Non Uniform Selection of Solutions for Upper Bounding the 3-SAT Threshold

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Abstract. We give a new insight into the upper bounding of the 3-SAT threshold by the first moment method. The best criteria developed so far to select the solutions to be counted discriminate among neighboring solutions on the basis of uniform information about each individual free variable. What we mean by uniform information, is information which does not depend on the solution: e.g. the number of positive/negative occurrences of the considered variable. What is new in our approach is that we use non uniform information about variables. Thus we are able to make a more precise tuning, resulting in a slight improvement on upper bounding the 3-SAT threshold for various models of formulas defined by their distributions.

1 Introduction

We consider the phase transition phenomenon that occurs in some random satisfiability problems, where the probability of satisfiability for a random formula suddenly goes from 1 to 0 at a given ratio $\frac{\#\text{clauses}}{\#\text{variables}}$. It was first experimentally observed that this transition would occur at a ratio near 4.25 for the standard 3-SAT model (see [1]). The same kind of transition was also observed in some variants of the standard model, e.g. when occurrences and signs of variables are balanced (see [2]).

The first important step towards the quest of the threshold is the work of Friedgut and Bourgain [3] establishing that the width of the transition window tends to zero as the number of variables tends to infinity.

An important breakthrough was then made by Achlioptas and Peres [4]: using a sophisticated technique based on the second moment method they located asymptotically the threshold of $k$-SAT for large constant $k$ at $2^k \ln 2 - O(k)$. However in the particular case of 3-SAT, there remains a gap between established lower and upper bounds.

The cornerstone method used for 25 years in order to establish upper bounds of the 3-SAT threshold is the so-called first moment method. Indeed we are interested in the probability that a formula has some solutions, but that probability is currently out of reach of human-tractable calculations; however the moments under this probability are much easier to estimate. The first moment method consists in bounding the probability we are interested in by the first moment of a certain quantity $X$ under this probability. The simplest quantity $X$ one can imagine as a candidate for the first moment method is the number of solutions. This gives an upper bound of 5.191 [5], which is far above the experimentally observed threshold at around 4.25. There has been ever since lots of efforts [6,7,8,9,10] intended to lower this upper bound by removing as many solutions as possible from the counted quantity $X$, the only requirement of the first moment method being to count at least 1 solution whenever a formula is satisfiable; thus the technique is to count only particular solutions, designed to be present whenever there is a solution, and not too complicated to count.

We obtain some new upper bounds in a variety of models of 3-CNF formulas (which we introduce later in section 2.1). In the particular case of the standard model we get an upper bound of 4.500. We must mention here the work of Díaz et al. [11]; gathering the technique of [10,12] with a pure literal elimination and a filtering on the typicality of clauses, they got an upper bound of 4.490. The fact is that our new technique is quite compatible with the pure literal elimination and the filtering on the typicality of clauses, but we only aim at emphasizing the positive effect of our new technique for selecting solutions, by comparing it to previous analogous techniques in several models of formulas.

The best implementations of the first moment method approximating the threshold of 3-SAT use local relationships between solutions, which involves solutions agreeing on the values of all variables but a constant number of them, in general one variable [8] or two [9].
We shall consider the set of solutions with local relationship as a graph which nodes are the solutions and an edge exists between two solutions if and only if both solutions agree on the values of all variables except one. Each edge will be labelled by the variable differing between both solutions.

For example the formula

\[ \Phi = \{ a \lor b \lor c, a \lor c \lor \overline{d}, a \lor \tau \lor \overline{d}, a \lor \overline{b} \lor \overline{d}, \overline{b} \lor c \lor \overline{d}, \overline{a} \lor \overline{b} \lor \tau, \overline{a} \lor \overline{b} \lor \overline{c} \} \]

has 7 solutions that can be represented by the non oriented graph of figure 1.

The techniques used so far amount to making an acyclic orientation of the above graph and to counting only the minimal solutions (those that do not have outgoing edges). The least is the number of minimal solutions the best is the upper bound obtained. In general, any graph can be oriented so as to obtain only one minimal element for every connected component (e.g. by a depth first search), but this orientation is obtained thanks to a sophisticated algorithm that is aware of the whole graph while in our case, the orientation must be decided locally.

The very first orientation [5,9] consisted in orienting an edge from the solution where the label variable is assigned 0 to the one where it is 1 regardless of which variable is considered. Later, in [12,11], an edge is oriented towards the value that makes true the most literals and this can be known thanks to the syntactic property of the number of occurrences of each variable in the formula. In both these types of orientation, the edges having the same labels are oriented the same way (e.g. from 0 to 1) anywhere in the graph. So we call such orientations uniform (see Figure 2(a)).

