# Analytical Forms for Most Likely Matrices Derived from Incomplete Information

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#### Abstract

Consider a rectangular matrix describing some type of communication or transportation between a set of origins and a set of destinations, or a classification of objects by two attributes. The problem is to infer the entries of the matrix from limited information in the form of constraints, generally the sums of the elements over various subsets of the matrix, such as rows, columns, etc, or from bounds on these sums, down to individual elements. Such problems are routinely addressed by applying the maximum entropy method to compute the matrix numerically, but in this paper we derive analytical, closed-form solutions. For the most complicated cases we consider the solution depends on the root of a non-linear equation, for which we provide an analytical approximation in the form of a power series. Some of our solutions extend to 3-dimensional matrices.

Besides being valid for matrices of arbitrary size, the analytical solutions exhibit many of the appealing properties of maximum entropy, such as precise use of the available data, intuitive behavior with respect to changes in the constraints, and logical consistency.

### 1 Introduction

Consider a set of n origins communicating with a set of m destinations. For our purposes it suffices that each origin is connected to each destination; the exact nature of the connection is not important. The communication may be in the form of transportation, e.g. the origins and destinations may be cities or other geographic locations, and people travel from one to another by some means, or commodities are transported from one to another in some fashion. Or the origins and destinations may be nodes connected by a communications network, with various sorts of traffic flowing from each source to each destination. In either

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of these cases, the transportation or communication can be represented by an rectangular  $n \times m$  trip or traffic matrix whose i, jth entry gives the number of trips, volume of traffic, units of a commodity, etc. from the *i*th origin to the *j*th destination. (The distinction between origins and destinations is not mandatory; one could take n = m and think just of a set of *n* locations.) In a different setting, we have a set of objects with two attributes, say height and weight, color and shape, success/failure of a test and test condition, and the objects are placed in a table according to the *n*-valued first attribute and the *m*-valued second attribute. In this setting the  $n \times m$  matrix is known as a (2-dimensional) contingency table whose (i, j)th entry is the number of objects whose 1st attribute has the *i*th value and 2nd attribute the *j*th value.

Whichever of these two settings obtains, we are interested in the situation where we have *limited* or incomplete information about the matrix: we do not know the individual elements, but know less detailed characteristics such as the totals of the rows and/or columns, or of some of them, the total sum of the matrix, or we have bounds on some of these quantities, or in addition we know the values of some individual elements or have bounds on them. The problem then is how to *infer* all the matrix elements from this information, and, in this paper, we are interested in solving the problem analytically. It is well known how to find numerical solutions to these inference problems by numerical entropy maximization.

Most likely matrices and maximum entropy We approach the problem by regarding the matrix as constructed from a known number of elements (trips, traffic units, etc), which we will think of as balls, to be placed into an  $n \times m$  array of boxes. We will refer to the number of ways (assignments of balls to boxes) in which a given matrix X can be built as its *number of realizations*, #(X). If the information I is known about X, we may also regard it as *constraints* that X has to satisfy, and we write #(X|I) for the number of realizations of X that accord with I or satisfy the constraints I. For example, if what we know about the  $2 \times 2$  matrix X,  $x_{ij} \in \mathbb{N}$ , is that its row sums are 7 and 3, some possibilities are

$$X_1 = \begin{pmatrix} 3 & 4 \\ 2 & 1 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 4 & 3 \\ 2 & 1 \end{pmatrix}, \quad X_3 = \begin{pmatrix} 4 & 3 \\ 1 & 2 \end{pmatrix}, \quad X_4 = \begin{pmatrix} 2 & 5 \\ 2 & 1 \end{pmatrix}, \quad X_5 = \begin{pmatrix} 1 & 6 \\ 3 & 0 \end{pmatrix}.$$

In fact there are 8 possible 1st rows and 4 possible 2nd rows, so 32 matrices satisfy these constraints. Further, for the above examples,  $\#(X_1|I) = \#(X_2|I) = \#(X_3|I) =$  $10!/(1!2!3!4!) = 12600, \ \#(X_4|I) = 10!/(5!2!2!1!) = 7560, \ \#(X_5|I) = 10!/(1!3!6!) = 840^{-1}$ . We will refer to the matrix  $\hat{X}$  for which #(X|I), given by a multinomial coefficient, is maximum, as the most likely matrix given the information/constraints I. "Most likely" may have probability connotations for some, but we use it only as a shorthand for "matrix that

 $<sup>^1\</sup>mathrm{We}$  assume that the balls are distinguishable. The boxes are distinguishable, being particular elements of a matrix.

can be realized in the greatest number of ways", which has nothing to do with probability, it is merely counting.

If the constraints are convex (in this paper they will be linear), and they specify the sum of all the elements, the discrete problem of maximizing #(X|I) can be turned into a continuous concave maximization problem via the Stirling approximation to the factorial: the log of the multinomial coefficient is approximated by the *entropy* of the  $x_{ij}$ . This continuous approximation is well-known, and in fact dates back to Boltzmann's (1847-1906) combinatorial formulation of statistical mechanics where molecules are assigned to boxes; see e.g. [Som67]. Thus our discrete most likely matrix problem connects to the extensive body of work on maximum entropy (MAXENT): see the works [Ros83], [Jay03] of E. T. Jaynes, the books [Tri69], [KK92], and the series of MAXENT conference proceedings [MAX98] and [MAX09]<sup>2</sup>, to name a few. So, as long as the total sum is known, the discrete most likely matrix problem and its continuous MAXENT analogue are equivalent to within the Stirling approximation, and we will sometimes refer to one, sometimes to the other.

The combinatorial rationale that we consider here is appealing because of its simplicity: it is just counting. In addition, MAXENT has intuitive appeal as maximizing uncertainty while conforming to precisely the available information. More importantly, it has a powerful *axiomatic* basis as well: see [Ski89], and [CG06] for recent developments.

**Summary and background** In this paper we derive analytical, closed-form solutions to a set of maximum entropy problems having to do with  $n \times m$  matrices subject to linear constraints. The constraints have the form of equalities or inequalities (upper bounds) on sums over various subsets of the matrix, e.g. rows, columns, the whole matrix, the diagonal, individual elements, etc. In §2 to §5 we consider known row, column, and total sums, as well as upper bounds on them. We observe that when the total sum is not known, the most likely matrix is not the MAXENT matrix, but it has a simple relationship to a certain MAXENT matrix. In §6 we consider upper bounds on row sums and on individual elements. Finally, in §7, we investigate the effect of having symmetric information in combination with bounds on sums and specified individual elements, including an extension to 3-dimensional matrices. Table 8.1 in §8 summarizes the types of constraints that we consider. In the most complicated cases the solutions depend on the root of a single non-linear equation, but even in those cases we find an analytical power series approximation to the root, hence to the matrix elements themselves. The analytical forms allow us to treat matrices of arbitrary size, reveal the exact structure of the most likely/MAXENT matrix, and allow us to see explicitly the robustness of the solution to changes in the constraints, and its behavior with respect to uncertainty in the data. These features demonstrate the *logical precision* of the MAXENT method and are inaccessible via numerical solutions.

An extensive and in-depth study of MAXENT matrices in transportation analysis is [ES90]; an introduction can be found in [KK92], and a recent reference is [BD08]. Various

<sup>&</sup>lt;sup>2</sup>The latter with the unfortunate adoption of Microsoft Word for the typesetting of mathematical papers.

aspects of matrices characterizing traffic in IP networks, including numerical estimation from incomplete data, are studied in [ACR+06], [ZRLD05], and the references therein<sup>3</sup>. A semi-analytical derivation of most likely traffic matrices subject to a total cost constraint is in [KO08]. With respect to contingency tables, [KK92] provides an introduction while [Goo63] derives fundamental results on the "vanishing of interactions" in MAXENT multidimensional tables. For a small sample of other applications of MAXENT see [CG02] and [Sen91] (economics and econometrics), [KT92] and [KMO93] (queueing problems), and [TJI02] (systems theory).

### 2 Specified row sums and some column sums

We begin by considering a small extension of a problem whose solution is already known in the literature in order to introduce the concepts and general methodology used in the rest of the paper. Phrasing the discussion in terms of an  $n \times m$  matrix X describing the traffic from n origins to m destinations, suppose we have the following information (or constraints) I about it:

- 1. The total traffic from each origin:  $\forall i, \sum_{j} x_{ij} = u_i$ .
- 2. The total traffic to each of the first  $\ell \leq m$  destinations:  $\forall j \leq \ell, \sum_i x_{ij} = v_j$

We assume that the information is consistent, i.e.  $\sum_i u_i \ge \sum_j v_j$ . This information also specifies the total traffic s in the network:  $s = \sum_i u_i$ .

To find the most likely traffic matrix  $\hat{X}$  that follows from the information I, given that the sum of all the entries is s, we construct X by distributing the s units of traffic into nmboxes so that  $x_{ij}$  of them go in box (i, j). The number of ways in which this can be done is

$$\left(\begin{array}{c}s\\x_{11},\ldots,x_{1m},x_{21},\ldots,x_{2m},\ldots,x_{n1},\ldots,x_{nm}\end{array}\right) = \frac{s!}{\prod_{i,j}x_{ij}!} = \#(X \mid s), \quad (2.1)$$

where the notation indicates that s is known. To render the maximization of  $\#(X \mid s)$  tractable, and, at the same time, achieve a relatively simple solution, we treat it as a *continuous* problem and maximize the log of  $\#(X \mid s)$  using the Stirling approximation

$$\ln x! = x \ln x - x + \frac{1}{2} \ln x + \ln \sqrt{2\pi} + \frac{\vartheta}{12x}, \quad \vartheta \in (0, 1),$$
(2.2)

which is defined for all x > 0 by  $x! = \Gamma(x + 1)$ . Using the first two terms of (2.2) and noting that  $\sum_{i,j} x_{ij} = s$  is given, the problem becomes

maximize 
$$-\sum_{i,j} x_{ij} \ln x_{ij},$$
 (2.3)

<sup>&</sup>lt;sup>3</sup>We say "estimation" because the methods used do not have the same logical standing as MAXENT. Also, the problem of estimating traffic in a real IP network is significantly more complex than the problems considered in this paper.

subject to

$$\sum_{j} x_{ij} = u_i \quad \text{for } i = 1, \dots, n, \qquad \sum_{i} x_{ij} = v_j \quad \text{for } j = 1, \dots, \ell.$$

