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.

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1. The conjecture and its statistical background

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

$$L(P) = \prod_{i=1}^{4} p_{ii}^4 \times \prod_{i \neq j} p_{ij}^2 \tag{1}$$

over the set of all 4×4-matrices $P = (p_{ij})$ 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

$$P = \frac{1}{40} \begin{pmatrix} 3 & 3 & 2 & 2 \\ 3 & 3 & 2 & 2 \\ 2 & 2 & 3 & 3 \\ 2 & 2 & 3 & 3 \end{pmatrix}$$

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 $(X_1, \dots, X_d)$ be a discrete multivariate random vector where each X_j takes value from a finite state set $S_j = \{1, \dots, s_j\}$. Let $\Omega = S_1 \times \cdots \times S_d$ be the sample space. For each $(x_1, \ldots, x_d) \in \Omega$, the joint probability mass function of $(X_1, \ldots, X_d)$ is denoted as

$$p(x_1, \ldots, x_d) = P\{(X_1, \ldots, X_d) = (x_1, \ldots, x_d)\}.$$

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

$$\begin{aligned} p(x_1, \ldots, x_d, h) &= P\{(X_1, \ldots, X_d, H) = (x_1, \ldots, x_d, h)\} \\ &= p(x_1|h) \cdots p(x_d|h)\lambda_h \end{aligned}$$

where λ_h is the marginal probability of $P\{H = h\}$ and $p(x_j|h)$ is the conditional probability $P\{X_j = x_j|H = h\}$. We denote this new r-class mixture model by $\mathcal{H}$. The marginal distribution of $(X_1, \ldots, X_d)$ in $\mathcal{H}$ is given by the probability mass function (which is also called *accounting equations* [8])

$$p(x_1, \ldots, x_d) = \sum_{h \in [r]} p(x_1, \ldots, x_d, h) = \sum_{h \in [r]} p(x_1|h) \cdots p(x_d|h)\lambda_h.$$

In practice, a collection of samples from Ω are observed. For each $(x_1, \ldots, x_d)$, let $n(x_1, \ldots, x_d) \in \mathbb{N}$ be the number of observed occurrences of $(x_1, \ldots, x_d)$ in the samples. While the parameters $p(x_1|h), \cdots, p(x_d|h)$, $\lambda_h, p(x_1, \ldots, x_d)$ 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

$$L(\mathcal{H}) = \prod_{(x_1, \ldots, x_d) \in \Omega} p(x_1, \ldots, x_d)^{n(x_1, \ldots, x_d)}.$$

Since each $p(x_1, \ldots, x_d)$ is nonnegative, it is equivalent but more convenient to use the log-likelihood function

$$l(\mathcal{H}) = \sum_{(x_1, \ldots, x_d) \in \Omega} n(x_1, \ldots, x_d) \ln p(x_1, \ldots, x_d), \tag{2}$$

where we define $\ln(0) = -\infty$. Finding the maxima of (2) is difficult and remains infeasible by current symbolic software [2, 9]. 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 $d = 2$, $S_1 = S_2 = \{\text{A,C,G,T}\}$, $s_1 = s_2 = 4$ 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

$$\begin{array}{c c} & \begin{array}{cccc} \text{A} & \text{C} & \text{G} & \text{T} \end{array} \\ \begin{array}{c} \text{A} \\ \text{C} \\ \text{G} \\ \text{T} \end{array} & \begin{pmatrix} 4 & 2 & 2 & 2 \\ 2 & 4 & 2 & 2 \\ 2 & 2 & 4 & 2 \\ 2 & 2 & 2 & 4 \end{pmatrix} \end{array}.$$

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 $P = (p_{ij})$ 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

$$L(P) = \prod_{i=1}^{n} p_{ii}^2 \times \prod_{i \neq j} p_{ij}. \tag{3}$$

The problem is

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

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

$$J = \begin{pmatrix} 1 & \dots & 1 \\ \vdots & & \vdots \\ 1 & \dots & 1 \end{pmatrix}.$$

Since the function (3) is a continuous function in p_{ij}'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 $p_{ij} = 0$.

