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<th>Title</th>
<th>TORIC IDEALS AND CONTINGENCY TABLES (Algebra, Languages and Computation)</th>
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TORIC IDEALS AND CONTINGENCY TABLES

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ABSTRACT. Fundamental questions on semigroup rings and toric ideals arising from contingency tables will be studied. In addition to discussing recent developments on such the topic, the algebraic background of contingency tables, including the algebraic aspects of Markov chains will be also explained.

1. ALGEBRAIC BACKGROUND OF CONTINGENCY TABLES

In commutative algebra, a Markov chain can be regarded as a system of binomial generators of the toric ideal arising from a contingency table.

An n-way contingency table is an n dimensional matrix whose entries are non-negative integers. For example, the following 2-way contingency table is given in [6, Table 2].

Example 1.1. Looking at the below 2-way contingency table $T$, we want to know whether “Eye color” and “Hair color” are correlated.

<table>
<thead>
<tr>
<th>Eye color \ Hair color</th>
<th>Black</th>
<th>Brunette</th>
<th>Red</th>
<th>Blonde</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brown</td>
<td>68</td>
<td>119</td>
<td>26</td>
<td>7</td>
<td>220</td>
</tr>
<tr>
<td>Blue</td>
<td>20</td>
<td>84</td>
<td>17</td>
<td>94</td>
<td>215</td>
</tr>
<tr>
<td>Hazel</td>
<td>15</td>
<td>54</td>
<td>14</td>
<td>10</td>
<td>93</td>
</tr>
<tr>
<td>Green</td>
<td>5</td>
<td>29</td>
<td>14</td>
<td>16</td>
<td>64</td>
</tr>
<tr>
<td>Total</td>
<td>108</td>
<td>286</td>
<td>71</td>
<td>127</td>
<td>592</td>
</tr>
</tbody>
</table>

In general, when an n-way contingency table is given, we are interested in n factor interaction. For the sake of simpleness, we explain the case $n = 2$ here. (See [1] for details.) We consider the following $I \times J$ contingency table $T_0$:

\[
\begin{array}{c|cccc|c}
X & Y_1 & Y_2 & \cdots & Y_J & \text{Total} \\
\hline
X_1 & n_{11} & n_{12} & \cdots & n_{1J} & n_{1+} \\
X_2 & n_{21} & n_{22} & \cdots & n_{2J} & n_{2+} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
X_I & n_{I1} & n_{I2} & \cdots & n_{IJ} & n_{I+} \\
\hline
\text{Total} & n_{+1} & n_{+2} & \cdots & n_{+J} & N
\end{array}
\]

Then we suppose the null hypothesis $H_0$ “there is no association between $X$ and $Y$,” and try to test it.
One of the popular methods which test the association of X and Y is the χ² test. In the χ² test, we compute the χ² statistic

$$\chi^2(T_0) = \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{(n_{ij} - \frac{n_{i+}n_{+j}}{N})^2}{\frac{n_{i+}n_{+j}}{N}}.$$  

If the hypothesis $H_0$ is true, then χ² statistic has asymptotic χ² distributions with degrees of freedom $(I - 1)(J - 1)$. Thus we compare $\chi^2(T_0)$ with the value $\alpha_{0.05}$ of the right-hand side 5% point of χ² distribution. If $\chi^2(T_0) < \alpha_{0.05}$, then we conclude that $H_0$ is true, and X and Y are independent.

However, it is known that, if $T_0$ is sparse, that is, there is a lot of cells with $n_{i+}n_{+j}/N < 5$, then the χ² approximation is bad. Hence χ² test is not good for contingency tables such that $N/IJ$ is small.

For such sparse contingency tables, we use the Fisher's exact test. Let $\mathcal{F}_{T_0}$ denote the set of tables with the same marginal distribution as $T_0$. For example, in Example 1.1, $\mathcal{F}_T$ is the set of all 4×4 matrix such that the sum of four rows is (108 286 71 127) and the sum of four columns is the transpose of (220 215 93 64). We now assume that $H_0$ is true and that $\mathcal{F}_{T_0}$ follows the multiple hypergeometric distribution. Here the multiple hypergeometric distribution is defined by

$$P(T) = \frac{\left(\prod_{i=1}^{I} n_{i+}!\right) \left(\prod_{j=1}^{J} n_{+j}!\right)}{N! \prod_{i,j} n_{ij}!}$$

for each $T \in \mathcal{F}_{T_0}$. For the Fisher's exact test, we compute $\chi^2(T)$ for all $T \in \mathcal{F}_{T_0}$ and P-value

$$P = \sum_{T \in \mathcal{F}_{T_0}, \chi^2(T) \geq \chi^2(T_0)} P(T)$$

of $T_0$. If $P > 0.05$, then we conclude that $H_0$ is true, and X and Y are independent.