The expression to be maximized is the *entropy* of the set of demands  $x_{ij}$ . (Usually, e.g. in information theory, entropy is defined for a vector whose entries sum to 1. What we use here is more properly referred to as *combinatorial*, as opposed to *information*, entropy<sup>4</sup>.) Because the entropy is a strictly concave function, the problem (2.3) has a unique solution which can be found by forming the Lagrangean (details in §A.1)

$$\Phi = -\sum_{i,j} x_{ij} \ln x_{ij} - \sum_i \lambda_i \left( \sum_j x_{ij} - u_i \right) - \sum_j \mu_j \left( \sum_i x_{ij} - v_j \right).$$

It follows that  $x_{ij} = e^{-\lambda_i - \mu_j - 1}$  if  $j \leq \ell$  and  $e^{-\lambda_i - 1}$  if  $j > \ell$ . Denoting  $e^{-\lambda_i - 1}$  by  $\lambda'_i$  and  $e^{-\mu_j}$  by  $\mu'_j$ , and then eliminating the primes to simplify the notation,

$$x_{ij} = \begin{cases} \lambda_i \mu_j, & j \le \ell \\ \lambda_i, & j > \ell \end{cases}, \qquad \lambda_i, \mu_j > 0.$$
(2.4)

The origin and destination constraints imply that

$$\lambda_i(\mu_1 + \dots + \mu_{\ell} + m - \ell) = u_i, \quad i = 1, \dots, n (\lambda_1 + \dots + \lambda_n)\mu_j = v_j, \quad j = 1, \dots, \ell.$$
 (2.5)

Adding the first set of constraints together and doing the same with the second set we get  $(\lambda_1 + \cdots + \lambda_n)(\mu_1 + \cdots + \mu_\ell + m - \ell) = u_1 + \cdots + u_n = s$  and  $(\lambda_1 + \cdots + \lambda_n)(\mu_1 + \cdots + \mu_\ell) = v_1 + \cdots + v_\ell$ . If we now let  $\lambda$  be the sum of the  $\lambda_i$  and  $\mu$  that of the  $\mu_j$ , it follows that if  $\ell < m$ 

$$\lambda = \frac{s - (v_1 + \dots + v_\ell)}{m - \ell}, \quad \mu = \frac{(n - \ell)(v_1 + \dots + v_\ell)}{s - (v_1 + \dots + v_\ell)}$$

So from (2.5),

$$\lambda_i = \frac{\left(s - (v_1 + \dots + v_\ell)\right)u_i}{(n - \ell)s}, \quad \mu_j = \frac{(m - \ell)v_j}{s - (v_1 + \dots + v_\ell)}.$$
(2.6)

Using this in (2.4), we finally get

$$\hat{x}_{ij} = \begin{cases} \frac{u_i v_j}{s}, & j \leq \ell, \\ \frac{s - (v_1 + \dots + v_\ell)}{m - \ell} \frac{u_i}{s}, & j > \ell, \end{cases} \quad i = 1, \dots, n.$$
(2.7)

<sup>4</sup>This usage goes back to Boltzmann's combinatorial formulation of statistical mechanics, see [Som67].

Now if  $\ell = m$ , (2.5) and the two equations following it become  $\lambda_i \mu = u_i$ ,  $\mu_j \lambda = v_j$ ,  $\lambda \mu = s$ , from which it follows that  $\lambda_i \mu_j = u_i v_j / s$ ; thus (2.7) is valid even when  $\ell = m$ . Therefore the most likely matrix  $\hat{X}$  consists of an  $n \times \ell$  left-hand part whose entries are given in the 1st line of (2.7), and a possibly empty right-hand part consisting of  $m - \ell$  identical columns, each of which is described by the 2nd line of (2.7).

The solution  $\hat{x}_{ij} = u_i v_j / s$  for all i, j is known as the gravity model for the traffic. This model has its origins in transportation analysis, in connection with the numbers of trips taken between n origins and m destinations, which are cities of known populations; Xis then referred to as a "trip matrix". See [KK92] for an introduction, and [ES90] for an in-depth treatment. In the context of contingency tables this model is known as the "independence model" under marginal constraints. An important generalization to multidimensional  $n_1 \times n_2 \times \cdots$  contingency tables is given in the classic paper [Goo63] of I. J. Good.

The form of  $\hat{X}$  is conceptually robust. For example, take the model with  $n = m = \ell$ and suppose the destination constraints are removed. Then all the  $\mu'_j$  in (2.4) can be taken equal to 1, and the solution is  $\hat{x}_{ij} = u_i/n, \forall j$ . Similarly, if the source constraints are removed,  $\hat{x}_{ij} = v_j/n, \forall i$ . And if both types of constraints are removed leaving just  $\sum_{i,j} x_{ij} = s$ , then  $\hat{x}_{ij} = s/n^2$ . We see that MAXENT yields independence and as much symmetry/uniformity as possible, subject to the given information.

### 3 Bounds on row sums

Suppose that the only information we have on the  $n \times m$  matrix X is upper bounds on the row sums:

$$\forall i, \quad \sum_{j} x_{ij} \leqslant u_i. \tag{3.1}$$

We will first show that with  $x_{ij} \in \mathbb{N}$ , the most likely matrix  $\hat{X}$  has its row sums in fact equal to  $u_1, \ldots, u_n$ . Indeed, let X be a matrix satisfying the constraints (3.1), and with  $\sum_{i,j} x_{ij} = s$ . Suppose that row i sums to strictly less than  $u_i$ . This means that there is a j such that if we increase  $x_{ij}$  by 1, the resulting matrix X' also satisfies the constraints. By (2.1), X' is more likely than X:

$$\frac{\#(X')}{\#(X)} = \frac{(s+1)!}{s!} \frac{x_{ij}!}{(x_{ij}+1)!} = \frac{s+1}{x_{ij}+1} > 1.$$

Proceeding in this way we can keep increasing the elements of the matrix while also increasing the value of #(X), until all constraints are satisfied with equality and the rows sum to exactly  $u_1, \ldots, u_n$ . This reduces the problem to the one considered in 2, where the total demand from each origin is known (as well as the total demand in the whole network). So the solution to (3.1) is simply

$$\forall i, \quad \hat{x}_{ij} = \frac{u_i}{n}.$$
(3.2)

This answer depends exactly on the given information and on nothing else. The argument we gave above also shows that *lower* bounds on the row sums are immaterial.

**Example 1** Suppose we have a  $10 \times 10$  matrix, and the upper bounds on the row sums are  $u_1, \ldots, u_{10} = 20, 20, 24, 30, 30, 36, 36, 36, 36, 40$ , measured in some units. We then find that the total number of matrices that accord with the information I is

$$M(I) = 30045015^2 \cdot 131128140 \cdot 847660528^2 \cdot 4076350421^4 \cdot 10272278170 \approx 2.41 \cdot 10^{89}.$$

(The number of solutions in  $\mathbb{N}$  of the equation  $x + x_2 + \cdots + x_{10} = u_i$  is simply the number of *compositions* of  $u_i$  into 10 parts, equal to  $\binom{u_i+9}{9}$ . And the inequality version can be handled by summing  $\binom{b+9}{9}$  over  $0 \leq b \leq u_i$ .) The most likely matrix  $\hat{X}$  is one of these 2.4 · 10<sup>89</sup> matrices. We can also find the number of matrices that satisfy (3.1) with equality. This turns out to be

 $M(I_{=}) = 10015005^{2} \cdot 38567100 \cdot 211915132^{2} \cdot 886163135^{4} \cdot 2054455634 \approx 2.20 \cdot 10^{83},$ 

and  $\hat{X}$  is one of these matrices. By (2.1) and (3.2),  $\hat{X}$  can be realized in  $\#(\hat{X}) = 308!/((2!)^2 2.4!(3!)^2 (3.6!)^4 4!)^{10} \approx 1.46 \cdot 10^{549}$  ways, where we took some liberties by allowing non-integral entries.

How much more likely is  $\hat{X}$  than a matrix X' which also obeys I and is the same as  $\hat{X}$  except that its 5th row is (2,2,2,2,2,4,4,4,4,4), a slight deviation from (3,...,3)? We see that  $\#(\hat{X})/\#(X') = (2!)^5/(4!)^5/(3!)^{10} \approx 4.21$ . If row 8 is (2,2,2,2,2,2,2,6,8,8) instead of (3.6,...,3.6), a larger deviation, the likelihood of X' is significantly smaller:  $\#(\hat{X})/\#(X') = (2!)^7 6!(8!)^2/(3.6!)^{10} \approx 813.9$ . Note that the units chosen for the  $u_i$  affect the size of the absolute numbers above, as well as the ratios; choosing finer units increases both the numbers and the ratios dramatically. For example, if all the  $u_i$  are multiplied by 10, the two likelihoods computed above become  $1.8 \cdot 10^7$  and  $4.2 \cdot 10^{32}$ .

### 4 Total sum and bounds on row sums

Now suppose that besides the upper bounds on the row sums we also know the total sum s:

$$\sum_{i,j} x_{ij} = s, \quad \text{and} \quad \forall i, \quad \sum_{j} x_{ij} \leqslant u_i.$$
(4.1)

For a solution to exist, we must have  $s \leq u_1 + \cdots + u_n$ . By Corollary A.1 we then have

$$x_{ij} = \lambda_i \mu, \qquad 0 < \lambda_i \leqslant 1. \tag{4.2}$$

To proceed, we consider the solution to a simpler problem: given  $a, b_1, \ldots, b_n > 0$ , what is the maximum entropy vector  $x^*$  satisfying  $x_1 + \cdots + x_n = a$  and  $\forall i, x_i \leq b_i$ ?

#### 4.1 The vector case

**Lemma 4.1** The maximum-entropy vector  $x^*$  satisfying  $\sum_i x_i = a$  and  $\forall i \ 0 \leq x_i \leq b_i$ , where  $a \leq b_1 + \cdots + b_n$ , is found as follows:

*i.* Arrange the  $b_i$  in increasing order, and permute the  $x_i$  accordingly.

*ii.* Find the largest 
$$j \in \{0, ..., n\}$$
 for which  $b_1 + \dots + b_j + (n-j)b_j \leq a$ . Let that be k.  
Then  $x_1^* = b_1, x_2^* = b_2, \dots, x_k^* = b_k$  and  $x_{k+1}^* = \dots = x_n^* = \frac{a - (b_1 + \dots + b_k)}{n-k}$ .