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 $\sum\limits_{j=1}^{n} p_{ij} = s_i$. Then $\sum\limits_{i=1}^{n} s_i = n^2$ and $\prod\limits_i s_i \leq n^n$ with equality if and only if $s_i = n$ for all i. Let $\bar{p}_{ij} = \frac{n}{s_i} p_{ij}$ and $\bar{P} = (\bar{p}_{ij})_{n \times n}$. Then $\mathrm{rank}(\bar{P}) = \mathrm{rank}(P)$ and $\sum\limits_{i,j} \bar{p}_{ij} = n^2$. However,

$$L(\bar{P}) = L(P) \cdot \left(\frac{n^n}{\prod\limits_i s_i} \right)^{n+1} \geq L(P)$$

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. $\square$

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 σ_1 and σ_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 $v_2 = (a_1, a_2, \ldots, a_n)^t$ and $\sigma_2 u_2 = (b_1, b_2, \ldots, b_n)^t$. Then P has the form

$$P = J + \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix} (a_1, a_2, \ldots, a_n) = \begin{pmatrix} 1 + a_1 b_1 & \cdots & 1 + a_n b_1 \\ \vdots & 1 + a_i b_j & \vdots \\ 1 + a_1 b_n & \cdots & 1 + a_n b_n \end{pmatrix}.$$

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

$$\sum_{i=1}^{n} a_i \cdot \sum_{i=1}^{n} b_i = 0. \tag{4}$$

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

Maximize: $\quad l(P) = 2 \sum\limits_{i=1}^{n} \ln(1 + a_i b_i) + \sum\limits_{i \neq j} \ln(1 + a_i b_j)$

Subject to: $\quad$ 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

$$\frac{\partial \Lambda(P, \lambda)}{\partial a_i} = \sum_{j=1}^{n} \frac{b_j}{1 + a_i b_j} + \frac{b_i}{1 + a_i b_i} + \lambda \sum_{j=1}^{n} b_j = 0, \quad 1 \leq i \leq n, \tag{5}$$

and

$$\frac{\partial \Lambda(P,\lambda)}{\partial b_j} = \sum_{i=1}^{n} \frac{a_i}{1+a_ib_j} + \frac{a_j}{1+a_jb_j} + \lambda \sum_{i=1}^{n} a_i = 0, \quad 1 \leq j \leq n. \tag{6}$$

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

$$\sum_{i=1}^{n} a_i = 0, \tag{7}$$

and

$$\sum_{i=1}^{n} b_i = 0. \tag{8}$$

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

Lemma 2. *A global maximum P must satisfy*

$$\sum_{j=1}^{n} \frac{b_j}{1+a_ib_j} + \frac{b_i}{1+a_ib_i} = 0, \quad 1 \leq i \leq n, \tag{9}$$

and

$$\sum_{i=1}^{n} \frac{a_i}{1+a_ib_j} + \frac{a_j}{1+a_jb_j} = 0, \quad 1 \leq j \leq n. \tag{10}$$

Doing some simple algebra yields

Corollary 3. *An optimal solution must satisfy*

$$\sum_{j=1}^{n} \frac{1}{1+a_ib_j} + \frac{1}{1+a_ib_i} = n+1, \quad 1 \leq i \leq n, \tag{11}$$

and

$$\sum_{i=1}^{n} \frac{1}{1+a_ib_j} + \frac{1}{1+a_jb_j} = n+1, \quad 1 \leq j \leq n. \tag{12}$$

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

The $2n$ equations derived by clearing denominators of the equations in Lemma 2 or Corollary 3 along with equations (7) and (8) form a system of $2n+2$ polynomial equations with $2n$ 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,

$$\sum_{j=1}^{n} \frac{1}{n} \cdot \frac{1}{1 + a_i b_j} \geq \frac{1}{\sum_{j=1}^{n} \frac{1}{n}(1 + a_i b_j)} = 1.$$

