# SOLVING THE 100 SWISS FRANCS PROBLEM 

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#### Abstract

Sturmfels offered 100 Swiss Francs in 2005 to a conjecture, which deals with a special case of the maximum likelihood estimation for a latent class model. This paper confirms the conjecture positively.


## 1. The conjecture and its statistical background

Sturmfels [11] proposed the following problem: Maximize the likelihood function

$$
\begin{equation*}
L(P)=\prod_{i=1}^{4} p_{i i}^{4} \times \prod_{i \neq j} p_{i j}^{2} \tag{1}
\end{equation*}
$$

over the set of all $4 \times 4$-matrices $P=\left(p_{i j}\right)$ whose entries are nonnegative and sum to 1 and whose rank is at most two. Based on numerical experiments by employing an expectation-maximization(EM) algorithm, Sturmfels [10, 11] conjectured that the matrix

$$
P=\frac{1}{40}\left(\begin{array}{llll}
3 & 3 & 2 & 2 \\
3 & 3 & 2 & 2 \\
2 & 2 & 3 & 3 \\
2 & 2 & 3 & 3
\end{array}\right)
$$

is a global maximum of $L(P)$. He offered 100 Swiss francs for a rigorous proof in a postgraduate course held at ETH Zürich in 2005.

Partial results were given in the paper in [5], where the general statistical background for this problem is also presented. This problem is a special case of the maximum likelihood estimation for a latent class model. More precisely, by following [5], let $\left(X_{1}, \ldots, X_{d}\right)$ be a discrete multivariate random vector where each $X_{j}$ takes value from a finite state set $S_{j}=\left\{1, \ldots, s_{j}\right\}$. Let $\Omega=S_{1} \times \cdots \times S_{d}$ be the sample

[^0]space. For each $\left(x_{1}, \ldots, x_{d}\right) \in \Omega$, the joint probability mass function of $\left(X_{1}, \ldots, X_{d}\right)$ is denoted as
$$
p\left(x_{1}, \ldots, x_{d}\right)=P\left\{\left(X_{1}, \ldots, X_{d}\right)=\left(x_{1}, \ldots, x_{d}\right)\right\} .
$$

The variables $X_{1}, \ldots, X_{d}$ may not be mutually independent generally. By introducing an unobservable variable $H$ defined on the set $[r]=\{1, \ldots r\}, X_{1}, \ldots, X_{d}$ become mutually independent. The joint probability mass function in the newly formed model is

$$
\begin{aligned}
p\left(x_{1}, \ldots, x_{d}, h\right) & =P\left\{\left(X_{1}, \ldots, X_{d}, H\right)=\left(x_{1}, \ldots, x_{d}, h\right)\right\} \\
& =p\left(x_{1} \mid h\right) \cdots p\left(x_{d} \mid h\right) \lambda_{h}
\end{aligned}
$$

where $\lambda_{h}$ is the marginal probability of $P\{H=h\}$ and $p\left(x_{j} \mid h\right)$ is the conditional probability $P\left\{X_{j}=x_{j} \mid H=h\right\}$. We denote this new $r$ class mixture model by $\mathcal{H}$. The marginal distribution of $\left(X_{1}, \ldots, X_{d}\right)$ in $\mathcal{H}$ is given by the probability mass function (which is also called accounting equations [8])

$$
p\left(x_{1}, \ldots, x_{d}\right)=\sum_{h \in[r]} p\left(x_{1}, \ldots, x_{d}, h\right)=\sum_{h \in[r]} p\left(x_{1} \mid h\right) \cdots p\left(x_{d} \mid h\right) \lambda_{h} .
$$

In practice, a collection of samples from $\Omega$ are observed. For each $\left(x_{1}, \ldots, x_{d}\right)$, let $n\left(x_{1}, \ldots, x_{d}\right) \in \mathbb{N}$ be the number of observed occurrences of $\left(x_{1}, \ldots, x_{d}\right)$ in the samples. While the parameters $p\left(x_{1} \mid h\right), \cdots$, $p\left(x_{d} \mid h\right), \lambda_{h}, p\left(x_{1}, \ldots, x_{d}\right)$ are unknown. The maximum likelihood estimation problem is to find the model parameters that can best explain the observed data, that is, to determine the global maxima of the likelihood function

$$
L(\mathcal{H})=\prod_{\left(x_{1}, \ldots, x_{d}\right) \in \Omega} p\left(x_{1}, \ldots, x_{d}\right)^{n\left(x_{1}, \ldots, x_{d}\right)}
$$

Since each $p\left(x_{1}, \ldots, x_{d}\right)$ is nonnegative, it is equivalent but more convenient to use the log-likelihood function

$$
\begin{equation*}
l(\mathcal{H})=\sum_{\left(x_{1}, \ldots, x_{d}\right) \in \Omega} n\left(x_{1}, \ldots, x_{d}\right) \ln p\left(x_{1}, \ldots, x_{d}\right), \tag{2}
\end{equation*}
$$

where we define $\ln (0)=-\infty$. Finding the maxima of (22) is difficult and remains infeasible by current symbolic software [2, 4]. We can only handle some special cases: small models or highly symmetric table. The 100 Swiss francs problem is the special case of $\mathcal{H}$ when $d=2$, $S_{1}=S_{2}=\{\mathrm{A}, \mathrm{C}, \mathrm{G}, \mathrm{T}\}, s_{1}=s_{2}=4$ and $r=2$. It is related to a DNA sequence alignment problem as described in [10]. In that example, the
contingency table for the observed counts of ordered pairs of nucleotides (i.e. AA, AC, AG, AT, CA, CC, $\cdots$ ) is

$$
\begin{aligned}
& \text { A C G T } \\
& \begin{array}{l}
\mathrm{A} \\
\mathrm{C} \\
\mathrm{G} \\
\mathrm{~T}
\end{array}\left(\begin{array}{llll}
4 & 2 & 2 & 2 \\
2 & 4 & 2 & 2 \\
2 & 2 & 4 & 2 \\
2 & 2 & 2 & 4
\end{array}\right) .
\end{aligned}
$$

So the likelihood function (2) in this example is exactly (1).
Even for this simple case, the problem is surprisingly difficult. We know that the global maxima must exist, as the region of the parameters is compact. By using an EM algorithm or Newton-Raphson method and starting from suitable initial points, one can find some local maxima of the likelihood function. However, the global maximum property is not guaranteed. We prove that Sturmfels' conjectured solution is indeed a global maximum.

Our paper is organized as follows. We first derive some general properties for optimal solutions in Section 2.1, then provide a theoretical solution to the conjecture in Sections 2.2. In 2.3, we make some comments about using Gröbner basis technique in solving this problem and provide a computational solution. Lastly, we suggest several new conjectures in more general cases.