The starting point for this result is noting that if the  $b_i$  are in increasing order, there is a unique  $\ell$  s.t.  $b_1 + \cdots + b_{\ell} < a \leq b_1 + \cdots + b_{\ell+1}$ . If so, a plausible high-entropy solution is to set the first  $\ell$  of the  $x_i$  (constrained to be smallest) equal to their upper bounds, and split the remainder of a, which does not exceed  $b_{\ell+1}$ , equally among the rest of the  $x_i$ , which are the more loosely constrained. Lemma 4.1 refines this idea: to actually achieve maximum entropy, only the first  $k < \ell$  of the  $x_i$  can be set to their upper bounds.

The significance of k is as follows. Suppose  $b_1 > a/n$ ; then k = 0, and  $b_2, \ldots, b_n$  are also > a/n. This means that the bounds on the  $x_i$  are loose enough to allow *complete* symmetry/uniformity: the MAXENT solution is  $x_1^* = \cdots = x_n^* = a/n$ . Now suppose that  $b_1 \leq a/n$  and  $b_1 + (n-1)b_2 > a$ , in which case k = 1. Then the bound  $b_1$  is restrictive enough to break the symmetry: the solution is  $x_1 = b_1, x_2 = \cdots = x_n = (a - b_1)/(n - 1)$ , symmetric apart from  $x_1$ . So, in general, k measures how many of the constraints on the individual  $x_i$  are *informative*, i.e. force the solution away from the total uniformity that would have obtained if only the constraint  $x_1 + \cdots + x_n = a$  had been present. Finally, k = n iff  $b_1 + \cdots + b_n = a$ . In that extreme, the solution is determined completely by the upper bounds:  $x^* = (b_1, \ldots, b_n)$ .

#### 4.2 Back to the matrix

Returning to the solution (4.2), we proceed along the lines of the proof of Lemma 4.1 in the Appendix. We treat the  $u_i$  as the  $b_i$  of the lemma: arrange the rows of X so that  $u_1 \leq u_2 \leq \cdots \leq u_n$ , and find the largest k s.t.

$$u_1 + \dots + u_k + (n-k)u_k \leqslant s. \tag{4.3}$$

It may be that k = 0, i.e.  $u_1 > s/n$ , but k cannot exceed n. As pointed out above, the number k measures how many of the row constraints are informative. Now consider the solution

$$\sum_{j} x_{1j} = u_1, \dots, \sum_{j} x_{kj} = u_k, \quad \lambda_{k+1} = \dots = \lambda_n = 1.$$
 (4.4)

From (4.2), this implies that for all j,  $x_{k+1,j} = \cdots = x_{nj} = \mu$ . Since the sum of all  $x_{ij}$  must be s,

$$u_1 + \dots + u_k + (n-k)m\mu = s$$
, so  $\mu = \frac{s - (u_1 + \dots + u_k)}{m(n-k)}$ .

Using this in (4.4),

$$\lambda_i = \frac{(n-k)u_i}{s - (u_1 + \dots + u_k)} \qquad i = 1, \dots, k,$$

and we must verify that  $\lambda_i \leq 1$ . But this holds if  $s > u_1 + \cdots + u_k + (n-k)u_i$ , which is true for any *i* because of (4.3).

In summary, with the rows of X arranged so that  $u_1 \leq u_2 \leq \cdots \leq u_n$ , the solution is

$$\hat{x}_{ij} = \begin{cases} \frac{u_i}{m}, & i \le k, \\ \frac{s - (u_1 + \dots + u_k)}{m(n-k)}, & i > k, \end{cases} \qquad (4.5)$$

where k is determined by (4.3). The non-informative  $u_{k+1}, \ldots, u_n$  do not appear.

According to (4.5),  $\hat{X}$  consists of k identical columns with the structure specified in the 1st line, followed by m - k identical columns with the structure specified in the 2nd line. Within each set, the columns are identical because we do not have any information that imposes a distinction. We also note that if  $s = \sum_i u_i$ , then k = n - 1, and we obtain the solution (3.2), as expected, since this value of s imposes no additional constraint. If  $s/n \leq \min_i u_i$ , the matrix is totally uniform:  $\hat{x}_{ij} = s/n^2$ .

Finally, the solution (4.5) translates immediately to the case where we have bounds on the columns, instead of the rows of the matrix.

**Example 2** We re-do Example 1, adding information on the total sum s. Here  $\sum_i u_i = 308$ . We see from the last column of the table that  $\#(\hat{X} \mid s)$  increases with s, as intuitively expected.

s	k	$\hat{x}_{1}$ .					$\hat{x}_{5}$ .				$\hat{x}_{10}$ .	$\log_{10} \#(\hat{X} s)$
308	10	20	20	24	30	30	36	36	36	36	40	549.2
307	9	20	20	24	30	30	36	36	36	36	39	547.3
304	9	20	20	24	30	30	36	36	36	36	36	541.8
303	9	20	20	24	30	30	35.8	35.8	35.8	35.8	35.8	539.9
275	5	20	20	24	30	30	30.2	30.2	30.2	30.2	30.2	487.2
274	5	20	20	24	30	30	30	30	30	30	30	485.3
273	3	20	20	24	29.86	29.86	29.86	29.86	29.86	29.86	29.86	483.4
272	3	20	20	24	29.71	29.71	29.71	29.71	29.86	29.71	29.71	481.5

Table 4.1: Row sums of the most likely  $10 \times 10$  matrix  $\hat{X}$  as a function of s. Within a row, all elements are equal. The stepwise line inside the table indicates the k-boundary. The last column of the table is computed by (2.1).

#### 4.3 Bounds on total sum and on row sums

Suppose that instead of knowing the total sum as above, we have only an upper bound u on it:

$$\sum_{i,j} x_{ij} \leqslant u, \quad \text{and} \quad \forall i, \quad \sum_{j} x_{ij} \leqslant u_i.$$
(4.6)

What has already been said in this section suffices to solve this problem also. First, if  $u > \sum_i u_i$ , then this constraint is immaterial and we have the problem of §3, whose solution is given by (3.2). So we are left with the case  $u \leq \sum_i u_i$ . Suppose that we pick a value s < u for the total demand, and then find  $\hat{X}$  as in §4.2. Example 2 showed that  $\#(\hat{X} \mid s)$  increases as s increases, suggesting that we should reduce to the problem (4.1) with s = u. Indeed, Lemma A.1 establishes this formally.

This is the first case where "most likely" is not equivalent to "having maximum entropy". However, we see that there is still a strong and simple connection: the most likely matrix is the MAXENT matrix with the largest total sum allowed by the constraints.

### 5 Bounds on row and column sums

Here we consider the situation where our information I consists just of upper bounds on both the row and column sums of the matrix:

$$\sum_{j} x_{ij} \leqslant u_i, \quad \sum_{i} x_{ij} \leqslant v_j, \qquad i, j = 1, \dots, n.$$

The number of realizations of a matrix subject to this information is given by expression (2.1), except in this case the total sum s is not known and has to be substituted by  $\sum_{i,j} x_{ij}$ . If we use the first two terms of (2.2) to approximate the log of

$$#(X|I) = \left(\begin{array}{c} x_{11} + \dots + x_{nm} \\ x_{11}, \dots, x_{1m}, x_{21}, \dots, x_{2m}, \dots, x_{n1}, \dots, x_{nm} \end{array}\right),$$

we find that it is given by the "entropy difference" function

$$G(X) = \left(\sum_{i,j} x_{ij}\right) \ln\left(\sum_{i,j} x_{ij}\right) - \sum_{i,j} x_{ij} - \sum_{i,j} (x_{ij} \ln x_{ij} - x_{ij})$$
  
$$= \left(\sum_{i,j} x_{ij}\right) \ln\left(\sum_{i,j} x_{ij}\right) - \sum_{i,j} x_{ij} \ln x_{ij}.$$
(5.1)

(When I includes the value of  $\sum_{i,j} x_{ij}$ , maximizing G(X) subject to I is equivalent to maximizing H(X) subject to I.) Proposition A.2 in the Appendix shows that G(X) is concave over the domain  $x_{ij} > 0$ . And by Corollary A.2, the elements of  $\hat{X}$  have the form

$$\hat{x}_{ij} = \left(\sum_{k,l} \hat{x}_{kl}\right) \lambda_i \mu_j, \quad \lambda_i, \mu_j \in (0,1].$$
(5.2)

Given the above, we note that there are two cases to consider w.r.t. to the bounds:

- 1. All rows sum to their bounds, and all columns sum to their bounds.
- 2. At least one row or one column sums to less than its bound.

Case 1 is possible only when  $\sum_{i} u_i = \sum_{j} v_j$ . If so, the solution s.t.  $\forall i, \sum_{j} x_{ij} = u_i$  and  $\forall j, \sum_{i} x_{ij} = v_j$  has been discussed in §2. Thus we need only consider case 2. We can establish the following property of  $\hat{X}$ :

**Proposition 5.1** The matrix  $\hat{X}$  is s.t. for any i, j pair, either row i sums to  $u_i$ , or column j sums to  $v_j$ . That is, there can be no pair i, j s.t. row i sums to  $< u_i$  and column j sums to  $< v_j$ .

By virtue of Proposition 5.1, if *one* column of  $\hat{X}$  sums to less than its bound, then *all* rows must sum to their bounds. The situation is symmetric w.r.t. rows and columns, so we will analyze just the column case, where one or more columns sum to less than their bounds.

So suppose that columns  $1, \ldots, k$  sum to their bounds, while columns  $k+1, \ldots, m$  sum to less than their bounds, with  $0 \leq k < m$ . Then we must have  $v = \sum_j v_j > \sum_i u_i = u$ . By Corollary A.2,  $\mu_{k+1} = \cdots = \mu_m = 1$  in (5.2). Also, as pointed out above, all rows must sum to their bounds, which implies that  $\sum_{k,l} x_{kl} = u$ .