Unfortunately, the Fisher's exact test also has a problem. In general, it is very difficult to enumerate all elements of $\mathcal{F}_{T_0}$. For example, in Example 1.1, $\mathcal{F}_T$ consists of 1,225,914,276,768,514 elements. In such a case, it is almost impossible to compute P-value of $T_0$ exactly.

Here we are in the position to introduce Markov Chain Monte Carlo method (called MCMC method for short). For the computation of P-value, we give up above exact calculation and make use of the Markov chain to do the sampling from $\mathcal{F}_{T_0}$.

Note that, if both $T$ and $T'$ belong to $\mathcal{F}_{T_0}$, then $T - T'$ is an integer $I \times J$ matrix such that the sum of all entries of each rows and each columns is zero. Let $\mathcal{M}_{I \times J}$ denote the set of all integer $I \times J$ matrices which satisfies that the sum of all entries of each rows and each columns is zero. Then a Markov basis is a finite subset $\{T_1, \ldots, T_t\} \subset \mathcal{M}_{I \times J}$ satisfying that, for any $T, T' \in \mathcal{F}_{T_0}$, there exist $T_{i_1}, \ldots, T_{i_A}$ with $\epsilon_k = \pm 1$ such that

$$T' = T + \sum_{k=1}^{A} \epsilon_k T_{i_k},$$
\[ T + \sum_{k=1}^{a} \varepsilon_k T_{ik} \in \mathcal{F}_{T_0} \]

for all \( 1 \leq a \leq A \).

If a Markov basis \( \{T_1, \ldots, T_\ell\} \) is given, then we can construct a Markov chain by the following algorithm:

**Metropolis–Hastings algorithm**

0. Choose \( T \in \mathcal{F}_{T_0} \) at random and set \( t = T \);

1. Repeat the following:
   1.1. Select \( T_i \) from the uniform distribution on \( \{T_1, \ldots, T_\ell\} \);
   1.2. Select \( \varepsilon \) from the uniform distribution on \( \{1, -1\} \) (independent of \( i \);
   1.3. If \( t + \varepsilon T_i \) is a nonnegative matrix, then set \( t = t + \varepsilon T_i \) with probability

   \[
   \min \left\{ \frac{P(t + \varepsilon T_i)}{P(t)}, 1 \right\}.
   \]

Let \( B = \{T_1, \ldots, T_\ell\} \) be a Markov basis and let \( G_{B,T_0} \) denote the graph with the vertex set \( \mathcal{F}_{T_0} \) where \( m \in \mathcal{F}_{T_0} \) and \( m' \in \mathcal{F}_{T_0} \) are joined by an edge if \( m - m' \in B \cup -B \). The most important point is that, the graph \( G_{B,T_0} \) must be connected. Otherwise, there exists an unreachable element of \( \mathcal{F}_{T_0} \) in Metropolis–Hastings algorithm. The infinite set \( \mathcal{M}_{I \times J} \) is regarded as the set of all integer solutions of some system of linear equations, and hence we can associate \( \mathcal{M}_{I \times J} \) with the "toric ideal" \( I_{A_{1}, \ldots, A_{n}} \).