## 2. Proof of the conjecture

2.1. General Properties. We focus on general $n \times n$ matrices $P=$ $\left(p_{i j}\right)$ in this section. For convenience we scale each entry of $P$ by $n^{2}$ so the entries sum to $n^{2}$, and take square root of the original likelihood function. So we may assume that

$$
\begin{equation*}
L(P)=\prod_{i=1}^{n} p_{i i}^{2} \times \prod_{i \neq j} p_{i j} \tag{3}
\end{equation*}
$$

The problem is

$$
\begin{array}{ll}
\text { Maximize: } & L(P) \\
\text { Subject to: } & \sum_{1 \leq i, j \leq n} p_{i j}=n^{2}, \text { and } \\
& p_{i j} \geq 0,1 \leq i, j \leq n .
\end{array}
$$

Suppose $P=\left(p_{i j}\right)_{n \times n}$ is a global maximum of $L(P)$. It is easy to see that $P$ cannot be the following $n \times n$ matrix

$$
J=\left(\begin{array}{ccc}
1 & \ldots & 1 \\
\vdots & & \vdots \\
1 & \ldots & 1
\end{array}\right)
$$

Since the function (3) is a continuous function in $p_{i j}$ 's, if one of the entries of $P$ approaches 0 , the product has to approach 0 too, as the other entries are bounded by $n^{2}$. Hence the optimal solutions must occur in interior points and we don't need to worry about the boundary where some $p_{i j}=0$.

Therefore, in the subsequent discussion, we may assume that $P \neq J$ and all its entries are positive. We show that $P$ must have certain symmetry properties.

Lemma 1. For an optimal solution $P$, its row sums and column sums must all equal $n$.

Proof. Let $\sum_{j=1}^{n} p_{i j}=s_{i}$. Then $\sum_{i=1}^{n} s_{i}=n^{2}$ and $\prod_{i} s_{i} \leq n^{n}$ with equality if and only if $s_{i}=n$ for all $i$. Let $\bar{p}_{i j}=\frac{n}{s_{i}} p_{i j}$ and $\bar{P}=\left(\bar{p}_{i j}\right)_{n \times n}$. Then $\operatorname{rank}(\bar{P})=\operatorname{rank}(P)$ and $\sum_{i, j} \bar{p}_{i j}=n^{2}$. However,

$$
L(\bar{P})=L(P) \cdot\left(\frac{n^{n}}{\prod_{i} s_{i}}\right)^{n+1} \geq L(P)
$$

with equality if and only if $s_{i}=n$ for all $i$. Since $P$ is a global maximum, $L(\bar{P}) \leq L(P)$. Therefore each row sum equals $n$. Similarly, each column sum equals $n$ as well.

We shall express $P$ in a form that involves fewer variables and has no rank constraint. Since $P$ has rank at most two, by singular value decomposition theorem, there are column vectors $u_{1}, u_{2}, v_{1}$ and $v_{2}$ of length $n$ such that

$$
P=\sigma_{1} u_{1} v_{1}^{t}+\sigma_{2} u_{2} v_{2}^{t}
$$

for some nonnegative numbers $\sigma_{1}$ and $\sigma_{2}$. By Proposition 1, $P$ has equal row and column sums, so $P$ has the vectors $(1,1, \ldots, 1)$ and $(1,1, \ldots, 1)^{t}$ as its left and right eigenvectors both with eigenvalue 1 .

Hence we may assume that $\sigma_{1}=1$ and $u_{1}=v_{1}=(1,1, \ldots, 1)^{t}$. Let $v_{2}=\left(a_{1}, a_{2}, \ldots, a_{n}\right)^{t}$ and $\sigma_{2} u_{2}=\left(b_{1}, b_{2}, \ldots, b_{n}\right)^{t}$. Then $P$ has the form

$$
P=J+\left(\begin{array}{c}
b_{1} \\
\vdots \\
b_{n}
\end{array}\right)\left(a_{1}, a_{2}, \ldots, a_{n}\right)=\left(\begin{array}{ccc}
1+a_{1} b_{1} & \ldots & 1+a_{n} b_{1} \\
\vdots & 1+a_{i} b_{j} & \vdots \\
1+a_{1} b_{n} & \cdots & 1+a_{n} b_{n}
\end{array}\right)
$$

In this form, $P$ has rank at most two. Also, the condition $\sum_{i j} p_{i j}=n^{2}$ becomes

$$
\begin{equation*}
\sum_{i=1}^{n} a_{i} \cdot \sum_{i=1}^{n} b_{i}=0 \tag{4}
\end{equation*}
$$

We have transformed the original problem to the following optimization problem:

Maximize: $\quad l(P)=2 \sum_{i=1}^{n} \ln \left(1+a_{i} b_{i}\right)+\sum_{i \neq j} \ln \left(1+a_{i} b_{j}\right)$
Subject to: Equation (4) and $1+a_{i} b_{j}>0,1 \leq i, j \leq n$.
The Lagrangian function would be

$$
\Lambda(P, \lambda)=l(P)+\lambda \sum_{i=1}^{n} a_{i} \cdot \sum_{i=1}^{n} b_{i}
$$

where $\lambda \in \mathbb{R}$. Any local extrema must satisfy

$$
\begin{equation*}
\frac{\partial \Lambda(P, \lambda)}{\partial a_{i}}=\sum_{j=1}^{n} \frac{b_{j}}{1+a_{i} b_{j}}+\frac{b_{i}}{1+a_{i} b_{i}}+\lambda \sum_{j=1}^{n} b_{j}=0, \quad 1 \leq i \leq n \tag{5}
\end{equation*}
$$

and

$$
\begin{equation*}
\frac{\partial \Lambda(P, \lambda)}{\partial b_{j}}=\sum_{i=1}^{n} \frac{a_{i}}{1+a_{i} b_{j}}+\frac{a_{j}}{1+a_{j} b_{j}}+\lambda \sum_{i=1}^{n} a_{i}=0, \quad 1 \leq j \leq n . \tag{6}
\end{equation*}
$$

By Lemma 1, for an optimal solution $P$, its row sums and column sums must be all equal to $n$. This means that

$$
\begin{equation*}
\sum_{i=1}^{n} a_{i}=0 \tag{7}
\end{equation*}
$$

and

$$
\begin{equation*}
\sum_{i=1}^{n} b_{i}=0 \tag{8}
\end{equation*}
$$

Plugging (7) and (8) into (5) and (6) respectively, we obtain the following lemma.

Lemma 2. A global maximum $P$ must satisfy

$$
\begin{equation*}
\sum_{j=1}^{n} \frac{b_{j}}{1+a_{i} b_{j}}+\frac{b_{i}}{1+a_{i} b_{i}}=0, \quad 1 \leq i \leq n \tag{9}
\end{equation*}
$$

and

$$
\begin{equation*}
\sum_{i=1}^{n} \frac{a_{i}}{1+a_{i} b_{j}}+\frac{a_{j}}{1+a_{j} b_{j}}=0, \quad 1 \leq j \leq n \tag{10}
\end{equation*}
$$

Doing some simple algebra yields
Corollary 3. An optimal solution must satisfy

$$
\begin{equation*}
\sum_{j=1}^{n} \frac{1}{1+a_{i} b_{j}}+\frac{1}{1+a_{i} b_{i}}=n+1, \quad 1 \leq i \leq n \tag{11}
\end{equation*}
$$

and

$$
\begin{equation*}
\sum_{i=1}^{n} \frac{1}{1+a_{i} b_{j}}+\frac{1}{1+a_{j} b_{j}}=n+1, \quad 1 \leq j \leq n \tag{12}
\end{equation*}
$$

Proof. Multiply (9) by $a_{i}$ and then add $\sum_{j=1}^{n} \frac{1}{1+a_{i} b_{j}}+\frac{1}{1+a_{i} b_{i}}$ to both sides, we can get (11).