If we consider the columns, (5.2) says that  $x_{ij} = u\lambda_i\mu_j$  for  $j \leq k$ , and  $x_{ij} = u\lambda_i$  for j > k. Adding these by sides over *i* we obtain

$$v_j = u\lambda\mu_j, \quad j \leqslant k \quad \text{and} \quad v_{k+1} > u\lambda, \dots, v_m > u\lambda,$$
(5.3)

where  $\lambda$  is the sum of the  $\lambda_i$ . Further, if we add all the columns,  $v_1 + \cdots + v_k + u\lambda + \cdots + u\lambda = u$ , whence

$$\lambda = \frac{u - (v_1 + \dots + v_k)}{(m - k)u}.$$
(5.4)

 $(\lambda = 1/m \text{ if } k = 0, \text{ i.e. if all columns sum to less than their bounds.})$  Turning to the rows, we have  $u\lambda_1\mu = u_1, \ldots, u\lambda_n\mu = u_n$ , where  $\mu$  is the sum of the  $\mu_j$ . Thus

$$\lambda_i \mu = \frac{u_i}{u} = r_i, \quad \text{and} \quad \lambda \mu = 1.$$
 (5.5)

We can now determine all the  $\lambda_i$  and  $\mu_j$ : from (5.5) and (5.3),

$$\lambda_i = \lambda r_i \quad \text{and} \quad \mu_j = \begin{cases} (1/\lambda)v_j/u, & j \le k.\\ 1, & j > k. \end{cases}$$
(5.6)

Note that neither  $\lambda_i$  nor  $\mu_j$  depend on  $v_{k+1}, \ldots, v_m$ . This means that we can take these bounds to be as large as we please, e.g.  $\infty$ , thus handling the case where no upper bound is specified for some of these columns.

It remains to take care of the fact that (5.2) requires  $\lambda_i, \mu_j \leq 1$ . It is easy to verify this for  $\lambda_i$ : it is the product of two factors, both < 1. The condition  $\mu_j \leq 1$  is equivalent to  $(m-k)v_j \leq u - (v_1 + \dots + v_k)$  for  $j \leq k$ . The inequalities in (5.3) impose another condition on k:  $(m-k)\min(v_{k+1}, \dots, v_m) > u - (v_1 + \dots + v_k)$ . Taking these two conditions together we see that k and the column bounds  $v_j$  must satisfy

$$\max(v_1,\ldots,v_k) \leqslant \frac{u-(v_1+\cdots+v_k)}{m-k} < \min(v_{k+1},\ldots,v_m),$$

where  $0 \leq k < m$ . Assume that the  $v_j$  are in increasing order<sup>5</sup>. Then this condition becomes

$$v_k \leqslant \frac{u - (v_1 + \dots + v_k)}{m - k} < v_{k+1}, \qquad 0 \leqslant k < m.$$
 (5.7)

The following result establishes the existence of a k satisfying (5.7):

**Proposition 5.2** Let  $v_1 \leq v_2 \leq \cdots \leq v_m$ , u < v, and  $v_1 \leq u/m$ . Then there is a unique  $k \in \{1, \ldots, m-1\}$  s.t.

$$(m-k)v_k \leq u - (v_1 + \dots + v_k) < (m-k)v_{k+1}$$

If  $v_1 > u/m$ , then k = 0.

Finally, if u < v, by (5.2), (5.4), and (5.6), the elements of  $\hat{X}$  are

$$\hat{x}_{ij} = \begin{cases} \frac{u_i v_j}{u}, & j \le k, \\ \frac{u - (v_1 + \dots + v_k)}{m - k} \frac{u_i}{u}, & j > k, \end{cases} \qquad i = 1, \dots, n$$
(5.8)

where k is given by Proposition 5.2. We note that k is the number of *informative* column constraints, in the sense that the solution depends on  $v_1, \ldots, v_k$  but not on  $v_{k+1}, \ldots$  (similar to the k in Lemma 4.1). In fact, some of  $v_{k+1}, \ldots, v_m$  may be infinite, i.e. there may be no upper bounds on some of columns  $k + 1, \ldots, m$ .

The reader may want to compare (5.8) with the result (2.7) for the model of §2. The comparison shows that even though for the problem we just solved "most likely" is not directly equivalent to "having maximum entropy", there is still a straightforward connection as we also saw in §4.3.

### 6 Bounds on individual elements

We first point out that whereas bounds on individual matrix elements provide the utmost flexibility in expressing constraints, they can have unintended consequences. Then we look at the most likely matrix subject to bounds on the row sums and on individual elements.

<sup>&</sup>lt;sup>5</sup>If the matrix is a contingency table, simply rearrange the columns. If it refers to n nodes, re-label the nodes.

#### 6.1 Expressive power and consistency

#### 6.1.1 Expressive power

Consider finding the most likely matrix  $\hat{X}$  subject just to the constraints

 $\forall i, j \quad x_{ij} \leqslant w_{ij},$ 

where W is a given  $n \times m$  matrix in N. Then it is easy to see by an argument similar to that of §3 that  $\hat{X}$  has elements  $\hat{x}_{ij} = w_{ij}$ . Thus the information W suffices to specify any possible most likely matrix. Conversely, to be able to specify an arbitrary matrix, information on every matrix element is necessary; W is one form of such information.

#### 6.1.2 Consistency

Imposing w-constraints that are satisfied with equality requires that the w- and u-constraints together satisfy certain conditions if the matrix  $\hat{X}$  is not to exhibit surprising behavior. For example, suppose we are trying to determine a  $3 \times 3$  matrix with row/column sums  $u_1, u_2, u_3$  and s.t.  $x_{11} = 0$ , as shown in Fig. 6.1, left. Then we must have  $x_{12} + x_{13} = u_1$  from row 1, and  $(x_{22} + x_{23} + x_{32} + x_{33}) + x_{12} + x_{13} = u_2 + u_3$  from columns 2 and 3. It follows that if  $u_1$  is not strictly less than  $u_2 + u_3$ , then  $x_{22} + x_{23} + x_{33} = 0$ , which means that all these elements are 0. So with certain  $u_1, u_2, u_3, x_{11} = 0$  may force other elements of the matrix to be 0 as well. This does not happen without the requirement  $x_{11} = 0$ : we know from §2 that for any  $u_1, u_2, u_3$  there is a  $\hat{X}$  with all elements non-zero.

					W	A	
0	$x_{12}$	$x_{13}$	$u_1$		,,		
$x_{21}$	$x_{22}$	$x_{23}$	$u_2$				1
$x_{31}$	$x_{32}$	$x_{33}$	$u_3$				
$u_1$	$u_2$	$u_3$			B	C	
					$u_1 \cdots u_k$	$u_{k+1}\cdots u_n$	

Figure 6.1: Matrices with some elements fixed by w-constraints.

More generally, suppose we have a constraint that forces a certain  $k \times k$  square submatrix of X to equal a matrix W. In the simplest case let W be in the upper left-hand corner of X as shown in Fig. 6.1, right. Then we have

$$\Sigma_W + \Sigma_A = u_1 + \dots + u_k, \qquad \Sigma_A + \Sigma_C = u_{k+1} + \dots + u_n,$$

assuming that  $\Sigma_W < u_1 + \cdots + u_k$ . It can be seen that unless u and W are s.t.  $u_1 + \cdots + u_k - \Sigma_W < u_{k+1} + \cdots + u_n$ , we must have  $\Sigma_C = 0$ , which would force the entire submatrix C to be 0.

If W is an arbitrary submatrix, let its rows and columns correspond to a set I of indices. Then the condition that must be satisfied so that C is not forced to 0 can be written as

$$u_I < \frac{u}{2} + \frac{w_{II}}{2},\tag{6.1}$$

where the subscripts indicate summation over the set. In terms of a traffic matrix, this condition says that the traffic originating in the set I must be less than half of the total, plus half of the traffic originating in I and terminating in I. As an example, suppose we require that there is no traffic among the locations in I; then (6.1) says that the traffic that leaves I cannot be more than half of the total traffic.

Related to the above, there is also a necessary and sufficient condition for the existence of a non-negative matrix with specified row and column sums and an arbitrary subset of elements specified to be 0: see Theorems 3.10 and 3.12 in Ch. 4 of [BP94]; see also §3.6 of [ES90].

#### 6.2 Bounds on row sums and on individual elements

Suppose we know the same bounds on the row sums as in 3, but, in addition, we have a bound on the size of each individual element:

$$\forall i \quad \sum_{j} x_{ij} \leqslant u_i, \quad \text{and} \quad \forall i, j \quad x_{ij} \leqslant w_{ij}.$$
 (6.2)

This problem is easy to solve because the constraints (6.2) are separable, so each row of the most likely matrix  $\hat{X}$  can be found *independently* of all the other rows. Fixing a particular row *i*, denote the  $x_{ij}$  by  $x_1, \ldots, x_m$ ,  $u_i$  by *a*, and the  $w_{ij}$  by  $b_1, \ldots, b_m$ . Then we have the problem of finding the most likely vector  $x^*$  that satisfies

$$x_1 + \dots + x_m \leqslant a, \qquad x_1 \leqslant b_1, \dots, x_m \leqslant b_m, \qquad a, b_i \in \mathbb{N}.$$
(6.3)

The solution to this problem is as follows. If  $a > b_1 + \cdots + b_m$ ,  $x^*$  is simply  $(b_1, \ldots, b_m)$ . If  $a \leq b_1 + \cdots + b_m$ , then  $x^*$  is found by replacing the inequality with an equality and reducing to the problem solved in 4. The formal details are given in Lemma A.1 in the Appendix.

### 7 Symmetric information

We now investigate some types of constraints that we have not looked at so far, but under the additional assumption that these constraints or information are *symmetric* w.r.t. rows and columns. By necessity, the matrices are  $n \times n$  square. Here is one motivation for considering symmetry. Suppose we are designing a "backbone" type, i.e. high capacity and geographically extensive, communications network connecting a set of n locations. The transmission facilities in such a network typically have the same capacity in each direction. To understand what capacities are needed for the links, we need an estimate of the traffic matrix. Given the symmetry of the capacities, we may assume, for example, that the total incoming and outgoing traffic for a given node are equal. The same considerations apply to a network of roads connecting a set of cities. Thus the symmetry of capacities allows us to act as if the traffic matrix were symmetric.

These considerations aside, the symmetric information allows us to go farther toward analytical solutions than would be possible otherwise. One of the questions we investigate via the analytical forms is the effect of fixing some elements on the "product of independent factors" structure of the MAXENT matrix.