The orientation that we use in this paper is less rigid: two edges labelled with the same variable can be oriented differently depending on the solutions involved (that is what we call non uniform orientation, see Figure 2(b)). Indeed we keep track of a set of 5 numbers associated with each variable and use it to discriminate among neighboring solutions. These 5 numbers provide information on the repartition of true and false occurrences of each variable in each type of clauses (clauses having 1, 2 or 3 true literals). Our intuition is that we should select solutions in which the least occurrences of true literals are critical. The less a clause has true literals, the more its true literals are critical. Such a property is by nature non uniform.

We develop our technique in a general framework allowing us to apply it to a wide variety of 3-CNF models of formulas defined by their distributions; thus we derive new bounds for some known models of formulas [2]. The existence of other non uniform orientations that may give a smaller number of minimal elements and then better bounds remains to be investigated.
In section 2 we present our framework and four different models of formulas; in section 3 we show how we make our non uniform selection of solutions, and sum up the bounds we obtain for each model. We give details on the calculation of the first moment and its constraints in section 4, as well as some hints on what led us to the weights we took for our non uniform selection.

2 Definitions and notations

We consider a generic random model of 3-CNF formulas having \( n \) variables and \( cn \) clauses. Models are parametrized by a probability distribution \( (d_{p,q})_{p,q \in \mathbb{N}} \) such that \( \sum_{p,q \in \mathbb{N}} d_{p,q} = 3c \). In each model a satisfiability threshold will appear for a specific value of \( c \) we want to estimate. Before we get formulas we draw configurations as follows:

1. each of the \( n \) variables is given \( p \) labelled positive occurrences and \( q \) labelled negative occurrences in a way that the overall proportion of variables with \( p \) positive occurrences and \( q \) negatives occurrences is \( d_{p,q} \);
2. a configuration can be seen as a matrix of \( 3cn \) bins containing literals occurrences; the repartition of literals into the \( 3cn \) bins is drawn uniformly among all \( (3cn)! \) permutations of labelled literals occurrences.

A legal formula is a configuration where occurrences are unlabelled and each clause contains at most one occurrence of each variable. For the models we consider in this paper and described in section 2.1, it was shown that an upper bound on the satisfiability threshold obtained for configurations also applies to legal formulas (see [11] for the standard model and [2] for models where \( p \) and \( q \) are bounded). So we shall work on configurations all along this paper.

2.1 Overview of Models

Standard Model: all literals are drawn uniformly and independently; it was shown in [12][13] that the resulting distribution is the 2D Poisson distribution: 

\[
d_{p,q} = \frac{(p+q)}{p} \frac{e^{-3c}}{(p+q)!} \left( \frac{3c}{p} \right)^{p+q}.
\]

By analogy with the standard model we now define several other models where we force an equilibrium between variables occurrences and/or signs. These can be seen as regular variants of 3-SAT (just like regular graphs). The equilibrium cannot be perfect because of parity or truncation reasons, but we circumvent it as follows. Of course one can check that all of these distributions sum up to 1 and have an average of 3c.

Model with Almost Balanced Signs: every variable appear with (almost) the same number of positive and negative occurrences; we define \( d_{p,q} \) by 

\[
d_{p,p} = e^{-3c} (3c)^{2p} \quad \text{and} \quad d_{p+1,p} = \frac{1}{2} e^{-3c} (3c)^{2p+1}.
\]

Model with Almost Balanced Occurrences: every variable appear with (almost) the same number occurrences; let \( t^* = [3c] \) and \( r^* = 3c - t^* \); we define \( d_{p,q} \) by 

\[
d_{p,t^*-p} = (1-r^*) \frac{(r^*)}{2t^*} \quad \text{and} \quad d_{p,t^*+1-p} = r^* \frac{(r^*)}{2t^*+1}.
\]

Model with Almost Balanced Signs and Occurrences: every variable appear with (almost) the same number occurrences and have exactly the same number of positive as negative occurrences (this model was examined in [2]); let \( p^* = \frac{3c}{2} \) and \( r^* = \frac{3c}{2} - p^* \). We define \( d_{p,q} \) by 

\[
d_{p^*,p^*} = 1 - r^* \quad \text{and} \quad d_{p^*+1,p^*+1} = r^*.
\]

2.2 Types of clauses and variables

Our selection method is based on different types of clauses: given any assignment, we call clause of type \( t \) a clause having \( t \) true literals under this assignment, and \( \beta_t \) the proportion of clauses of type \( t \).