The $2 n$ equations derived by clearing denominators of the equations in Lemma 2 or Corollary 3 along with equations (7) and (8) form a system of $2 n+2$ polynomial equations with $2 n$ unknowns, whose solutions contain all global maxima. From computational point of view, we may find all the solutions to this system of equations, say utilizing Gröbner basis method, and then pick a global maximum. At the time we submitted this paper (in 2008), we could not solve the system for $n=4$ using Maple on a computer with moderate computation power. With both the advance in computer hardware and efficient implementations of algorithms for computing Gröbner basis, the system for $n=4$ now became solvable. A computational solution for this problem is attached in Section 2.3, However, the system for $n=5$ remains unsolvable using our computers.

Our strategy below is to prove that $P$ should have high symmetry. Firstly $a_{i}$ 's and $b_{i}$ 's are in the same order: if $a_{i}>a_{j}>0$, then $b_{i}>$ $b_{j}>0$ correspondingly (Lemma 4 and 5). For the case $n=4$ once we force $a_{1}=b_{1}$ by scaling, we can eventually prove $a_{i}=b_{i}$ for all other $i$ 's (Lemma 7 and 9). With four $a_{i}$ 's remained, we prove that the $a_{i}$ 's with
the same signs must be identical. Finally one can solve the system by hand. Note that Fienberg et. al. [5] derived results similar to Lemmas 4 and 5, but our approaches are simpler and completely different.

Lemma 4. For every $i$,
(1) $a_{i}=0$ if and only if $b_{i}=0$, and
(2) $a_{i}>0$ if and only if $b_{i}>0$.

Proof. For the first part, plugging in $a_{i}=0$ to the equation (9), we have $\sum_{j=1}^{n} b_{j}+b_{i}=0$, thus $b_{i}=0$. Similarly, if $b_{i}=0$ then $a_{i}=0$.
For the second part, note that $g(x)=\frac{1}{x}$ is concave up in $(0, \infty)$. By Jensen's Inequality,

$$
\sum_{j=1}^{n} \frac{1}{n} \cdot \frac{1}{1+a_{i} b_{j}} \geq \frac{1}{\sum_{j=1}^{n} \frac{1}{n}\left(1+a_{i} b_{j}\right)}=1
$$

That is,

$$
\sum_{j=1}^{n} \frac{1}{1+a_{i} b_{j}} \geq n
$$

Compare with equation (11), we get

$$
\frac{1}{1+a_{i} b_{i}} \leq 1
$$

so $a_{i} b_{i} \geq 0$. We conclude that $a_{i}>0$ if and only if $b_{i}>0$.
Lemma 5. For $i$ and $j$,
(1) $a_{i}=a_{j}$ if and only if $b_{i}=b_{j}$, and
(2) $a_{i}>a_{j}$ if and only if $b_{i}>b_{j}$.

Proof. For the first part, suppose $b_{i}=b_{j}$. Then, by (10),

$$
\sum_{k=1}^{n} \frac{a_{k}}{1+a_{k} b_{i}}+\frac{a_{i}}{1+a_{i} b_{i}}=0 \text { and } \sum_{k=1}^{n} \frac{a_{k}}{1+a_{k} b_{j}}+\frac{a_{j}}{1+a_{j} b_{j}}=0
$$

Then $\frac{a_{i}}{1+a_{i} b_{i}}=\frac{a_{j}}{1+a_{j} b_{j}}$, so $a_{i}=a_{j}$. Then, using (9), we have $b_{i}=b_{j}$.
For the second part, switch $b_{i}, b_{j}$ in $P$ to form a new matrix $\bar{P}$. Then we should have $L(P) \geq L(\bar{P})$ due to our assumption that $P$ is a global
maximum. Note that

$$
\begin{aligned}
L(P)-L(\bar{P})= & C_{1} \cdot\left(\left(1+a_{i} b_{i}\right)^{2}\left(1+a_{i} b_{j}\right)\left(1+a_{j} b_{i}\right)\left(1+a_{j} b_{j}\right)^{2}\right. \\
& \left.-\left(1+a_{i} b_{j}\right)^{2}\left(1+a_{i} b_{i}\right)\left(1+a_{j} b_{j}\right)\left(1+a_{j} b_{i}\right)^{2}\right) \\
= & C_{2} \cdot\left(\left(1+a_{i} b_{i}\right)\left(1+a_{j} b_{j}\right)-\left(1+a_{i} b_{j}\right)\left(1+a_{j} b_{i}\right)\right) \\
= & C_{2} \cdot\left(a_{i} b_{i}+a_{j} b_{j}-a_{i} b_{j}-a_{j} b_{i}\right) \\
= & C_{2} \cdot\left(a_{i}-a_{j}\right)\left(b_{i}-b_{j}\right)
\end{aligned}
$$

where $C_{1}, C_{2}$ are products of some entries of $P$, so $C_{1}, C_{2}$ are positive. Thus $\left(a_{i}-a_{j}\right)\left(b_{i}-b_{j}\right) \geq 0$. Note that $a_{i}=a_{j}$ if and only if $b_{i}=b_{j}$ by part(1), we conclude that $a_{i}>a_{j}$ if and only if $b_{i}>b_{j}$.
2.2. Theoretical solution. We complete the theoretical proof for the conjecture in this section. From now on we focus on the case when $n=4$. By Lemma 55 we can always assume $a_{1} \geq a_{2} \geq a_{3} \geq a_{4}$ and $b_{1} \geq b_{2} \geq b_{3} \geq b_{4}$. We know $a_{1} \neq 0$, otherwise $b_{1}=0$ by Lemma (4, hence $a_{i}=b_{j}=0$, which result in $P=J$. We also have $\frac{a_{1}}{b_{1}}>0$, so we can replace $\left(a_{1}, a_{2}, a_{3}, a_{4}\right)$ in $P$ by $\sqrt{\frac{a_{1}}{b_{1}}}\left(a_{1}, a_{2}, a_{3}, a_{4}\right)$ and $\left(b_{1}, b_{2}, b_{3}, b_{4}\right)^{t}$ by $\sqrt{\frac{b_{1}}{a_{1}}}\left(b_{1}, b_{2}, b_{3}, b_{4}\right)^{t}$. It turns out that $1+\sqrt{\frac{a_{1}}{b_{1}}} a_{i} \sqrt{\frac{b_{1}}{a_{1}}} b_{i}=1+a_{i} b_{j}$ for any $i$ and $j$, so we may always assume $a_{1}=b_{1}$. Thus $P$ can be expressed as the form

$$
\left(\begin{array}{cccc}
1+a_{1}^{2} & 1+a_{2} a_{1} & 1+a_{3} a_{1} & 1+a_{4} a_{1}  \tag{13}\\
1+a_{1} b_{2} & 1+a_{2} b_{2} & 1+a_{3} b_{2} & 1+a_{4} b_{2} \\
1+a_{1} b_{3} & 1+a_{2} b_{3} & 1+a_{3} b_{3} & 1+a_{4} b_{3} \\
1+a_{1} b_{4} & 1+a_{2} b_{4} & 1+a_{3} b_{4} & 1+a_{4} b_{4}
\end{array}\right) .
$$

If $a_{2} \leq 0$, we then replace $\left(a_{1}, a_{2}, a_{3}, a_{4}\right)$ in $P$ by $\left(-a_{4},-a_{3},-a_{2},-a_{1}\right)$ and $\left(b_{1}, b_{2}, b_{3}, b_{4}\right)^{t}$ by $\left(-b_{4},-b_{3},-b_{2},-b_{1}\right)^{t}$. The new matrix with $-a_{4} \geq$ $-a_{3} \geq 0$ has the same likelihood function as $P$. Thus we may assume $a_{1} \geq a_{2} \geq 0$. Without loss of generality, we may make the following assumption.