#### 7.1 Total sum and bounds on row and column sums

Here the sum of row i is bounded by  $u_i$ , and so is the sum of column i. By Corollary A.1, the matrix elements are of the form

$$x_{ij} = \lambda_i \mu_j \nu, \qquad \lambda_i, \mu_j \in (0, 1],$$

where  $\lambda_i, \mu_i$  correspond to the row and column constraints respectively, and  $\nu$  to the constraint on the total sum. We will show that the solution is essentially the same as that obtained in §4 for the non-symmetric, row-only case. So define k by (4.3), and consider the solution

1. Constraints  $1, \ldots, k$  are satisfied as equalities for both rows and columns (so we must have  $\lambda_1, \ldots, \lambda_k \leq 1$  and  $\mu_1, \ldots, \mu_k \leq 1$ ), and

2. 
$$\lambda_{k+1} = \cdots = \lambda_n = 1$$
, and  $\mu_{k+1} = \cdots = \mu_n = 1$ .

It follows that the matrix must look like

$$\begin{bmatrix} [\lambda_i \mu_j \nu]_{k \times k} & [\lambda_i \nu]_{k \times n-k} \\ [\mu_j \nu]_{n-k \times k} & [\nu]_{n-k \times n-k} \end{bmatrix} = \begin{bmatrix} A & B \\ C & D \end{bmatrix}.$$

Note that rows k + 1, ..., n are identical, and so are columns k + 1, ..., n. Let  $\Sigma_A, ..., \Sigma_D$  denote the sums of the elements of the submatrices. Clearly,

$$\Sigma_A + \Sigma_B = u_1 + \dots + u_k, \quad \Sigma_A + \Sigma_C = u_1 + \dots + u_k, \quad \Sigma_A + \Sigma_B + \Sigma_C + \Sigma_D = s.$$

Therefore  $\Sigma_B = \Sigma_C$  and  $u_1 + \cdots + u_k + \Sigma_B + \Sigma_D = s$ . Substituting for the elements of B and D, we find that

$$\nu = \frac{s - (u_1 + \dots + u_k)}{(n - k)(\lambda_1 + \dots + \lambda_k + n - k)}.$$

And from  $\Sigma_B = \Sigma_C$  it follows that  $\lambda_1 + \cdots + \lambda_k = \mu_1 + \cdots + \mu_k$ . Now the constraint on row i < k is  $\lambda_i(\lambda_1 + \cdots + \lambda_k + n - k)\nu = u_i$ . Using the expression for  $\nu$  in this we find that  $\lambda_i = (n-k)u_i/(s-(u_1+\cdots+u_k))$ , and this is <1 as required. Similarly, from the constraint for column j < k we find that  $\mu_j = (n-k)u_j/(s-(u_1+\cdots+u_k))$ . We see that  $\mu_j = \lambda_j$ . Therefore we need only deal with the  $\lambda_j$ . Substituting the values of the  $\lambda_i$  in the expression for  $\nu$ , we finally arrive at the solution

$$\hat{x}_{ij} = \begin{cases} \frac{u_i u_j}{s}, & (i,j) \in A, \\ \frac{(s - (u_1 + \dots + u_k))u_i}{(n - k)s}, & (i,j) \in B, \\ \frac{(s - (u_1 + \dots + u_k))u_j}{(n - k)s}, & (i,j) \in C, \\ \frac{(s - (u_1 + \dots + u_k))^2}{(n - k)^2 s}, & (i,j) \in D, \end{cases}$$

$$(7.1)$$

where k is defined by (4.3). This solution is symmetric, and the reader can verify that it satisfies all the constraints. The A, B, C matrices have the gravity form, the B and C matrices are the transpose of one another, and the D matrix is constant. Finally, note that we did not assume the symmetry in the solution, it followed as a consequence of the symmetric information.

#### 7.2 Given row and column sums, partially fixed diagonal

Assume that the sum of row and column i is  $u_i$ , and that the first  $m \leq n$  of the diagonal elements are fixed to be 0. Then, with  $s = u_1 + \cdots + u_n$  still denoting the total sum, the matrix elements other than the first m on the diagonal must be given by

$$\hat{x}_{ij} = s\lambda_i\mu_j, \quad \lambda_i, \mu_j > 0.$$

Including the factor s is a convenience, as will become clear. For the above solution to be possible the consistency condition (6.1) must be satisfied: each  $u_i$  must be strictly less than half of s. We shall assume this to be the case. If  $\lambda$  is the sum of the  $\lambda_i$  and  $\mu$  that of the  $\mu_j$ , and  $r_i = u_i/s$ , the row and column constraints can be written as

$$\lambda_i(\mu - \mu_i) = r_i, \quad i \leqslant m, \qquad \lambda_i \mu = r_i, \quad i > m, \mu_j(\lambda - \lambda_j) = r_j, \quad j \leqslant m, \qquad \mu_j \lambda = r_j, \quad j > m.$$

$$(7.2)$$

Here  $r_1 + \cdots + r_n = 1$  and  $r_i < 1/2$  for all *i*. Noting that (7.2) is unchanged if we exchange the  $\lambda_i$  and the  $\mu_i$  leads us to consider a solution with  $\mu_i = \lambda_i$ . Then (7.2) reduces to

$$\lambda_i(\lambda - \lambda_i) = r_i, \quad i \leqslant m, \qquad \lambda_i \lambda = r_i, \quad i > m.$$
(7.3)

(7.3) implies that for  $i \leq m$  we have  $\lambda_i = (\lambda \pm \sqrt{\lambda^2 - 4r_i})/2$ , whereas for i > m,  $\lambda_i = r_i/\lambda$ . Suppose we pick the root with the "-" for  $i = 1, \ldots, m$ . Adding the expressions for the  $\lambda_i$  by sides and dividing both sides of the result by  $\lambda \neq 0$  we see that  $\lambda$  must satisfy the equation

$$\sqrt{1 - 4r_1/\lambda^2} + \dots + \sqrt{1 - 4r_m/\lambda^2} - 2\frac{r_{m+1} + \dots + r_n}{\lambda^2} = m - 2.$$
 (7.4)

An exact analytical solution of (7.4) is impractical, but we can find an approximation. To begin with, we observe that the l.h.s. of (7.4) is a monotone increasing function of  $\lambda$  so the root of (7.4) is unique<sup>6</sup>. Second, at the expense of restricting the  $r_i$  somewhat, we can localize the root:

**Proposition 7.1** Suppose that each of  $r_1, \ldots, r_n$  is in (0, 1/3), and  $r_1 + \cdots + r_n = 1$ . Then for any  $n \ge 3$  and any  $m \le n$ , equation (7.4) has a root in the interval  $(2\sqrt{r_{\max}}, 4/3)$ , where  $r_{\max}$  is the largest of the  $r_i$ .

To see the necessity for some additional restriction on the  $r_i$ , suppose that m = n and that we extend (0, 1/3) to (0, 1/2). Then consider the set  $r_1 = \frac{1}{2}$  and  $r_2 = \cdots = r_n = \frac{1}{2(n-1)}$ ; it can be seen that (7.4) has no solution in  $(\sqrt{2}, \infty)$ .

In terms of the root  $\lambda$  of (7.4) the final solution is

$$\hat{x}_{ij} = \begin{cases} \frac{s\lambda^2}{4} \left(1 - \sqrt{1 - 4r_i/\lambda^2}\right) \left(1 - \sqrt{1 - 4r_j/\lambda^2}\right), & i, j \leq m \text{ and } i \neq j, \\ \frac{sr_i}{2} \left(1 - \sqrt{1 - 4r_j/\lambda^2}\right), & i > m, j \leq m, \\ \frac{sr_j}{2} \left(1 - \sqrt{1 - 4r_i/\lambda^2}\right), & i \leq m, j > m, \\ sr_i r_j/\lambda^2, & i, j > m. \end{cases}$$
(7.5)

We see that the  $\hat{x}_{ij}$  for  $i, j \leq m$  have a product form, but, in general, the factors are *not* independent. We know from §2 that irrespective of symmetry, the dependence disappears if we don't fix any diagonal elements. Fixing these elements imposes a global dependence as we saw in §6.

**Example 3** We consider the two extreme cases m = n and m = 1. In addition, suppose that all the  $u_i$  are equal.

First let m = n. Then all  $r_i$  are 1/n and  $\lambda = \sqrt{n/(n-1)}$ . From the first line of (7.5) the matrix  $\hat{X}$  has the form

$$\frac{s}{n(n-1)} \left( \begin{array}{cccc} 0 & 1 & 1 & \dots & 1\\ 1 & 0 & 1 & \dots & 1\\ \vdots & \vdots & \vdots & \vdots & \vdots\\ 1 & 1 & 1 & \dots & 0 \end{array} \right).$$

<sup>&</sup>lt;sup>6</sup>This is also true because the solution to our strictly concave maximization problem is unique.

Compare this with the case where the diagonal is not fixed to 0, and the solution is  $\hat{x}_{ij} = s/n^2$ .

Now let m = 1. This is the simplest possible case: we have a square matrix with all row and column sums equal, except that the single element  $d_{11}$  is fixed to be 0. From (7.4) we find  $\lambda = (n-1)/\sqrt{n(n-2)}$ . From the last three lines of (7.5) we see that now  $\hat{X}$  is

$$\frac{s}{n(n-1)} \begin{pmatrix} 0 & 1 & 1 & \dots & 1\\ 1 & \frac{n-2}{n-1} & \frac{n-2}{n-1} & \dots & \frac{n-2}{n-1}\\ \vdots & \vdots & \vdots & \dots & \vdots\\ 1 & \frac{n-2}{n-1} & \frac{n-2}{n-1} & \dots & \frac{n-2}{n-1} \end{pmatrix}.$$

**Example 4** Now consider the case m = n, but with the  $r_i$  arbitrary. We obtain an analytical approximation to the solution. If we let  $\xi = 4/\lambda^2$ , (7.4) becomes

$$\sqrt{1 - r_1 \xi} + \dots + \sqrt{1 - r_n \xi} = n - 2, \qquad \xi \in (9/4, 1/r_{\text{max}}),$$
(7.6)

where the lower bound on  $\xi$  comes from Proposition 7.1. This equation has the form  $f(\xi) = c$ , and if  $\xi_0$  is an approximation to its solution, the reversion technique in Ch. 1 of [Hen88] can be used to find the following power series for  $\xi$ : with  $\rho_i = \sqrt{1 - r_i \xi_0}$  and  $\delta = f(\xi_0) - c = \rho_1 + \cdots + \rho_n - n + 2$ ,

$$\xi = \xi_0 + \frac{2}{r_1/\rho_1 + \dots + r_n/\rho_n} \delta - \frac{r_1^2/\rho_1^3 + \dots + r_n^2/\rho_n^3}{(r_1/\rho_1 + \dots + r_n/\rho_n)^3} \delta^2 - \dots$$
(7.7)

It is known that this series converges, and it can be shown that  $\delta < 1$  for any  $\xi_0 \in (9/4, 1/r_{\text{max}})^7$ . By (7.5) the non-diagonal matrix elements are given by  $\frac{s}{\xi}(1-\sqrt{1-r_i\xi})(1-\sqrt{1-r_i\xi})$ , and (7.7) lets us find power series expansions for them in terms of  $\delta$ . We do not show these series here, but the expansions to first order result in manageable expressions. The accuracy of the expansions remains to be investigated.