A configuration in \( \mathbb{R}^d \) is a finite set \( A = \{a_1, \ldots, a_n\} \subset \mathbb{Z}^d \) which is contained in a hyperplane in \( \mathbb{R}^d \) without the origin. Let \( K[t, t^{-1}] = K[t_1, t_1^{-1}, \ldots, t_d, t_d^{-1}] \) denote the Laurent polynomial ring in \( d \) variables over a field \( K \). We associate a configuration \( A \subset \mathbb{Z}^d \) with the semigroup ring \( K[A] = K[a_1, \ldots, a_n] \subset K[t, t^{-1}] \), where \( t^a = t_1^{a_1} \cdots t_d^{a_d} \) if \( a = (a_1, \ldots, a_d) \). Let \( K[x] = K[x_1, \ldots, x_n] \) denote the polynomial ring in \( n \) variables over \( K \). The toric ideal \( I_A \) of \( A \) is the kernel of the surjective homomorphism \( \pi : K[x] \to K[A] \) defined by setting \( \pi(x_i) = t^{a_i} \) for \( 1 \leq i \leq n \). A polynomial \( f \in K[x] \) of the form \( u - v \), where \( u \) and \( v \) are monomials, is called a *binomial*. It is known [14] that the toric ideal \( I_A \) is generated by the binomials \( u - v \) with \( \pi(u) = \pi(v) \).

A configuration \( A \) is called *unimodular* if the initial ideal of \( I_A \) is generated by squarefree monomials with respect to any monomial order. A configuration \( A \) is called *compressed* if the initial ideal of \( I_A \) is generated by squarefree monomials with respect to any reverse lexicographic order. We are interested in the following conditions:

(i) \( A \) is unimodular;
(ii) \( A \) is compressed;
(iii) there exists a monomial order \(<\) such that the initial ideal of \( I_A \) with respect to \(<\) is generated by squarefree monomials;
(iv) \( K[A] \) is normal.
Then (i) $\implies$ (ii) $\implies$ (iii) $\implies$ (iv) holds and each of the converse of them is false in general. We refer the reader to [8], [9] and [10] for further information.

On the other hand, a binomial $f$ belonging to $I_A$ is called indispensable ([15] and [11]) if, for an arbitrary system $F$ of binomial generators of $I_A$, either $f$ or $-f$ appears in $F$. If $f$ is indispensable, then $-f$ is indispensable. Hence the set of indispensable binomials is of the form $F \cup -F$, where $F \cap -F = \emptyset$. In abuse of terminology, such a set $F$ will be called the set of indispensable binomials of $I_A$.

In the present paper, we study the configuration arising from a $r_1 \times r_2 \times \cdots \times r_n$ contingency table, where $r_1 \geq r_2 \geq \cdots \geq r_n \geq 2$. Let $A_{r_1, r_2, \ldots, r_n}$ be the set of vectors

$$e_{i_1i_2\cdots i_n}^{(1)} \oplus e_{i_1i_2\cdots i_n}^{(2)} \oplus \cdots \oplus e_{i_1i_2\cdots i_{n-1}}^{(n)},$$

where each $i_k$ belongs to $[r_k] = \{1, 2, \ldots, r_k\}$ and $e_{i_1i_2\cdots i_{n-1}}^{(k)}$ is a unit coordinate vector of $\mathbb{Z}^{r_1 \times \cdots \times r_{k-1} \times r_{k+1} \times \cdots \times r_n}$. The toric ideal $I_{A_{r_1, r_2, \ldots, r_n}}$ is the kernel of the homomorphism

$$\pi : K[[x_{i_1i_2\cdots i_n} \mid i_k \in [r_k]]] \longrightarrow K[[t_{i_1i_2\cdots i_{n-1}}^{(k)} \mid k \in [n], i_k \in [r_k]]]$$

defined by $\pi(x_{i_1i_2\cdots i_n}) = t_{i_1i_2\cdots i_{n-1}}^{(1)}t_{i_1i_2\cdots i_{n-1}}^{(2)} \cdots t_{i_1i_2\cdots i_{n-1}}^{(n)}$.

**Proposition 1.2.** Work with the same notation as above. Then $B \subset M_{r_1 \times \cdots \times r_n}$ is a Markov basis for an arbitrary $T$ if and only if the toric ideal $I_{A_{r_1, \ldots, r_n}}$ is generated by the binomials $x^{\beta^+} - x^{\beta^-} \in K[x]$ with $\beta^+ - \beta^- \in B$.

**2. Recent Developments**

In the present section, we discuss the recent developments ([12]) on semigroup rings and toric ideals arising from contingency tables. First, using the formula in [13, p. 162], we can compute the dimension of $K[A_{r_1, \ldots, r_n}]$.