Assumption 6. We can always assume the following
(1) $a_{1} \geq a_{2} \geq a_{3} \geq a_{4}$ and $b_{1} \geq b_{2} \geq b_{3} \geq b_{4}$,
(2) $a_{1}=b_{1}>0$, and
(3) $a_{1} \geq a_{2} \geq 0$.

The results in the rest of this section are all based on Assumption 6 , Our first goal is to prove $a_{2}=b_{2}$.

Lemma 7. $a_{2}=b_{2}$.
Proof. If one of $a_{2}, b_{2}$ is 0 , then $a_{2}=b_{2}=0$ by Lemma 4. We assume that both $a_{2}, b_{2}$ are nonzero.

Apply Corollary 3 to the first row of matrix (13). We have

$$
\frac{2}{1+a_{1}^{2}}+\frac{1}{1+a_{2} a_{1}}+\frac{1}{1+a_{3} a_{1}}+\frac{1}{1+a_{4} a_{1}}=5
$$

Also

$$
a_{1}^{2}+a_{2} a_{1}+a_{3} a_{1}+a_{4} a_{1}=0 .
$$

From the two equations above we get

$$
\begin{equation*}
a_{3} a_{1} \cdot a_{4} a_{1}=f_{1}\left(a_{1} a_{1}, a_{1} a_{2}\right) \tag{14}
\end{equation*}
$$

where $f_{1}$ is a bivariate function in $x, y$ defined as

$$
f_{1}(x, y)=\frac{2-x-y}{5-\frac{2}{1+x}-\frac{1}{1+y}}+x+y-1
$$

Similarly, apply Corollary 3 to the second row of matrix (13). We get

$$
\frac{1}{1+a_{1} b_{2}}+\frac{2}{1+a_{2} b_{2}}+\frac{1}{1+a_{3} b_{2}}+\frac{1}{1+a_{4} b_{2}}=5 .
$$

Along with

$$
a_{1} b_{2}+a_{2} b_{2}+a_{3} b_{2}+a_{4} b_{2}=0,
$$

we get

$$
\begin{equation*}
a_{3} b_{2} \cdot a_{4} b_{2}=f_{1}\left(a_{2} b_{2}, a_{1} b_{2}\right) \tag{15}
\end{equation*}
$$

Since $a_{1}, b_{2}$ are nonzero, we combine equations (14) and (15) to get

$$
\begin{equation*}
\frac{f_{1}\left(a_{1}^{2}, a_{1} a_{2}\right)}{a_{1}^{2}}=\frac{f_{1}\left(a_{2} b_{2}, a_{1} b_{2}\right)}{b_{2}^{2}} . \tag{16}
\end{equation*}
$$

Normalizing (16) we can derive a trivariate polynomial equation, say

$$
\begin{equation*}
f_{2}\left(a_{1}, a_{2}, b_{2}\right)=0 \tag{17}
\end{equation*}
$$

Symmetrically apply Corollary 3 to the first column and the second column 13, we get

$$
\begin{equation*}
\frac{f_{1}\left(a_{1}^{2}, a_{1} b_{2}\right)}{a_{1}^{2}}=\frac{f_{1}\left(a_{2} b_{2}, a_{1} a_{2}\right)}{a_{2}^{2}} . \tag{18}
\end{equation*}
$$

One can see that equation (18) is obtainable by switching $a_{2}$ with $b_{2}$ in equation (16). Thus we have

$$
\begin{equation*}
f_{2}\left(a_{1}, b_{2}, a_{2}\right)=0 . \tag{19}
\end{equation*}
$$

Subtracting (19) from (17) yields

$$
f_{2}\left(a_{1}, a_{2}, b_{2}\right)-f_{2}\left(a_{1}, b_{2}, a_{2}\right)=0
$$

Since we only switched $a_{2}$ and $b_{2}$ in polynomial $f_{2}$, there must be a factor $a_{2}-b_{2}$ for $f_{2}\left(a_{1}, a_{2}, b_{2}\right)-f_{2}\left(a_{1}, b_{2}, a_{2}\right)$, say

$$
\begin{equation*}
\left(a_{2}-b_{2}\right) f_{3}\left(a_{1}, a_{2}, b_{2}\right)=0, \tag{20}
\end{equation*}
$$

where

$$
\begin{aligned}
f_{3}\left(a_{1}, a_{2}, b_{2}\right)= & \left(20 a_{1}^{4} b_{2}^{2}+15 a_{1}^{3} b_{2}+3 a_{1}^{2} b_{2}^{2}+2 a_{1} b_{2}-4 b_{2}^{2}\right) a_{2}^{2} \\
+ & \left(3 a_{1}^{4} b_{2}+15 a_{1}^{3} b_{2}^{2}+2 a_{1}^{3}+10 a_{1}^{2} b_{2}+2 a_{1} b_{2}^{2}-3 a_{1}-b_{2}\right) a_{2} \\
& -4 a_{1}^{4}+2 a_{1}^{3} b_{2}-a_{1}^{2}-3 a_{1} b_{2}-2 .
\end{aligned}
$$

Thus $a_{2}=b_{2}$ if $f_{3}\left(a_{1}, a_{2}, b_{2}\right) \neq 0$. This is true because we have some bounds for $a_{1}^{2}, a_{1} a_{2}, a_{1} b_{2}$ as presented in Lemma 8 below, which can be applied to get

$$
\begin{aligned}
f_{3}\left(a_{1}, a_{2}, b_{2}\right)= & \left(20 a_{1}^{4} b_{2}^{2}+15 a_{1}^{3} b_{2}+3 a_{1}^{2} b_{2}^{2}+2 a_{1} b_{2}-4 b_{2}^{2}\right) a_{2}^{2} \\
& +\left(3 a_{1}^{4} b_{2}+15 a_{1}^{3} b_{2}^{2}+2 a_{1}^{3}+10 a_{1}^{2} b_{2}+2 a_{1} b_{2}^{2}-3 a_{1}-b_{2}\right) a_{2} \\
& -4 a_{1}^{4}+2 a_{1}^{3} b_{2}-a_{1}^{2}-3 a_{1} b_{2}-2 \\
< & \frac{20}{5^{4}}+\frac{15}{5^{3}}+\frac{3}{4} a_{2}^{2} b_{2}^{2}+\frac{2}{5} a_{2} b_{2}-4 a_{2}^{2} b_{2}^{2} \\
& +\frac{3}{2^{2} 5^{2}}+\frac{15}{5^{3}}+\frac{2}{2^{2} 5}+\frac{10}{5^{2}}+\frac{2}{5} a_{2} b_{2}-a_{2} b_{2} \\
& +\frac{2}{2^{2} 5}-2 \\
< & -\frac{13}{4} a_{2}^{2} b_{2}^{2}-\frac{1}{5} a_{2} b_{2}-\frac{549}{500} \\
< & 0 .
\end{aligned}
$$

Therefore, $f_{3}\left(a_{1}, a_{2}, b_{2}\right) \neq 0$ and $a_{2}=b_{2}$, just as needed.