Moreover we want to have some control on the number of occurrences of variables in the different types of clauses; to do so we need 6 numbers per variable, so we say that a variable is of type \( (i,j,k,l,m,v) \) if it is assigned \( v \) and has:

\[
\begin{align*}
&i \quad \text{true occurrences in clauses of type 1}; \\
&j \quad \text{true occurrences in clauses of type 2}; \\
&k \quad \text{true occurrences in clauses of type 3}; \\
&l \quad \text{false occurrences in clauses of type 1}; \\
&m \quad \text{false occurrences in clauses of type 2}; \\
\end{align*}
\]

\[
\begin{array}{cccccc}
\text{true} & & & & & \text{false} \\
\beta_1 & \beta_2 & \beta_3 & & & \\
\end{array}
\]
Remark 1. For each variable we have \( i + j + k = p \) and \( l + m = q \) or vice versa (according to the value \( v \) assigned to the variable).

Then we put some weights onto the solutions as follows: in a given solution each variable of type \((i, j, k, l, m, v)\) receives a weight \( \omega_{i,j,k,l,m,v} \). The weight of a solution will be the product of the weights of all variables. It turns out that in the end we shall take binary weights, yielding in fact an orientation between solutions. We explain the choice of the weights in sections 3 and 4.4. Then we apply the first moment method to the random variable \( X \) equal to the sum of the weights of the solutions.

3 Selection of Solutions

Let us recall how the first moment method works: we want to show that \( \text{Pr}(Y \geq a) \) is small but we don’t have access to \( \text{Pr}(Y \geq a) \). Instead we use some \( \text{EX} \). It suffices then to ensure that \( \text{Pr}(Y \geq a) \leq \text{EX} \). For our problem 3-SAT, \( Y \) is the number of solutions, \( a = 1 \) and \( X \) is the total weight on the solutions. Since \( X \geq 0 \), Markov’s inequality yields that \( \text{Pr}(X \geq 1) \leq \text{EX} \); so if we choose \( X \) such that \( Y \geq 1 \) implies \( X \geq 1 \), we have \( \text{Pr}(Y \geq 1) \leq \text{Pr}(X \geq 1) \leq \text{EX} \).

Then our goal will be to tune the weights so that \( \text{EX} \to 0 \) for the least ratio \( c = \#\text{clauses} / \#\text{variables} \).

3.1 Construction of a Correct Weighting Scheme

Of course we must put some constraints onto the weights in order that the weighting scheme can be correct for the first moment method: namely the sum of the weights of the solutions of a satisfiable formula must be at least 1. However the constraints we choose here might not be necessary for the first moment method to hold.

Let us recall that given a solution, a variable is called free when the assignment obtained by inverting its value (0/1) remains a solution. Thus in our framework, a variable is free iff its \( i \) number is 0. How does the tuple \((0, j, k, l, m, v)\) for a free variable \( x \) behave when the value \( v \) is inverted to \( 1-v \)? \( (i(x) \leftarrow 0, j(x) \leftrightarrow l(x), k(x) \leftrightarrow m(x) \) and \( v(x) \leftarrow 1-v \).

1. the first constraint we put is that \( \omega_{i,j,k,l,m,v} = 1 \) as soon as \( i \geq 1 \); that is, we put significant weights only onto free variables. The reason for this is that free variables allow to move between solutions.

2. the second constraint is that

\[
\omega_{0,j,k,l,m,v} + \omega_{0,l,m,j,k,1-v} = 1 \tag{1}
\]

that is, the sum of the weights of a free variable in a couple of solutions differing only on that variable is 1. We impose this condition by analogy with the conditions on weights given in [13].

As suggested by the analysis given in section 4.4 we shall take \( \omega_{0,j,k,l,m,v} = 1_{P(j,k,l,m,v)} \) for a certain predicate \( P(j,k,l,m,v) \) linked with the sign of \( \alpha_1 \rho_{j,l} + \alpha_2 \rho_{k,m} \) (where \( \alpha_1 \) and \( \alpha_2 \) are any real constants and \( \rho \) is an operator defined as \( \rho_{a,b} = a-b \)).

The fact that we imposed \( \omega_{0,j,k,l,m,v} + \omega_{0,l,m,j,k,1-v} = 1 \) tells us that given a solution and a free variable \( x \) at the value \( v \), the predicate \( P \) is satisfied by \( x \) at the value \( v \) or (exclusively) by \( x \) at the value \( 1-v \). Thus we are able to define an orientation between neighboring solutions.