**Proposition 2.1.** The dimension of $K[A_{r_1, \ldots, r_n}]$ is equal to

$$(1) \quad n = 2$$(unimodular, Segre product of polynomial rings),

$$(2) \quad n \geq 3$$(Lawrence lifting)

$$(3) \quad r_1 \times r_2 \times 2 \times \cdots \times 2$$

(computed by Aoki–Takemura [2], [3]).

In particular, for all of (1) – (3), a minimal set of binomial generators is unique.

**Conjecture 2.2.** The toric ideal of the configuration $A_{r_1, r_2, \ldots, r_n}$ is generated by indispensable binomials.

On the other hand, Boffi–Rossi [5] computed a lexicographic Gröbner basis of the toric ideal $I_{A_{333}}$ whose initial ideal is generated by squarefree monomials. We now discuss the following two properties of the toric ideal of the configuration $A_{333}$.
Theorem 2.3. No reduced Gröbner basis of $I_{A_{333}}$ coincides with the set of indispensable binomials (= the minimal set of binomial generators) of $I_{A_{333}}$.

Theorem 2.4. The configuration $A_{333}$ is compressed.

We characterize the configurations $A_{r_1r_2\ldots r_n}$ for which there exists a monomial order $<$ such that the reduced Gröbner basis of $I_{A_{r_1r_2\ldots r_n}}$ with respect to $<$ is the set of indispensable binomials of $I_{A_{r_1r_2\ldots r_n}}$.

Theorem 2.5. Let $n \leq 3$. Then the following conditions are equivalent for $A_{r_1r_2\ldots r_n}$:

(i) either $n = 2$ or $r_3 = 2$;
(ii) $A_{r_1r_2\ldots r_n}$ is unimodular;
(iii) there exists a monomial order $<$ such that the reduced Gröbner basis of $I_{A_{r_1r_2\ldots r_n}}$ with respect to $<$ is the set of indispensable binomials of $I_{A_{r_1r_2\ldots r_n}}$;
(iv) there exists a monomial order $<$ such that the reduced Gröbner basis of $I_{A_{r_1r_2\ldots r_n}}$ with respect to $<$ is a minimal set of binomial generators of $I_{A_{r_1r_2\ldots r_n}}$.

We study normality of semigroup rings arising from contingency tables. We classify all normal semigroup rings $K[A_{r_1r_2\ldots r_n}]$ except for $K[A_{553}]$, $K[A_{543}]$ and $K[A_{443}]$.

Theorem 2.6. Work with the same notation as above. Then we have

<table>
<thead>
<tr>
<th>$r_1 \times r_2$ or $r_1 \times r_2 \times 2 \times \cdots \times 2$</th>
<th>unimodular</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r_1 \times 3 \times 3$</td>
<td>normal</td>
</tr>
<tr>
<td>$5 \times 5 \times 3$ or $5 \times 4 \times 3$ or $4 \times 4 \times 3$</td>
<td>UNKNOWN if normal or not</td>
</tr>
<tr>
<td>otherwise, i.e.,</td>
<td></td>
</tr>
<tr>
<td>$n \geq 4$ and $r_3 \geq 3$</td>
<td></td>
</tr>
<tr>
<td>$n = 3$ and $r_3 \geq 4$</td>
<td></td>
</tr>
<tr>
<td>$n = 3$, $r_3 = 3$, $r_1 \geq 6$ and $r_2 \geq 4$</td>
<td>not normal</td>
</tr>
</tbody>
</table>

Even though a unique minimal set of generators of $I_{A_{r_13}}$ is given in [3], it seems to be difficult to know if $K[A_{543}]$ and $K[A_{443}]$ are normal. On the other hand, we do not know if $A_{r_133}$ with $r_1 \geq 4$ are compressed.

Question 2.7. Are $K[A_{553}]$, $K[A_{543}]$ and $K[A_{443}]$ normal?

Question 2.8. Is $A_{r_133}$ compressed for $r_1 \geq 4$?

References

[3] S. Aoki and A. Takemura, The list of indispensable moves of the unique minimal Markov basis for $3 \times 4 \times K$ and $4 \times 4 \times 4$ contingency tables with fixed two-dimensional marginals, METR Technical Report, 03-38.

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