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

$$\begin{aligned}
L(P) - L(\bar{P}) &= C_1 \cdot ((1+a_ib_i)^2(1+a_ib_j)(1+a_jb_i)(1+a_jb_j)^2 \\
&\quad -(1+a_ib_j)^2(1+a_ib_i)(1+a_jb_j)(1+a_jb_i)^2) \\
&= C_2 \cdot ((1+a_ib_i)(1+a_jb_j) - (1+a_ib_j)(1+a_jb_i)) \\
&= C_2 \cdot (a_ib_i + a_jb_j - a_ib_j - a_jb_i) \\
&= C_2 \cdot (a_i - a_j)(b_i - b_j)
\end{aligned}$$

where C_1, C_2 are products of some entries of P, so C_1, C_2 are positive. Thus $(a_i - a_j)(b_i - b_j) \geq 0$. 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 $b_i > b_j$. $\square$

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 5, 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 (a_1, a_2, a_3, a_4) in P by $\sqrt{\frac{a_1}{b_1}}(a_1, a_2, a_3, a_4)$ and $(b_1, b_2, b_3, b_4)^t$ by $\sqrt{\frac{b_1}{a_1}}(b_1, b_2, b_3, b_4)^t$. It turns out that $1 + \sqrt{\frac{a_1}{b_1}}a_i\sqrt{\frac{b_1}{a_1}}b_i = 1 + a_ib_j$ for any i and j, so we may always assume $a_1 = b_1$. Thus P can be expressed as the form

$$\begin{pmatrix}
1+a_1^2 & 1+a_2a_1 & 1+a_3a_1 & 1+a_4a_1 \\
1+a_1b_2 & 1+a_2b_2 & 1+a_3b_2 & 1+a_4b_2 \\
1+a_1b_3 & 1+a_2b_3 & 1+a_3b_3 & 1+a_4b_3 \\
1+a_1b_4 & 1+a_2b_4 & 1+a_3b_4 & 1+a_4b_4
\end{pmatrix}. \tag{13}$$

If $a_2 \leq 0$, we then replace (a_1, a_2, a_3, a_4) in P by $(-a_4, -a_3, -a_2, -a_1)$ and $(b_1, b_2, b_3, b_4)^t$ by $(-b_4, -b_3, -b_2, -b_1)^t$. 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

$$\frac{2}{1+a_1^2}+\frac{1}{1+a_2a_1}+\frac{1}{1+a_3a_1}+\frac{1}{1+a_4a_1}=5.$$

Also

$$a_1^2+a_2a_1+a_3a_1+a_4a_1=0.$$

From the two equations above we get

$$a_3a_1\cdot a_4a_1=f_1(a_1a_1,a_1a_2) \tag{14}$$

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

$$\frac{1}{1+a_1b_2}+\frac{2}{1+a_2b_2}+\frac{1}{1+a_3b_2}+\frac{1}{1+a_4b_2}=5.$$

Along with

$$a_1b_2+a_2b_2+a_3b_2+a_4b_2=0,$$

we get

$$a_3b_2\cdot a_4b_2=f_1(a_2b_2,a_1b_2). \tag{15}$$

Since a_1,b_2 are nonzero, we combine equations (14) and (15) to get

$$\frac{f_1(a_1^2,a_1a_2)}{a_1^2}=\frac{f_1(a_2b_2,a_1b_2)}{b_2^2}. \tag{16}$$

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

$$f_2(a_1,a_2,b_2)=0. \tag{17}$$

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

$$\frac{f_1(a_1^2,a_1b_2)}{a_1^2}=\frac{f_1(a_2b_2,a_1a_2)}{a_2^2}. \tag{18}$$

One can see that equation (18) is obtainable by switching a_2 with b_2 in equation (16). Thus we have