## Lemma 8.

(1) $a_{1}^{2} \leq \frac{1}{2}$,
(2) $0 \leq a_{1} a_{2} \leq \frac{1}{5}$, and
(3) $0 \leq a_{1} b_{2} \leq \frac{1}{5}$.

Proof. (1) Let $A_{i}=1+a_{1} a_{i}$ for $i=1, \ldots, 4$, then $\sum_{i=1}^{4} A_{i}=4, A_{1} \geq$ $A_{2} \geq 1, A_{3} \geq A_{4}>0$ and

$$
\frac{2}{A_{1}}+\frac{1}{A_{2}}+\frac{1}{A_{3}}+\frac{1}{A_{4}}=5
$$

Since

$$
\frac{1}{A_{3}}+\frac{1}{A_{4}} \geq \frac{4}{A_{3}+A_{4}}=\frac{4}{4-A_{1}-A_{2}}
$$

we have

$$
\begin{equation*}
5=\frac{2}{A_{1}}+\frac{1}{A_{2}}+\frac{1}{A_{3}}+\frac{1}{A_{4}} \geq \frac{2}{A_{1}}+\frac{1}{A_{2}}+\frac{4}{4-A_{1}-A_{2}} . \tag{21}
\end{equation*}
$$

Let

$$
g\left(A_{2}\right)=\frac{1}{A_{2}}+\frac{4}{4-A_{1}-A_{2}}
$$

where $g$ is a function in $\mathbb{R}[x]$. Then

$$
\frac{\partial g\left(A_{2}\right)}{\partial A_{2}}=-\frac{1}{A_{2}^{2}}+\frac{4}{\left(4-A_{1}-A_{2}\right)^{2}}
$$

Note that $A_{1} \geq A_{2} \geq 1$, thus $4-A_{1}-A_{2} \leq 2$ and $\frac{\partial g\left(A_{2}\right)}{\partial A_{2}} \geq 0$. Therefore $g\left(A_{2}\right) \geq g(1)$ for $A_{2} \geq 1$, that is,

$$
\frac{1}{A_{2}}+\frac{4}{4-A_{1}-A_{2}} \geq 1+\frac{4}{3-A_{1}} .
$$

Hence by inequality (21),

$$
5 \geq \frac{2}{A_{1}}+\frac{1}{A_{2}}+\frac{4}{4-A_{1}-A_{2}} \geq \frac{2}{A_{1}}+1+\frac{4}{3-A_{1}}
$$

We get $2 A_{1}^{2}-5 A_{1}+3 \leq 0$, i.e. $1 \leq A_{1} \leq \frac{3}{2}$. Thus $a_{1}^{2} \leq \frac{1}{2}$.
(2) Assume $A_{2}=1+a_{1} a_{2}>\frac{6}{5}$. Then $g\left(A_{2}\right)>g\left(\frac{6}{5}\right)$. That is,

$$
5 \geq \frac{2}{A_{1}}+\frac{1}{A_{2}}+\frac{4}{4-A_{1}-A_{2}}>\frac{2}{A_{1}}+\frac{5}{6}+\frac{4}{\frac{14}{5}-A_{1}}
$$

The solution set of $A_{1}$ is $(-\infty, 0) \cup\left(\frac{28}{25}, \frac{6}{5}\right) \cup\left(\frac{14}{5}, \infty\right)$. Note that $A_{1}>0$ and $A_{1}=1+a_{1}^{2} \leq \frac{3}{2}$, we then get $\frac{28}{25}<A_{1}<\frac{6}{5}$, which contradicts with $A_{1} \geq A_{2}$. Thus $A_{2} \leq \frac{6}{5}$ and $0 \leq a_{1} a_{2} \leq \frac{1}{5}$.
(3) This result is followed by letting $A_{1}=1+a_{1}^{2}$ and $A_{i}=1+a_{1} b_{i}$ for $i \geq 2$. The above proofs in part (1) and (2) remain good.

Lemma 9. $a_{i}=b_{i}$ for $i=3,4$.

Proof. Let $A_{i}=1+a_{i} b_{1}$ for $i=1, \ldots, 4$. Then

$$
\sum_{i=1}^{4} A_{i}=4
$$

and

$$
\frac{2}{A_{1}}+\frac{1}{A_{2}}+\frac{1}{A_{3}}+\frac{1}{A_{4}}=5 .
$$

By the two equations above, since $A_{3} \geq A_{4}$, we can derive explicit expression for $A_{3}, A_{4}$ in the variables $A_{1}, A_{2}$, say $A_{3}=h_{1}\left(A_{1}, A_{2}\right)$ and $A_{4}=h_{2}\left(A_{1}, A_{2}\right)$. If we let $B_{i}=1+a_{1} b_{i}$, we can get $B_{3}=h_{1}\left(B_{1}, B_{2}\right)$ and $B_{4}=h_{2}\left(B_{1}, B_{2}\right)$ in a similar manner. Note that $A_{1}=B_{1}$ and $A_{2}=1+a_{2} b_{1}=1+b_{2} a_{1}=B_{2}$, we deduce that $A_{i}=B_{i}$ for $i=3,4$. Since $a_{1}=b_{1}>0, a_{i}=b_{i}$ for $i=3,4$.

By Lemmas 7 and 9, we have $a_{i}=b_{i}$ for all $i$. Hence $P$ can be expressed as

$$
P=\left(\begin{array}{cccc}
1+a_{1}^{2} & 1+a_{2} a_{1} & 1+a_{3} a_{1} & 1+a_{4} a_{1} \\
1+a_{1} a_{2} & 1+a_{2}^{2} & 1+a_{3} a_{2} & 1+a_{4} a_{2} \\
1+a_{1} a_{3} & 1+a_{2} a_{3} & 1+a_{3}^{2} & 1+a_{4} a_{3} \\
1+a_{1} a_{4} & 1+a_{2} a_{4} & 1+a_{3} a_{4} & 1+a_{4}^{2}
\end{array}\right)
$$

where

$$
\begin{equation*}
\sum_{i=1}^{4} a_{i}=0 \tag{22}
\end{equation*}
$$

By Corollary 3 we have the following system of equations

$$
\left\{\begin{array}{l}
\frac{2}{1+a_{1}^{2}}+\frac{1}{1+a_{2} a_{1}}+\frac{1}{1+a_{3} a_{1}}+\frac{1}{1+a_{4} a_{1}}=5  \tag{23}\\
\frac{1}{1+a_{1} a_{2}}+\frac{2}{1+a_{2}^{2}}+\frac{1}{1+a_{3} a_{2}}+\frac{1}{1+a_{4} a_{2}}=5 \\
\frac{1}{1+a_{1} a_{3}}+\frac{1}{1+a_{2} a_{3}}+\frac{2}{1+a_{3}^{2}}+\frac{1}{1+a_{4} a_{3}}=5 \\
\frac{1}{1+a_{1} a_{4}}+\frac{1}{1+a_{2} a_{4}}+\frac{1}{1+a_{3} a_{4}}+\frac{2}{1+a_{4}^{2}}=5
\end{array}\right.
$$

With (22) and (23), we claim that
Lemma 10. $a_{i}=a_{j}$ if $a_{i} a_{j}>0$.