Now consider a numerical example with u = (40, 20, 30, 40). We have  $r = (\frac{4}{13}, \frac{2}{13}, \frac{3}{13}, \frac{4}{13})$ , so solving (7.6) we find  $\xi \approx 2.88018 \in (\frac{9}{4}, \frac{13}{4})$ . If we take  $\xi_0 = 9/4$ , (7.7) gives  $\xi \approx 2.25 + 0.749023 - 0.112889 = 2.8861$ . Then the form  $\frac{s}{\xi}(1 - \sqrt{1 - r_i\xi})(1 - \sqrt{1 - r_j\xi})$  yields

	1	0	7.59	12.59	19.82	\		/ 12.31	6.15	9.23	12.31	
$\hat{\mathbf{v}}$	= (	7.59	0	4.82	7.59		, vs.	6.15	3.08	4.62	6.15	
$\Lambda =$		12.59	4.82	0	12.59	,		9.23	4.62	6.92	9.23	,
		19.82	7.59	12.59	0 /			12.31	6.15	9.23	12.31	)

the MAXENT matrix without the 0-diagonal constraint, whose elements are simply  $sr_ir_j$ . As we also saw in Example 3, the result of fixing the diagonal to 0 cannot be regarded as a (small) perturbation of the  $sr_ir_j$  form.

<sup>&</sup>lt;sup>7</sup>Note that  $\rho_i < 1 - 1/2r_i\xi_0$ , so  $\rho_1 + \dots + \rho_n < n - \xi_0/2$ .

**Generalization** (a) The solution (7.5) is valid also when the  $u_i$  are upper bounds on the row sums, instead of specifying their values. In that case Corollary A.1 requires that  $\lambda_i \leq 1$ , which is true if

 $\forall i \quad 2\sqrt{r_i} \leqslant \lambda \leqslant 2 \qquad \text{or} \qquad \lambda > 2.$ 

But this holds by virtue of Proposition 7.1.

(b) The diagonal elements can be set to arbitrary values  $w_{11}, \ldots, w_{nn}$ , if the  $r_i$  are re-defined as  $(u_i - w_{ii})/s$ . This actually requires a slight extension of Proposition 7.1; see Proposition 7.2 below. And it can be verified that if we set  $w_{ii} = u_i^2/s$  we get the expected solution  $\hat{x}_{ij} = sr_ir_j$ .

#### 7.3 3-dimensional matrices with fixed diagonal

The development of §7.2 can be extended to 3-dimensional matrices. These can be thought of as contingency tables involving elements with 3 attributes, or as trip matrices where a trip is characterized by an origin and a destination as in the 2-dimensional case, and, in addition, by a class of vehicle, say, or as traffic matrices where traffic flows have origins, destinations, and a size class, such as "small", "medium", "large". Whatever the three attributes, we will index them by i, j, k. We will consider the case where the whole diagonal is 0 and the available information is the sums over all (i, k) sections and all (j, k) sections of the matrix:

$$\forall i \quad \sum_{j \neq i} x_{ijk} = u_{ik}, \qquad \forall j \quad \sum_{i \neq j} x_{ijk} = v_{jk}.$$

In the case of a traffic matrix for example, this means that we know the total number of flows originating at i and of size class k, and the total number ending at j of size class k. The matrix elements will then be

 $x_{ijk} = s\lambda_{ik}\mu_{jk}$  for  $i \neq j$ , and 0 otherwise,

where the  $\lambda_{ik}$  and  $\mu_{jk}$  are s.t.

$$\forall i \quad s \sum_{j \neq i} \lambda_{ik} \mu_{jk} = u_{ik}, \qquad \forall j \quad s \sum_{i \neq j} \lambda_{ik} \mu_{jk} = v_{jk}.$$

Now let this information be symmetric w.r.t *i* and *j*, i.e.  $v_{ik} = u_{ik}$ . Further, define  $r_{ik} = u_{ik}/s$ . Then the above constraints can be written as

$$\forall i \quad \lambda_{ik}(\mu_{.k} - \mu_{ik}) = r_{ik}, \qquad \forall j \quad \mu_{jk}(\lambda_{.k} - \lambda_{jk}) = r_{jk},$$

where the dot indicates summation over the corresponding index. Since the index j in the second set of constraints could have equally well been written i, we are led to consider a solution with  $\mu_{ik} = \lambda_{ik}$  and the single set of constraints

$$\forall i \quad \lambda_{ik}(\lambda_{.k} - \lambda_{ik}) = r_{ik}.$$

Proceeding as we did after (7.3),  $\lambda_{ik} = (\lambda_{.k} - \sqrt{\lambda_{.k}^2 - 4r_{ik}})/2$ . Adding these over *i* and setting  $\xi_k = 4/\lambda_{.k}^2$ , we arrive at a generalization of (7.6):

$$\forall k \quad \sqrt{1 - r_{1k}\xi_k} + \dots + \sqrt{1 - r_{nk}\xi_k} = n - 2.$$

This is completely analogous to what we found in Example 4, except that here we have one equation for each of the  $\xi_k$ . The final expression for the elements of the matrix is

$$x_{ijk} = \frac{4}{\xi_k} \left( 1 - \sqrt{1 - r_{ik}\xi_k} \right) \left( 1 - \sqrt{1 - r_{jk}\xi_k} \right) \quad \text{for } i \neq j, \text{ and } 0 \text{ otherwise.}$$

Note that the matrix sections corresponding to different values of k are independent of one another. The above development generalizes to the case where only the first m < n of the diagonal elements are fixed, and in the other ways discussed in §7.2.

#### 7.4 Given row and column sums, fixed diagonal blocks

We generalize the development of §7.2 to equality constraints expressed by a block-diagonal matrix W with blocks  $W_1, \ldots, W_m, m \ge 3$ . This means that the *n* nodes are partitioned into *m* sets  $I_1, \ldots, I_m$ , and the submatrix of X that has rows and columns in  $I_j$  is constrained to equal  $W_j$ . So X looks like

where the rest of the entries are determined by the *u*-constraints and, as previously, are given by  $s\lambda_i\lambda_j$ . Thus for the nodes in the set  $I_1$  we have the equations

$$s\lambda_1(\text{sum of }\lambda_j, j \notin I_1) = u_1 - (\text{sum of first row of }W_1),$$
  
 $s\lambda_2(\text{sum of }\lambda_j, j \notin I_1) = u_2 - (\text{sum of second row of }W_1),$ 

etc. Let  $\lambda_{I_1}$  denote  $\sum_{i \in I_1} \lambda_i$ , and similarly for  $\lambda_{I_2}$ , etc. Also let  $\lambda = \lambda_{I_1} + \cdots + \lambda_{I_m}$ . Then the above equations can be written as

$$s\lambda_1(\lambda - \lambda_{I_1}) = u_1 - w_{1I_1}, \quad s\lambda_2(\lambda - \lambda_{I_2}) = u_2 - w_{2I_1}, \quad \dots$$

where the meaning of the additional notation should be clear. If we now add these equations by sides, the result can be written compactly as

$$\lambda_{I_1}(\lambda - \lambda_{I_1}) = r_{I_1}, \quad \text{where} \quad r_{I_1} = (u_{I_1} - w_{I_1I_1})/s,$$

and where subscripts that are sets indicate summation over the respective sets. If we do the same thing for the rows in  $I_2, \ldots, I_m$ , we arrive at the system of equations

$$\lambda_{I_1}(\lambda - \lambda_{I_1}) = r_{I_1}, \quad \lambda_{I_2}(\lambda - \lambda_{I_2}) = r_{I_2}, \quad \dots, \quad \lambda_{I_m}(\lambda - \lambda_{I_m}) = r_{I_m}$$

which has exactly the form (7.3) except that here the  $r_{I_i}$  don't sum to 1, but to

$$\sigma = 1 - \frac{1}{s} \sum_{i=1}^{m} w_{I_i I_i} < 1.$$

Of course, the  $u_{I_i}$  and  $w_{I_iI_i}$  are assumed to satisfy the consistency condition (6.1). Proceeding just as in §7.2, we have

$$\lambda_{I_j} = \frac{1}{2} \left( \lambda - \sqrt{\lambda^2 - 4r_{I_j}} \right)$$

so that  $\lambda$  is the root of the equation

$$\sqrt{1 - 4r_{I_1}/\lambda^2} + \dots + \sqrt{1 - 4r_{I_m}/\lambda^2} = m - 2, \tag{7.8}$$

about which we have a generalization of Proposition 7.1:

**Proposition 7.2** Suppose that  $r_{I_1} + \cdots + r_{I_m} = \sigma < 1$ , and each  $r_{I_j}$  is in  $(0, \sigma/3)$ . Then for  $m \ge 3$  equation (7.8) has a root in  $(2\sqrt{r_{\max}}, 4\sqrt{\sigma}/3)$ , where  $r_{\max}$  is the largest of the  $r_{I_j}$ .

Given the root  $\lambda$  of (7.8), if  $i \in I_k$ ,  $\lambda_i$  is given by  $2r_i/(\lambda + \sqrt{\lambda^2 - 4r_{I_k}})$ . But this expression also equals  $r_i(\lambda - \sqrt{\lambda^2 - 4r_{I_k}})/(2r_{I_k})$ . So the solution to our problem is: for  $i \in I_k, j \in I_\ell, k \neq \ell$ ,

$$\hat{x}_{ij} = \frac{s}{4} \frac{\lambda^2 r_i r_j}{r_{I_k} r_{I_\ell}} \left( 1 - \sqrt{1 - 4r_{I_k} / \lambda^2} \right) \left( 1 - \sqrt{1 - 4r_{I_\ell} / \lambda^2} \right),$$
  

$$r_i = \frac{u_i - w_{iI_k}}{s}, \quad r_{I_k} = \sum_{i \in I_k} r_i = \frac{u_{I_k} - w_{I_k I_k}}{s}.$$
(7.9)

Suppose that all blocks are of size 1, so m = n and the constraints are  $x_{ii} = w_{ii}$ . Then it is easily seen that (7.9) gives the same result as (7.5). An analytical approximation to the solution of (7.8), and to the matrix elements themselves, can be found by the power series (7.7).