$$f_2(a_1,b_2,a_2)=0. \tag{19}$$

Subtracting (19) from (17) yields

$$f_2(a_1,a_2,b_2)-f_2(a_1,b_2,a_2)=0.$$

Since we only switched a_2 and b_2 in polynomial f_2, there must be a factor a_2-b_2 for $f_2(a_1,a_2,b_2)-f_2(a_1,b_2,a_2)$, say

$$(a_2-b_2)f_3(a_1,a_2,b_2)=0, \tag{20}$$

where

$$\begin{aligned} f_3(a_1,a_2,b_2) = &\quad (20a_1^4b_2^2+15a_1^3b_2+3a_1^2b_2^2+2a_1b_2-4b_2^2)a_2^2 \\ &+ (3a_1^4b_2+15a_1^3b_2^2+2a_1^3+10a_1^2b_2+2a_1b_2^2-3a_1-b_2)a_2 \\ &- 4a_1^4+2a_1^3b_2-a_1^2-3a_1b_2-2. \end{aligned}$$

Thus $a_2=b_2$ if $f_3(a_1,a_2,b_2)\neq 0$. This is true because we have some bounds for a_1^2, a_1a_2, a_1b_2 as presented in Lemma 8 below, which can be applied to get

$$\begin{aligned} f_3(a_1,a_2,b_2) = &\quad (20a_1^4b_2^2+15a_1^3b_2+3a_1^2b_2^2+2a_1b_2-4b_2^2)a_2^2 \\ &+ (3a_1^4b_2+15a_1^3b_2^2+2a_1^3+10a_1^2b_2+2a_1b_2^2-3a_1-b_2)a_2 \\ &- 4a_1^4+2a_1^3b_2-a_1^2-3a_1b_2-2 \\ < &\quad \frac{20}{5^4}+\frac{15}{5^3}+\frac{3}{4}a_2^2b_2^2+\frac{2}{5}a_2b_2-4a_2^2b_2^2 \\ &+ \frac{3}{2^25^2}+\frac{15}{5^3}+\frac{2}{2^25}+\frac{10}{5^2}+\frac{2}{5}a_2b_2-a_2b_2 \\ &+ \frac{2}{2^25}-2 \\ < &\ -\frac{13}{4}a_2^2b_2^2-\frac{1}{5}a_2b_2-\frac{549}{500} \\ < &\ 0. \end{aligned}$$

Therefore, $f_3(a_1,a_2,b_2)\neq 0$ and $a_2=b_2$, just as needed. □

Lemma 8.

1. $a_1^2 \le \frac{1}{2}$,
2. $0 \le a_1a_2 \le \frac{1}{5}$, *and*
3. $0 \le a_1b_2 \le \frac{1}{5}$.

Proof. (1) Let $A_i = 1 + a_1a_i$ for $i = 1,\dots,4$, then $\sum_{i=1}^{4} A_i = 4$, $A_1 \ge A_2 \ge 1$, $A_3 \ge A_4 > 0$ and

$$\frac{2}{A_1}+\frac{1}{A_2}+\frac{1}{A_3}+\frac{1}{A_4}=5.$$

Since

$$\frac{1}{A_3}+\frac{1}{A_4}\ge\frac{4}{A_3+A_4}=\frac{4}{4-A_1-A_2},$$

we have

$$5=\frac{2}{A_1}+\frac{1}{A_2}+\frac{1}{A_3}+\frac{1}{A_4}\ge\frac{2}{A_1}+\frac{1}{A_2}+\frac{4}{4-A_1-A_2}. \tag{21}$$

Let

$$g(A_2)=\frac{1}{A_2}+\frac{4}{4-A_1-A_2},$$

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

$$\frac{\partial g(A_2)}{\partial A_2}=-\frac{1}{A_2^2}+\frac{4}{(4-A_1-A_2)^2}.$$