Proof. Let

$$
F(x)=\frac{1}{1+a_{1} x}+\frac{1}{1+a_{2} x}+\frac{1}{1+a_{3} x}+\frac{1}{1+a_{4} x}+\frac{1}{1+x^{2}}-5=0 .
$$

Normalizing $F(x)$ yields a polynomial (the numerator) of degree 6 in $x$ whose constant is 0 and whose coefficient of the term $x$ is $\sum_{i=1}^{4} a_{i}=0$. So $a_{1}, a_{2}, a_{3}, a_{4}, 0,0$ are all the zeros of $F(x)$. Suppose there exists consecutive $i, j$ such that $a_{i}>a_{j}>0$ (or $a_{j}<a_{i}<0$ respectively). Then $F(x)$ is continuous in the interval $\left(-\frac{1}{a_{j}},-\frac{1}{a_{i}}\right)$. Note that

$$
\lim _{x \rightarrow-\frac{1}{a_{j}}}{ }^{+} F(x)=\infty \text { and } \lim _{x \rightarrow-\frac{1}{a_{i}}}{ }^{-} \text {. } F(x)=-\infty .
$$

There must be a zero lying in $\left(-\frac{1}{a_{j}},-\frac{1}{a_{i}}\right)$, say $a_{0}$. Then $a_{0}<-\frac{1}{a_{i}}$ (or $a_{0}>-\frac{1}{a_{j}}$ respectively), i.e. $1+a_{i} a_{0}<0$ (or $1+a_{j} a_{0}<0$ respectively). Since $a_{0} \neq 0, x_{0}$ must be one of $a_{k}, k=1, \ldots, 4$. Thus $1+a_{i} a_{0}$ (or $1+a_{j} a_{0}$, respectively) is an entry in matrix $P$, contradicting the fact that each entry of $P$ is positive. Therefore if $i, j$ are consecutive and $a_{i} a_{j}>0$, we must have $a_{i}=a_{j}$. Hence $a_{i} a_{j}>0$ implies $a_{i}=a_{j}$ for any $i, j$.

With Lemma 10 it is handy to solve the system (23). Under Assumption (6) there are only 4 possible patterns of signs for $\left(a_{1}, a_{2}, a_{3}, a_{4}\right)$. If the signs are $(+,+,+,-)$, then $a_{1}=a_{2}=a_{3}=-\frac{1}{3} a_{4}$. Substitute this to any equation in (23) yields $a_{1}=a_{2}=a_{3}=\frac{1}{\sqrt{15}}$ and $a_{4}=-\frac{3}{\sqrt{15}}$. The matrix would be

$$
P_{1}=\left(\begin{array}{cccc}
\frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\
\frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\
\frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\
\frac{4}{5} & \frac{4}{5} & \frac{4}{5} & \frac{8}{5}
\end{array}\right) .
$$

For the case when the signs are $(+,+,-,-)$, we get $a_{1}=\frac{1}{\sqrt{5}}$ and the matrix would be

$$
P_{2}=\left(\begin{array}{cccc}
\frac{6}{5} & \frac{6}{5} & \frac{4}{5} & \frac{4}{5} \\
\frac{6}{5} & \frac{6}{5} & \frac{4}{5} & \frac{4}{5} \\
\frac{4}{5} & \frac{4}{5} & \frac{6}{5} & \frac{6}{5} \\
\frac{4}{5} & \frac{4}{5} & \frac{6}{5} & \frac{6}{5}
\end{array}\right) .
$$

When the signs are $(+,+, 0,-), a_{1}=\frac{1}{2 \sqrt{2}}$, and the matrix would be

$$
P_{3}=\left(\begin{array}{cccc}
\frac{9}{8} & \frac{9}{8} & 1 & \frac{3}{4} \\
\frac{9}{8} & \frac{9}{8} & 1 & \frac{3}{4} \\
1 & 1 & 1 & 1 \\
\frac{3}{4} & \frac{3}{4} & 1 & \frac{3}{2}
\end{array}\right) .
$$

And when the signs are $(+, 0,0,-), a_{1}=\frac{1}{\sqrt{3}}$ and the matrix would be

$$
P_{4}=\left(\begin{array}{cccc}
\frac{4}{3} & 1 & 1 & \frac{2}{3} \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
\frac{2}{3} & 1 & 1 & \frac{4}{3}
\end{array}\right)
$$

The matrices obtaining local maximum of the likelihood function must be among the matrices above. We conclude that matrix $P_{2}$ obtains the global maximum. Finally, multiplying matrix $P_{2}$ by $\frac{1}{16}$ yields

$$
P=\frac{1}{40}\left(\begin{array}{llll}
3 & 3 & 2 & 2 \\
3 & 3 & 2 & 2 \\
2 & 2 & 3 & 3 \\
2 & 2 & 3 & 3
\end{array}\right)
$$

2.3. Approach via Gröbner bases. Gröbner basis technique is a general approach for solving systems of equations. Buchberger introduced in 1965 the first algorithm for computing Gröbner basis (see [1]), and subsequently there have been extensive efforts in improving its efficiency. It is not our purpose here to give a detailed survey of all the algorithms in the literature, but we mention two important algorithms F4 (Faugère 1999, [3]) and F5 (Faugère 2002, [4]) where signatures are introduced to detect useless S-pairs without performing reductions. F5 is believed to be the fastest algorithm in the last decade. Most recently, Gao, Guan and Volny (2010, [6]) introduced an incremental algorithm (G2V) that is simpler and several times faster than F5, and Gao, Volny and Wang (2010, [7]) developed a more general algorithm that avoids the incremental nature of F5 and G2V and is flexible in signature orders. All these algorithms are for general polynomial systems. If a large system of polynomials have certain structures, it is not known
how to use these algorithms to take advantage of the structures of the polynomial system.

After we submitted our paper (in 2008), one of the referees pointed out that it is possible to compute the Gröbner basis for our polynomial system with $n=4$. We give more details on this computation. The solution starts from Equations (7-10), using the scaling at of the beginning of Section 2.2. Without the scaling the solutions are infinite. For this one needs to assume $a_{1}=b_{1} \neq 0$. Note that this assumption relies on Lemmas 4 and 5 we proved. It takes about ten minutes for the whole computation in Maple on a moderate computer.