Finally, the solution (7.9) holds even when the  $u_i$  are upper bounds on the row and column sums. In that case Corollary A.1 requires  $\lambda_{I_j} \leq 1$ , which holds if  $\forall j, 2\sqrt{r_{I_j}} \leq \lambda \leq 2$ . But this last condition obtains by virtue of Proposition 7.2.

# 8 Conclusion

Table 8.1 summarizes the problems for which we obtained results in this paper. We saw that the most likely/MAXENT matrices exhibit as much independence, symmetry, and uniformity as possible subject to the available information or constraints. Further, they are robust with respect to changes in the information/constraints. Lastly, given independent constraints on the rows and columns, the matrix elements have a "product of independent factors" form, unless some of them are fixed, in which case the independence disappears.

Rectangular matrices/contingency tables
Given row sums and some column sums
Bounds on row sums
Total sum and bounds on row sums
Bounds on total sum and row sums
Bounds on row and column sums
Bounds on row sums and on individual elements
Square matrices with symmetric information
Total sum and bounds on row and column sums
Given row sums and partially-fixed diagonal,
with extension to 3d matrices
Given row sums and fixed diagonal blocks

Table 8.1: Summary of cases solved.

The types of constraints that we considered were relatively simple, as befits an initial exploration of the space of analytical solutions. The aim was to have enough basic results to establish a framework for further investigations, perhaps motivated by constraints arising in concrete problems.

Finally, even though we used the discrete balls-and-boxes framework throughout, all that is said in this paper applies also to deriving 2-dimensional *discrete probability distributions* from incomplete information, if we think of the balls as "probability quanta" thrown into the boxes. Jaynes [Jay03] calls this the "Wallis derivation" of MAXENT probability distributions.

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## A Auxiliary results and Proofs

### A.1 Optimal solutions of concave programs

We review some standard terminology and results.

Suppose C is a convex set in  $\mathbb{R}^n$ . A concave program is the problem of maximizing a concave function f on this set, subject to a number of equality and inequality constraints:

$$\max_{x \in C} f(x) \quad \text{subject to} \\ g_i(x) = 0, \quad i = 1, \dots, \ell, \qquad h_j(x) \leq 0, \quad j = 1, \dots, m,$$
(A.1)

where the  $g_i$  are *linear* on C (and assumed linearly independent) and the  $h_j$  are *convex* on C. All  $x \in C$  satisfying the constraints are called *feasible*. The Lagrangean function associated with the concave program (A.1) is

$$\Phi(x,\alpha,\beta) = f(x) - \sum_{i} \alpha_{i} g_{i}(x) - \sum_{j} \beta_{j} h_{j}(x).$$
(A.2)

The following result (Theorem 2.30 in [ADSZ88], or  $\S5.5.3$  of [BV04]) gives sufficient conditions for solving a concave program in which all functions are differentiable on (the interior of) C:

**Theorem 1** If  $x^*$  is feasible, and there are  $\alpha^*, \beta^*$  such that

$$\nabla_x \Phi(x^*, \alpha^*, \beta^*) = 0, \qquad \beta_j^* h_j(x^*) = 0 \quad \text{and} \quad \beta_j^* \ge 0 \quad \forall j,$$

then  $x^*$  solves the concave program (A.1).

Also recall that if a strictly concave function on a convex set has a maximum, the maximizing point is unique (Theorem 2.22 in [ADSZ88]).

**Corollary A.1** Suppose the function f in (A.2) is the entropy, and all the constraints are linear and involve coefficients that are either 0 or 1. Then the elements of  $x^*$  have the form

$$x_k^* = \prod_{i \in E_k} \alpha'_i \prod_{j \in I_k} \beta'_j, \quad where \quad \alpha'_i > 0, \beta'_j \in (0, 1],$$

where  $E_k$  is the set of indices of the equalities  $g_i$  in which  $x_k$  appears, and  $I_k$  is the set of indices of the inequalities  $h_j$  where  $x_k$  appears. The *j*-th inequality constraint can be satisfied either as a strict inequality or as an equality, and we must have

$$h_j(x^*) \ln \beta'_j = 0.$$
 (A.3)

**Corollary A.2** If the function f in (A.2) is the entropy difference function G of (5.1) and the constraints are as in Corollary A.1, then

$$x_k^* = \left(\sum_{1 \leqslant \ell \leqslant n} x_\ell^*\right) \prod_{i \in E_k} \alpha_i' \prod_{j \in I_k} \beta_j', \qquad \alpha_i' > 0, \beta_j' \in (0, 1],$$

where the  $\beta'_{i}$  must satisfy (A.3).

#### A.2 Proofs for §4

#### Proof of Lemma 4.1

The Lagrangean is

$$\Phi = -\sum_{i} x_{i} \ln x_{i} - \lambda_{1}(x_{1} - b_{1}) - \dots - \lambda_{n}(x_{n} - b_{n}) - \mu(x_{1} + \dots + x_{n} - a)$$

Setting  $\nabla \Phi$  to 0, we have for all *i* 

$$x_i = e^{-\lambda_i - \mu - 1} \rightsquigarrow \lambda_i \mu. \tag{A.4}$$

By Corollary A.1, for a point  $(x_1, \ldots, x_n)$  given by (A.4) to solve the problem the following must hold

- a)  $(x_1, \ldots, x_n)$  must be feasible,
- b) By (A.3), we must have  $\lambda_i \in (0, 1]$  for all i, and  $(x_i b_i) \ln \lambda_i = 0$ .

Now arrange the  $b_i$  and  $x_i$  as stated in part (i) of the lemma. Consider the solution

$$x_i = b_i = \lambda_i \mu, \quad \text{with } \lambda_i \leq 1, \qquad i = 1, \dots, k$$
  

$$x_i = \mu, \qquad \text{with } \lambda_i = 1, \quad i = k+1, \dots, n$$
(A.5)

in accordance with (b) above, where k is as yet undetermined. Putting (A.5) into the equality constraint we get  $b_1 + \cdots + b_k + (n-k)\mu = a$ . It follows that

$$x_{k+1} = \dots = x_n = \mu = \frac{a - (b_1 + \dots + b_k)}{n - k}.$$
 (A.6)

Now let k be chosen as in part (ii) of the lemma. Then the solution  $(x_1, \ldots, x_n)$  given by (A.5), (A.6) is feasible as required in (a) above: by the definition of k,  $b_1 + \cdots + b_{k+1} + (n-k-1)b_{k+1} > a$ , which is equivalent to  $\mu < b_{k+1}$ .

To satisfy (b), we need to check that  $\lambda_i \leq 1$  for i = 1, ..., k. From (A.5) and (A.6),

$$\lambda_i = \frac{(n-k)b_i}{a - (b_1 + \dots + b_k)} \quad \text{and} \quad \lambda_i \leq 1 \quad \Leftrightarrow \quad a - (b_1 + \dots + b_k) \ge (n-k)b_i.$$

But this last condition holds  $\forall i \leq k$  by the definition of k. We have found a solution  $x^*$ , and because the entropy function is strictly concave, this solution is unique and we are done. It remains to show that it is possible to find a k as required in part (ii) of the lemma. This is done in Proposition A.1 below.

**Proposition A.1** Given  $b_0 = 0 < b_1 \leq b_2 \leq \cdots \leq b_n$  and  $0 < a \leq b_1 + \cdots + b_n$ , there is a  $k \in \{0, \ldots, n\}$  s.t. the inequality

$$a - (b_1 + \dots + b_j) \ge (n - j)b_j$$

holds for all  $j \leq k$  and for no larger j.

**Proof** Consider the function  $\varphi(j) = a - (b_1 + \dots + b_j) - (n - j)b_j$ ,  $j \in \{0, 1, \dots, n\}$ . It is easy to see that  $\varphi(j) \ge \varphi(j+1)$  for all j, so this function is monotone decreasing. Further,  $\varphi(0) = a > 0$  and  $\varphi(n) = a - (b_1 + \dots + b_n) \le 0$ . So there is a  $k \le n$  s.t.  $\varphi(j) \ge 0$  for  $j \le k$ , and  $\varphi(j) < 0$  for j > k, as claimed. Note that k = n iff  $b_1 + \dots + b_n = a$ .  $\Box$ 

#### A.3 Proofs for §5

Proposition A.2 The function

$$G(x_1, \dots, x_n) = \left(\sum_i x_i\right) \ln\left(\sum_i x_i\right) - \sum_i x_i - \sum_i (x_i \ln x_i - x_i)$$
$$= \left(\sum_i x_i\right) \ln\left(\sum_i x_i\right) - \sum_i x_i \ln x_i$$

is concave over the domain  $x_1 > 0, \ldots, x_n > 0$ .

This is probably known somewhere in the information theory literature, but I don't know where. So a proof is presented below.

**Proof** By Theorem 2.14 of [ADSZ88] it suffices to show that  $\mathcal{H}(x) = \nabla^2 G(x)$ , the Hessian of G, is negative semi-definite. We find

$$\mathcal{H}(x) = \frac{1}{x_1 + \dots + x_n} U_n - \operatorname{diag}\left(\frac{1}{x_1}, \dots, \frac{1}{x_n}\right),$$

where  $U_n$  is a matrix all of whose entries are 1, and for an arbitrary vector  $y = (y_1, \ldots, y_n)$ we must have  $y^T \mathcal{H}^{\dagger} \leq 0$ . To establish this, first write  $\mathcal{H}$  as

$$\mathcal{H}(x) = \frac{1}{x_1 + \dots + x_n} \left( U_n - \operatorname{diag}\left(\frac{x_1 + \dots + x_n}{x_1}, \dots, \frac{x_1 + \dots + x_n}{x_n}\right) \right)$$

Now define  $\xi_i = x_i/(x_1 + \cdots + x_n)$ . The condition  $y^T \mathcal{H}^{\dagger} \leq 0$  is then equivalent to

$$(y_1 + \dots + y_n)^2 \leq y_1^2 / \xi_1 + \dots + y_n^2 / \xi_n,$$
 (A.7)

where the  $\xi_i$  are positive and sum to 1. The truth of (A.7) follows from the fact that  $y_1^2/\xi_1 + \cdots + y_n^2/\xi_n$  is a convex function of  $\xi_1, \ldots, \xi_n$  over the domain  $\xi_1 > 0, \ldots, \xi_n > 0$ , and its minimum under the constraint  $\xi_1 + \cdots + \xi_n = 1$  occurs at  $\xi_i^* = y_i/(y_1 + \cdots + y_n)$ . So the least value of the r.h.s. of (A.7) as a function of  $\xi_1, \ldots, \xi_n$  is  $(y_1 + \cdots + y_n)^2$ .  $\Box$ 

#### **Proof of Proposition 5.1**

We first give a straightforward proof assuming that  $x_{ij} \in \mathbb{N}$ . Suppose there is a matrix X s.t. for some i, j row i sums to less than  $u_i$  and column j to less than  $v_j$ . Further, let X

have total sum s. Consider the matrix X' formed by adding 1 to  $x_{ij}$ . First, if X satisfies the constraints, so does X'. Second,  $\#(X'|I)/\#(X|I) = (s+1)/(x_{ij}+1) > 1$ . Thus X' has more realizations than X, and so X cannot be the most likely matrix  $\hat{X}$ .