Note that $A_1 \geq A_2 \geq 1$, thus $4 - A_1 - A_2 \leq 2$ and $\frac{\partial g(A_2)}{\partial A_2} \geq 0$. Therefore $g(A_2) \geq g(1)$ 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 $2A_1^2 - 5A_1 + 3 \leq 0$, 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 $g(A_2) > g(\frac{6}{5})$. 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 $(-\infty, 0) \cup (\frac{28}{25}, \frac{6}{5}) \cup (\frac{14}{5}, \infty)$. 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. $\square$

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 $A_3 = h_1(A_1, A_2)$ and $A_4 = h_2(A_1, A_2)$. If we let $B_i = 1 + a_1 b_i$, we can get $B_3 = h_1(B_1, B_2)$ and $B_4 = h_2(B_1, B_2)$ 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 $i = 3, 4$. $\square$

By Lemmas 7 and 9, we have $a_i = b_i$ for all i. Hence P can be expressed as

$$P = \begin{pmatrix} 1 + a_1^2 & 1 + a_2 a_1 & 1 + a_3 a_1 & 1 + a_4 a_1 \\ 1 + a_1 a_2 & 1 + a_2^2 & 1 + a_3 a_2 & 1 + a_4 a_2 \\ 1 + a_1 a_3 & 1 + a_2 a_3 & 1 + a_3^2 & 1 + a_4 a_3 \\ 1 + a_1 a_4 & 1 + a_2 a_4 & 1 + a_3 a_4 & 1 + a_4^2 \end{pmatrix}$$

where

$$\sum_{i=1}^{4} a_i = 0. \tag{22}$$

By Corollary 3 we have the following system of equations

$$\begin{cases} \dfrac{2}{1+a_1^2} + \dfrac{1}{1+a_2a_1} + \dfrac{1}{1+a_3a_1} + \dfrac{1}{1+a_4a_1} = 5, \\ \dfrac{1}{1+a_1a_2} + \dfrac{2}{1+a_2^2} + \dfrac{1}{1+a_3a_2} + \dfrac{1}{1+a_4a_2} = 5, \\ \dfrac{1}{1+a_1a_3} + \dfrac{1}{1+a_2a_3} + \dfrac{2}{1+a_3^2} + \dfrac{1}{1+a_4a_3} = 5, \\ \dfrac{1}{1+a_1a_4} + \dfrac{1}{1+a_2a_4} + \dfrac{1}{1+a_3a_4} + \dfrac{2}{1+a_4^2} = 5. \end{cases} \tag{23}$$

With (22) and (23), we claim that

Lemma 10. *$a_i = a_j$ if $a_ia_j > 0$.*

Proof. Let

$$F(x) = \frac{1}{1+a_1x} + \frac{1}{1+a_2x} + \frac{1}{1+a_3x} + \frac{1}{1+a_4x} + \frac{1}{1+x^2} - 5 = 0.$$

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 $(-\frac{1}{a_j}, -\frac{1}{a_i})$. Note that

$$\lim_{x \to -\frac{1}{a_j}^+} F(x) = \infty \quad \text{and} \quad \lim_{x \to -\frac{1}{a_i}^-} F(x) = -\infty.$$

There must be a zero lying in $(-\frac{1}{a_j}, -\frac{1}{a_i})$, say a_0. Then $a_0 < -\frac{1}{a_i}$ (or $a_0 > -\frac{1}{a_j}$ respectively), i.e. $1 + a_ia_0 < 0$ (or $1 + a_ja_0 < 0$ respectively). Since $a_0 \neq 0$, x_0 must be one of a_k, $k = 1, \ldots, 4$. Thus $1 + a_ia_0$ (or $1 + a_ja_0$, respectively) is an entry in matrix P, contradicting the fact that each entry of P is positive. Therefore if i, j are consecutive and $a_ia_j > 0$, we must have $a_i = a_j$. Hence $a_ia_j > 0$ 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 (a_1, a_2, a_3, a_4). 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

$$P_1 = \begin{pmatrix} \frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\ \frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\ \frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\ \frac{4}{5} & \frac{4}{5} & \frac{4}{5} & \frac{8}{5} \end{pmatrix}.$$