Precisely, one can construct an ideal

$$
\mathcal{J}_{0}=\left\langle a_{1}-b_{1}, \sum_{i=1}^{4} a_{i}, \sum_{i=1}^{4} b_{i}, h_{1}, \cdots, h_{8}\right\rangle \subset \mathbb{C}[X]
$$

where $h_{i}$ is a numerator on the left hand side of Equations 9, 10, $\mathbb{C}$ is the complex field and $X$ represents the list of unknowns: $a_{1}, \cdots, a_{4}, b_{1}, \cdots, b_{4}$. Let

$$
\mathcal{J}_{1}=\mathcal{J}_{0}+\left\langle 1-u \cdot a_{1}\right\rangle \subset \mathbb{C}[X, u]
$$

where $u$ is a new variable. Then $a_{1} \neq 0$ for any solution of $\mathcal{J}_{1}$. We compute the Gröbner basis $G_{1}$ of $\mathcal{J}_{1}$ in an elimination term order with $u>X$. Let $G_{2}=G_{1} \cap \mathbb{C}[X]$. Then $G_{2}$ is a Gröbner basis of $\mathcal{J}_{1} \cap$ $\mathbb{C}[X]$. Now $\left\langle G_{2}\right\rangle$ is a zero-dimensional ideal, and its rational univariate representation can be computed. In this step, a univariate polynomial $r(v)$ with a new variable $v$ is computed, whose roots can represent all the solutions of $\left\langle G_{2}\right\rangle$. It has degree of 398, with 56 real roots. By substituting each real root to the representations, there are 18 roots making that some entries of $P$ equal 0 thus $L(P)=0$. Each of the
remaining solutions gives one of the following:

$$
\begin{array}{ll}
P_{1}=\left(\begin{array}{cccc}
\frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\
\frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\
\frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\
\frac{4}{5} & \frac{4}{5} & \frac{4}{5} & \frac{8}{5}
\end{array}\right), & P_{2}=\left(\begin{array}{cccc}
\frac{6}{5} & \frac{6}{5} & \frac{4}{5} & \frac{4}{5} \\
\frac{6}{5} & \frac{6}{5} & \frac{4}{5} & \frac{4}{5} \\
\frac{4}{5} & \frac{4}{5} & \frac{6}{5} & \frac{6}{5} \\
\frac{4}{5} & \frac{4}{5} & \frac{6}{5} & \frac{6}{5}
\end{array}\right), \\
P_{3}=\left(\begin{array}{cccc}
\frac{9}{8} & \frac{9}{8} & 1 & \frac{3}{4} \\
\frac{9}{8} & \frac{9}{8} & 1 & \frac{3}{4} \\
1 & 1 & 1 & 1 \\
\frac{3}{4} & \frac{3}{4} & 1 & \frac{3}{2}
\end{array}\right), & P_{4}=\left(\begin{array}{cccc}
\frac{4}{3} & 1 & 1 & \frac{2}{3} \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
\frac{2}{3} & 1 & 1 & \frac{4}{3}
\end{array}\right),
\end{array}
$$

up to a permutation of variables $a_{i}$ 's and $b_{i}$ 's. It is straightforward to check that $P_{2}$ is the optimal solution.

We also tried to the case for $n=5$, but our computation did not finish after more than one day, mainly because the computation for the first Gröbner basis $G_{1}$ did not finish. Gröbner basis encodes both real and complex solutions. For our system with $n=4$, there are far more complex solutions than real solutions. For a system of polynomials with finitely many complex solutions, it is expected that in general, the more solutions with the system, the harder to compute Gröbner basis (for any term order). Also, even if a final Gröbasis is small, the intermediate polynomials may be large (in number of nonzero terms as well as the size of the coefficients), hence the algorithms can not finish in reasonable time in practice, in fact, it's more likely that the computer is out of memory quickly. For our theoretical approach (by hand), we were able to explore some partial structure in our polynomial system. For example, we have a polynomial of the form $\left(a_{2}-b_{2}\right) f_{3}\left(a_{1}, a_{2}, b_{2}\right)$ in the proof for Lemma 7. Our approach is to justify that the factor $f_{3}\left(a_{1}, a_{2}, b_{2}\right)$, a trivariate polynomial with 17 terms, is nonzero by applying some bounds from Lemma 8, so that we can derive the simplest equation $a_{2}-b_{2}=0$. In the proof we used the fact that we are looking only for real solutions. However, it is possible that $f_{3}\left(a_{1}, a_{2}, b_{2}\right)$ is zero for some complex solutions. The locus of all solutions may be much more complicated than that of real solutions, hence the Gröbner basis is much more time consuming to compute.

## 3. Some comments on more general likelihood functions

In this section, we consider some generalization of the likelihood problem. We let the exponent in the likelihood function (3) be symbolic, and consider the function

$$
\begin{equation*}
L(P)=\prod_{i=1}^{n} p_{i i}^{s} \times \prod_{i \neq j} p_{i j}^{t} \tag{24}
\end{equation*}
$$

where $P=\left(p_{i j}\right)$ is still an $n \times n$ matrix as before. The question is how the optimal solution depends on $(s, t)$. Even for the case when $n=4$, it seems hard to find the optimal solutions. In the following, we describe some possible solutions in the form of conjectures.

Conjecture 11. For given $0<t<s$ where $t$, $s$ are two integers, among the set of all non-negative $4 \times 4$ matrices whose rank is at most 2 and whose entries sum to 1 , the matrix

$$
P=\frac{1}{4 s+12 t}\left(\begin{array}{cccc}
\frac{s+t}{2} & \frac{s+t}{2} & t & t \\
\frac{s+t}{2} & \frac{s+t}{2} & t & t \\
t & t & \frac{s+t}{2} & \frac{s+t}{2} \\
t & t & \frac{s+t}{2} & \frac{s+t}{2}
\end{array}\right)
$$

is a global maximum for the likelihood function $L(P)$ in (24) when $n=$ 4.

The results in Section 2.1 remain good for this likelihood function. The equation (10) becomes

$$
\frac{b_{1}}{1+a_{i} b_{1}}+\frac{b_{2}}{1+a_{i} b_{2}}+\frac{b_{3}}{1+a_{i} b_{3}}+\frac{b_{4}}{1+a_{i} b_{4}}+\frac{\left(\frac{s}{t}-1\right) a_{i}}{1+a_{i} b_{i}}=0 .
$$

But the bounds in Lemma 8 involve the fraction $\frac{s}{t}$ and become complicated. A similar equation to (20) can be derived, but the nonzero factor is difficult to claim. Hopefully we may also prove $a_{2}=b_{2}$. Then $a_{3}=b_{3}$ and $a_{4}=b_{4}$ can be derived in a similar manner to Lemma 9 , So does Lemma 10. Finally we can find 4 local extrema and need only compare them to obtain the global maximum. In the case when the signs of $\left(a_{1}, a_{2}, a_{3}, a_{4}\right)$ are $(+,+,+,-)$, we have the equation

$$
a_{1}^{2}\left((3 s+9 t) a_{1}^{2}-(s-t)\right)=0 .
$$

Thus $a_{1}=\sqrt{\frac{s-t}{3 s+9 t}}$, and the matrix would be

$$
P_{1}=\left(\begin{array}{llll}
\frac{4 s+8 t}{3 s+9 t} & \frac{4 s+8 t}{3 s+9 t} & \frac{4 s+8 t}{3 s+9 t} & \frac{12 t}{3 s+9 t} \\
\frac{4 s+8 t}{3 s+9 t} & \frac{4 s+8 t}{3 s+9 t} & \frac{4+8 t}{3 s+9 t} & \frac{12 t}{3 s+9 t} \\
\frac{4 s+8 t}{3 s+9 t} & \frac{4 s+8 t}{3 s+9 t} & \frac{4 s+8 t}{3 s+9 t} & \frac{12 t}{3 s+9 t} \\
\frac{12 t}{3 s+9 t} & \frac{12 t}{3 s+9 t} & \frac{12 t}{3 s+9 t} & \frac{12 s}{3 s+9 t}
\end{array}\right) .
$$

