one of w_i' $(i = 1, 2)$ is a proper subwalk of w_i, a contradiction to the primitiveness of w_i. Therefore, w is primitive. □

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