For the case when the signs are $(+,+,-,-)$, we get $a_1 = \frac{1}{\sqrt{5}}$ and the matrix would be

$$P_2 = \begin{pmatrix} \frac{6}{5} & \frac{6}{5} & \frac{4}{5} & \frac{4}{5} \\ \frac{6}{5} & \frac{6}{5} & \frac{4}{5} & \frac{4}{5} \\ \frac{4}{5} & \frac{4}{5} & \frac{6}{5} & \frac{6}{5} \\ \frac{4}{5} & \frac{4}{5} & \frac{6}{5} & \frac{6}{5} \end{pmatrix}.$$

When the signs are $(+,+,0,-)$, $a_1 = \frac{1}{2\sqrt{2}}$, and the matrix would be

$$P_3 = \begin{pmatrix} \frac{9}{8} & \frac{9}{8} & 1 & \frac{3}{4} \\ \frac{9}{8} & \frac{9}{8} & 1 & \frac{3}{4} \\ 1 & 1 & 1 & 1 \\ \frac{3}{4} & \frac{3}{4} & 1 & \frac{3}{2} \end{pmatrix}.$$

And when the signs are $(+,0,0,-)$, $a_1 = \frac{1}{\sqrt{3}}$ and the matrix would be

$$P_4 = \begin{pmatrix} \frac{4}{3} & 1 & 1 & \frac{2}{3} \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ \frac{2}{3} & 1 & 1 & \frac{4}{3} \end{pmatrix}.$$

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

$$P = \frac{1}{40} \begin{pmatrix} 3 & 3 & 2 & 2 \\ 3 & 3 & 2 & 2 \\ 2 & 2 & 3 & 3 \\ 2 & 2 & 3 & 3 \end{pmatrix}.$$

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 Section2.2. 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

$$\mathcal{J}_0 = \langle a_1 - b_1, \sum_{i=1}^{4} a_i, \sum_{i=1}^{4} b_i, h_1, \cdots, h_8 \rangle \subset \mathbb{C}[X]$$

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

$$\mathcal{J}_1 = \mathcal{J}_0 + \langle 1 - u \cdot a_1 \rangle \subset \mathbb{C}[X, u]$$

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 $\langle G_2 \rangle$ 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 $\langle G_2 \rangle$. 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:

$$P_1 = \begin{pmatrix} \frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\ \frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\ \frac{16}{15} & \frac{16}{15} & \frac{16}{15} & \frac{4}{5} \\ \frac{4}{5} & \frac{4}{5} & \frac{4}{5} & \frac{8}{5} \end{pmatrix}, \qquad P_2 = \begin{pmatrix} \frac{6}{5} & \frac{6}{5} & \frac{4}{5} & \frac{4}{5} \\ \frac{6}{5} & \frac{6}{5} & \frac{4}{5} & \frac{4}{5} \\ \frac{4}{5} & \frac{4}{5} & \frac{6}{5} & \frac{6}{5} \\ \frac{4}{5} & \frac{4}{5} & \frac{6}{5} & \frac{6}{5} \end{pmatrix},$$

$$P_3 = \begin{pmatrix} \frac{9}{8} & \frac{9}{8} & 1 & \frac{3}{4} \\ \frac{9}{8} & \frac{9}{8} & 1 & \frac{3}{4} \\ 1 & 1 & 1 & 1 \\ \frac{3}{4} & \frac{3}{4} & 1 & \frac{3}{2} \end{pmatrix}, \qquad P_4 = \begin{pmatrix} \frac{4}{3} & 1 & 1 & \frac{2}{3} \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ \frac{2}{3} & 1 & 1 & \frac{4}{3} \end{pmatrix},$$