To give a proof assuming that the elements of X are non-negative reals, by Corollary A.2 we must have  $\hat{x}_{ij} = (\sum_{k,l} \hat{x}_{kl}) \lambda_i \mu_j$ . Now if there is a pair i, j s.t.  $\sum_j \hat{x}_{ij} - u_i < 0$  and  $\sum_i \hat{x}_{ij} - v_j < 0$ , we must have  $\lambda_i = \mu_j = 1$ , so  $\hat{x}_{ij} = \sum_{k,l} \hat{x}_{kl}$ . Thus all other elements of  $\hat{X}$  must be 0. Further,  $\hat{x}_{ij} \leq \min(u_i, v_j)$ . But it is easy to see that this matrix cannot have the most realizations.

#### **Proof of Proposition 5.2**

Consider the function  $\varphi(\ell) = u - (v_1 + \dots + v_\ell) - (n-\ell)v_{\ell+1}$ . It is easy to check that  $\varphi(\ell) \nearrow$  as  $\ell \nearrow$ . Further,  $\varphi(0) = u - nv_1 \ge 0$  if  $u/n \ge v_1$ . Finally,  $\varphi(n-1) = u - (v_1 + \dots + v_n) < 0$ . Thus there is a least  $\ell$ , s.t.  $\varphi(\ell) < 0$ ,  $1 \le \ell < n-1$ , and  $\varphi(\ell-1) \ge 0$ . Let that  $\ell$  be k. The two conditions  $\varphi(k) < 0$  and  $\varphi(k-1) \ge 0$  establish what is claimed.

#### A.4 Proofs for §6.2

The following result is a variation of Lemma 4.1: it says that the most likely vector with sum bounded by a and elements bounded by the vector b is the MAXENT vector with sum equal to a and elements bounded by b.

**Lemma A.1** The most likely vector  $x^* = (x_1^*, \ldots, x_m^*)$  satisfying  $\forall i \ 0 \leq x_i \leq b_i$  and  $x_1 + \cdots + x_m \leq a, \ a, b_i \in \mathbb{N}$ , is found as follows. If  $a \leq b_1 + \cdots + b_m$ , the inequality in this constraint can be replaced by equality and then  $x^*$  is given by Lemma 4.1. If  $a > b_1 + \cdots + b_m$ , then  $x^* = (b_1, \ldots, b_m)$ .

**Proof** First we reduce the problem in  $\mathbb{N}$  to another problem in  $\mathbb{N}$ . Suppose that  $a \leq b_1 + \cdots + b_m$ . Let  $y = (y_1, \ldots, y_m), y_i \in \mathbb{N}$  be the most likely vector summing to  $\alpha \leq a-1$  and satisfying  $y_i \leq b_i$ . Pick a  $y_j$  s.t.  $y_j < b_j$ ; this exists because y sums to  $\alpha$ , which is strictly less than  $b_1 + \cdots + b_m$ . But then the vector  $y' = (y_1, \ldots, y_{j-1}, y_j + 1, y_{j+1}, \ldots, y_m)$  sums to  $\alpha + 1$ , satisfies the *b*-constraints, and by the argument given in §3,  $\#(y' \mid \alpha + 1) > \#(y \mid \alpha)$ . So by increasing the allowed sum  $\alpha$  we get a more likely vector. It follows that the most likely vector  $x^*$  in  $\mathbb{N}$  satisfying the constraints sums to exactly a, and (an approximation in  $\mathbb{R}$ ) can therefore be found by Lemma 4.1.

Now let  $a > b_1 + \cdots + b_m$ . In that case the *a*-constraint is irrelevant and we have precisely the problem solved in §3 for a matrix; so  $x^* = (b_1, \ldots, b_m)$ .

#### A.5 Proofs for $\S7.2$

#### A.5.1 Proof of Proposition 7.1

We already noted that the function

$$f(\lambda) = \sqrt{1 - 4r_1/\lambda^2} + \dots + \sqrt{1 - 4r_m/\lambda^2} - 2(r_{m+1} + \dots + r_n)/\lambda^2 - (m-2)$$

is monotone increasing for any  $m \leq n$ . We will now show that f(4/3) > 0 and  $f(2\sqrt{r_{\text{max}}}) \leq 0$ .

f > 0 at 4/3 This reduces to showing that

$$\sqrt{1 - 9/4r_1} + \dots + \sqrt{1 - 9/4r_m} - 9/8(r_{m+1} + \dots + r_n) > m - 2.$$
 (A.8)

The l.h.s. has the form  $\sum_{i} \varphi_i(r_i)$  where  $\varphi_i(\cdot)$  is concave, so it is a concave function of  $r_1, \ldots, r_n$  (Prop. 2.16 of [ADSZ88]) over the convex domain defined by  $r_1 + \cdots + r_n = 1$  and  $0 < r_i \leq 1/3$ . Therefore its minimum occurs on the boundary of the domain ([ADSZ88], Prop. 2.25.) The boundary consists of all points s.t. three of the  $r_i$  are 1/3 and the rest are 0. There are several cases to consider. First, it is easy to check that (A.8) holds for m = 0 and m = 1.

Next let m = 2. What we want to prove reduces to  $\sqrt{1 - 9/4r_1} + \sqrt{1 - 9/4r_2} - 9/8(r_3 + \cdots + r_n) > 0$ . The possibilities for the boundary are  $r_1 = r_2 = r_3 = 1/3$ , or  $r_1 = 1/3, r_3 = r_4 = 1/3$ , or  $r_3 = r_4 = r_5 = 1/3$ , and the desired inequality holds under any of these conditions.

Lastly suppose that  $m \ge 3$ , and, without loss of generality, that  $r_1 = r_2 = r_3 = 1/3$ . Then (A.8) becomes 3/2 + m - 3 > m - 2, which is true. Next, let  $r_1 = r_2 = 1/3$ ,  $r_{m+1} = 1/3$ ; (A.8) becomes 1 + m - 2 - 3/8 > m - 2, which is also true. The remaining two cases are  $r_1 = 1/3$ ,  $r_{m+1} = r_{m+2} = 1/3$ , and  $r_{m+1} = r_{m+2} = r_{m+3} = 1/3$ , and (A.8) holds for both.

 $f \leq 0$  at  $2\sqrt{r_{\text{max}}}$  Without loss of generality we may assume that  $r_{\text{max}} = r_1$  because this makes the notation simpler. Then  $f(2\sqrt{r_{\text{max}}}) < 0$  reduces to establishing

$$\sqrt{1 - r_2/r_1} + \dots + \sqrt{1 - r_m/r_1} - \frac{r_{m+1} + \dots + r_n}{2r_1} \leqslant m - 2.$$
 (A.9)

We will find the maximum of the function on the l.h.s., treating  $r_1$  as known for the moment. Using Theorem 1, the l.h.s. is a concave function of  $r_2, \ldots, r_n$ , and under the constraint  $r_2 + \cdots + r_n = 1 - r_1$  it has a unique maximum at the point determined by

$$\frac{1}{2r_1} = \frac{1}{2r_1} \left( 1 - \frac{r_2}{r_1} \right)^{-3/2} = \cdots = \frac{1}{2r_1} \left( 1 - \frac{r_m}{r_1} \right)^{-3/2}$$

Thus the maximum occurs at the point  $r_2 = \cdots = r_m = 0$  and  $r_{m+1} + \cdots + r_n = 1 - r_1$ , where the value of the function is  $m - 1 - (1 - r_1)/(2r_1)$ . Therefore (A.9) will hold iff  $r_1 \leq 1/3$ .

The above proof assumed that m < n. When m = n, (A.9) becomes

$$\sqrt{1 - r_2/r_1} + \dots + \sqrt{1 - r_n/r_1} \leqslant n - 2.$$
 (A.10)

As before, the l.h.s. is a concave function for fixed  $r_1$ , and its maximum occurs at  $r_2 = \cdots = r_n = (1 - r_1)/(n - 1)$ . Thus (A.10) holds if

$$(n-1)\sqrt{1-\frac{1-r_1}{(n-1)r_1}} \le n-2,$$

which is true if  $r_1 \leq 1/3$ .

**Proof of Proposition 7.2** We re-use the proof of Proposition 7.1. Define  $f(\lambda) = \sqrt{1 - 4r_{I_1}/\lambda^2} + \cdots + \sqrt{1 - 4r_{I_m}/\lambda^2} - (m-2)$ . Setting  $\rho_i = r_{I_i}/\sigma$ , this becomes

$$f(\lambda) = \sqrt{1 - 4\sigma\rho_1/\lambda^2} + \dots + \sqrt{1 - 4\sigma\rho_m/\lambda^2} - (m - 2), \qquad \sum_i \rho_i = 1.$$

Then  $f(4\sqrt{\sigma}/3) > 0$  is equivalent to  $\sqrt{1-9/4\rho_1} + \cdots + \sqrt{1-9/4\rho_m} > m-2$ ; but this is a special case of (A.8). It remains to show that  $f(2\sqrt{r_{\max}}) = f(2\sqrt{\sigma\rho_{\max}}) \leq 0$ . Assuming w.l.o.g. that  $\rho_{\max} = \rho_1$ , this reduces to  $\sqrt{1-\rho_2/\rho_1} + \cdots + \sqrt{1-\rho_2/\rho_m} \leq m-2$ , which follows from (A.10).

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