In the case when the signs are $(+,+,-,-)$, we get $a_{1}=\sqrt{\frac{s-t}{s+3 t}}$ and the matrix would be

$$
P_{2}=\left(\begin{array}{llll}
\frac{2 s+2 t}{s+3 t} & \frac{2 s+2 t}{s+3 t} & \frac{4 t}{s+3 t} & \frac{4 t}{s+3 t}  \tag{25}\\
\frac{2 s+2 t}{s+3 t} & \frac{2 s+2 t}{s+3 t} & \frac{4 t}{s+3 t} & \frac{4 t}{s+3 t} \\
\frac{4 t}{s+3 t} & \frac{4 t}{s+3 t} & \frac{2 s+2 t}{s+3 t} & \frac{2 s+2 t}{s+3 t} \\
\frac{4 t}{s+3 t} & \frac{4 t}{s+3 t} & \frac{2 s+2 t}{s+3 t} & \frac{2 s+2 t}{s+3 t}
\end{array}\right) .
$$

One can prove that $L\left(P_{1}\right)<L\left(P_{2}\right)$ by some calculus technique, for example, taking the partial derivative of $\frac{L\left(P_{1}\right)}{L\left(P_{2}\right)}$ with respect to $s$. In similar approaches one can also show that $L\left(P_{3}\right)<L\left(P_{2}\right)$ and $L\left(P_{4}\right)<$ $L\left(P_{2}\right)$ where $P_{3}, P_{4}$ are the corresponding matrices for the cases when signs are $(+,+, 0,-)$ and $(+, 0,0,-)$ respectively. Thus the matrix in (25) is a global maximum.

More generally, let $(u)_{l_{1} \times l_{2}}$ be a block matrix with every entry being $u$ where $l_{1} \times l_{2} \in \mathbb{N}^{2}$ and $u>0$.

Conjecture 12. Let $n \geq 2$ and $0<t<s$. Then the matrix

$$
P=\frac{1}{n s+(n-1) n t}\left(\begin{array}{cc}
\left(\frac{s-t}{\left\lceil\frac{n}{2}\right\rceil}+t\right)_{\left\lceil\frac{n}{2}\right\rceil \times\left\lceil\frac{n}{2}\right\rceil} & (t)_{\left\lceil\frac{n}{2}\right\rceil \times\left\lfloor\frac{n}{2}\right\rfloor} \\
(t)_{\left\lfloor\frac{n}{2}\right\rfloor \times\left\lceil\frac{n}{2}\right\rceil} & \left(\frac{s-t}{\left\lfloor\frac{n}{2}\right\rfloor}+t\right)_{\left\lfloor\frac{n}{2}\right\rfloor \times\left\lfloor\frac{n}{2}\right\rfloor}
\end{array}\right)
$$

is a global maximum for $L(P)$ in (24).

Conjecture 13. Let $n \geq 2$ and $0<s \leq t$. Then the matrix

$$
P=\left(\begin{array}{ccccc}
\frac{2 s}{n^{2}(s+t)} & \frac{1}{n^{2}} & \cdots & \frac{1}{n^{2}} & \frac{2 t}{n^{2}(s+t)} \\
\frac{1}{n^{2}} & \frac{1}{n^{2}} & \cdots & \frac{1}{n^{2}} & \frac{1}{n^{2}} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\frac{1}{n^{2}} & \frac{1}{n^{2}} & \cdots & \frac{1}{n^{2}} & \frac{1}{n^{2}} \\
\frac{2 t}{n^{2}(s+t)} & \frac{1}{n^{2}} & \cdots & \frac{1}{n^{2}} & \frac{2 s}{n^{2}(s+t)}
\end{array}\right)
$$

is a global maximum for $L(P)$ in (24).

Acknowledgment. The authors were partially supported by the National Science Foundation under grants DMS-0302549 and DMS-1005369 and National Security Agency under grant H98230-08-1-0030. We would like to thank Bernd Sturmfels for his encouragement and anonymous referees for their helpful comments, in particular one of them provided Maple codes to us.

## References

[1] Buchberger, B. Gröbner-Basis: An Algorithmic Method in Polynomial Ideal Theory. Reidel Publishing Company, Dodrecht - Boston - Lancaster (1985)
[2] Catanese, F., Hoşten, S., Khetan, A., Sturmfels, B.: The maximum likelihood degree, Am. J. Math. 128, 671-697 (2006)
[3] Faugère, J. C. A new efficient algorithm for computing Gröbner basis (F4). J Pure Appl Algebra 139(1-3), 61-88 (1999)
[4] Faugère, J. C. A new efficient algorithm for computing Gröbner basis without reduction to zero (F5). In ISSAC '02: Proceedings of the 2002 international symposium on Symbolic and algebraic computation. New York, NY, USA, ACM, pp. 75-83 (2002)
[5] Fienberg, S., Hersh, P., Rinaldo, A., Zhou, Y.: Maximum likelihood estimation in latent class models for contingency table data, in Algebraic and geometric methods in statistics (eds Gibilisco P. et al), Cambridge University Press (2009)
[6] Gao, S., Guan, Y., and Volny IV, F.: A new incremental algorithm for computing Gröbner basis. In ISSAC'10: Proceedings of the 2010 International Symposium on Symbolic and Algebraic Computation. Munich, Germany, ACM, pp. 13-19 (2010)
[7] Gao, S., Volny IV, F., and Wang, S.: A new algorithm for computing Gröbner bases. Submitted (2010)
Available at http://www.math.clemson.edu/~sgao/pub.html
[8] Henry, N.W., Lazarsfeld, P.F.: Latent Structure Analysis, Houghton Mufflin Company (1968)
[9] Hoşten, S., Khetan, A., Sturmfels, B.: Solving the likelihood equations, Found. Comput Math 5, 389-407 (2005)
[10] Pachter, L., Sturmfels, B.: Algebraic Statistics for Computational Biology, Cambridge University Press (2005)
[11] Sturmfels, B.: Open problems in Algebraic Statistics, in Emerging Applications of Algebraic Geometry, (eds Putinar M. and Sullivant S. ), I.M.A. Volumes in Mathematics and its Applications, 149, Springer, New York, pp. 351-364 (2008)

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[^0]:    1991 Mathematics Subject Classification. Primary 65H10; Secondary 62P10, 62F30.

    Key words and phrases. Maximum likelihood estimation, latent class model, solving polynomial equations, algebraic statistics.