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 $(a_2 - b_2)f_3(a_1, a_2, b_2)$ in the proof for Lemma 7. Our approach is to justify that the factor $f_3(a_1, a_2, b_2)$, 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 $f_3(a_1, a_2, b_2)$ 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

$$L(P) = \prod_{i=1}^{n} p_{ii}^{s} \times \prod_{i \neq j} p_{ij}^{t}, \tag{24}$$

where $P = (p_{ij})$ 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 4×4 matrices whose rank is at most 2 and whose entries sum to 1, the matrix*

$$P = \frac{1}{4s + 12t} \begin{pmatrix} \frac{s+t}{2} & \frac{s+t}{2} & t & t \\ \frac{s+t}{2} & \frac{s+t}{2} & t & t \\ t & t & \frac{s+t}{2} & \frac{s+t}{2} \\ t & t & \frac{s+t}{2} & \frac{s+t}{2} \end{pmatrix}$$

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

$$\frac{b_1}{1 + a_i b_1} + \frac{b_2}{1 + a_i b_2} + \frac{b_3}{1 + a_i b_3} + \frac{b_4}{1 + a_i b_4} + \frac{(\frac{s}{t} - 1)a_i}{1 + a_i b_i} = 0.$$

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 (a_1, a_2, a_3, a_4) are $(+,+,+,-)$, we have the equation

$$a_1^2((3s+9t)a_1^2 - (s-t)) = 0.$$

Thus $a_1 = \sqrt{\frac{s-t}{3s+9t}}$, and the matrix would be

$$P_1 = \begin{pmatrix} \frac{4s+8t}{3s+9t} & \frac{4s+8t}{3s+9t} & \frac{4s+8t}{3s+9t} & \frac{12t}{3s+9t} \\ \frac{4s+8t}{3s+9t} & \frac{4s+8t}{3s+9t} & \frac{4s+8t}{3s+9t} & \frac{12t}{3s+9t} \\ \frac{4s+8t}{3s+9t} & \frac{4s+8t}{3s+9t} & \frac{4s+8t}{3s+9t} & \frac{12t}{3s+9t} \\ \frac{12t}{3s+9t} & \frac{12t}{3s+9t} & \frac{12t}{3s+9t} & \frac{12s}{3s+9t} \end{pmatrix}.$$

In the case when the signs are $(+,+,-,-)$, we get $a_1 = \sqrt{\frac{s-t}{s+3t}}$ and the matrix would be

$$P_2 = \begin{pmatrix} \frac{2s+2t}{s+3t} & \frac{2s+2t}{s+3t} & \frac{4t}{s+3t} & \frac{4t}{s+3t} \\ \frac{2s+2t}{s+3t} & \frac{2s+2t}{s+3t} & \frac{4t}{s+3t} & \frac{4t}{s+3t} \\ \frac{4t}{s+3t} & \frac{4t}{s+3t} & \frac{2s+2t}{s+3t} & \frac{2s+2t}{s+3t} \\ \frac{4t}{s+3t} & \frac{4t}{s+3t} & \frac{2s+2t}{s+3t} & \frac{2s+2t}{s+3t} \end{pmatrix}. \tag{25}$$

One can prove that $L(P_1) < L(P_2)$ by some calculus technique, for example, taking the partial derivative of $\frac{L(P_1)}{L(P_2)}$ with respect to s. In similar approaches one can also show that $L(P_3) < L(P_2)$ and $L(P_4) < L(P_2)$ 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*

$$P = \frac{1}{ns + (n-1)nt} \begin{pmatrix} (\frac{s-t}{\lceil \frac{n}{2} \rceil} + t)_{\lceil \frac{n}{2} \rceil \times \lceil \frac{n}{2} \rceil} & (t)_{\lceil \frac{n}{2} \rceil \times \lfloor \frac{n}{2} \rfloor} \\ (t)_{\lfloor \frac{n}{2} \rfloor \times \lceil \frac{n}{2} \rceil} & (\frac{s-t}{\lfloor \frac{n}{2} \rfloor} + t)_{\lfloor \frac{n}{2} \rfloor \times \lfloor \frac{n}{2} \rfloor} \end{pmatrix}$$

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

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

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

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

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