Let us say that variable \( x \) is obedient when \( P \) is satisfied. We put an arc between 2 solutions differing only on 1 (free) variable \( x \) from the solution \( S_d \) (where \( x \) is disobedient) to the solution \( S_o \) (where \( x \) is obedient), and we call that relation \( S_d > S_o \). The notation \( > \) is not randomly chosen.

Namely our weighting scheme counts 1 for a solution when it does not have any disobedient free variables, and 0 otherwise; but what can ensure that whenever there is a solution, there is also a solution where all free variables are obedient? It suffices that the relation \( > \) is circuit-free. Then the transitive closure of \( > \) is an order, and we are precisely counting the minimal solutions in that order. Minimal solutions exist because the set of all solutions is finite. So let us see how we can make the relation \( > \) circuit-free.

Recapitulation of Existing Methods.

All Solutions: This method consists in computing the first moment on all solutions: \( P(j,k,l,m,v) \equiv 1 \).

Negatively Prime Solutions (NPS): This method consists in counting only solutions which free variables are assigned 1. That is \( P(j,k,l,m,v) \equiv v > 0 \). This method was introduced in [8].

NPS with Imbalance: This method was introduced in [12] and combined to some other ingredients in [11]. This method consists in allowing free variables to take only a value such that the number of true occurrences is larger than the number of negative occurrences of this variable (and in case of equality, ties are broken in favor of the value 1). In other words \( P(j,k,l,m,v) \equiv (\rho_{j,l} + \rho_{k,m,v}) >_{\text{lex}} (0,0) \), where \( >_{\text{lex}} \) denotes the lexicographical order.
Our Method. May we choose arbitrary real coefficients $\alpha_1$ and $\alpha_3$ in the expression of $\alpha_1 \rho_{j,l} + \alpha_3 \rho_{k,m}$ in order that the first moment method should hold? It turns out that it is the case, and here is a proof of it.

We make the following observation: how does the population of the 3 different types of clauses evolve when a free variable $x$ is flipped? $\beta_1 = \rho_{j,l}(x)$, $\beta_2 = (\rho_{k,m} - \rho_{j,l})(x)$ and $\beta_3 = -\rho_{k,m}(x)$.

Thus $\alpha_1 \rho_{j,l} + \alpha_3 \rho_{k,m}$ is the variation of $\alpha_1 \beta_1 - \alpha_3 \beta_3$; so we may define our predicate $P$ in the following way:

$$P(j, k, l, m, v) \equiv (\alpha_1 \rho_{j,l} + \alpha_3 \rho_{k,m}, v) > \text{lex} (0, 0);$$

thanks to $v$ we break ties when $\alpha_1 \rho_{j,l} + \alpha_3 \rho_{k,m} = 0$, so that the underlying relation $>$ between solutions is circuit-free: namely going from $S_d$ to $S_o$ when $S_d > S_o$ strictly increases $(-\alpha_1 \beta_1 + \alpha_3 \beta_3, v)$ for $>_{\text{lex}}$.

Moreover the exclusion between $P(j, k, l, m, v)$ and $P(l, m, j, k, 1-v)$ is satisfied, which means that whenever there is a solution with a disobedient free variable, it suffices to flip the value of this variable so that it becomes obedient. We investigated the best ratio between $\alpha_1$ and $\alpha_3$ by numerical experiments.

### 3.2 Summary of Results

| model                  | standard | almost balanced signs | almost balanced occurrences | almost balanced signs and occurrences |
|------------------------|----------|-----------------------|----------------------------|---------------------------------------|
| all solutions          | 5.040    | 3.858                 | 5.046                      | 3.783                                 |
| NPS \(v > 0\)          | 4.552    | 3.521                 | 4.662                      | 3.548                                 |
| NPS+imbalance \((\rho_{j,l} + \rho_{k,m}, v) > (0, 0)\) | 4.506    | 3.514                 | 4.628                      | 3.548                                 |
| our method \((\alpha \rho_{j,l} + \rho_{k,m}, v) > (0, 0)\) | 4.500    | 3.509                 | 4.623                      | 3.546                                 |
| our $\alpha$           | $\alpha = 2.00$ | $1.01 \leq \alpha \leq 1.16$ | $2.01 \leq \alpha \leq 2.24$ | $\alpha \geq 1.01$ |

As one can see in table 1 our method yields in all models a slight improvement on the bounds obtained by former methods. Note that for some models there is a range of values for $\alpha$ which give the same upper bound.

In the model where signs as well as occurrences are balanced, the method of NPS+imbalance is of course the same as the method of NPS, whereas our method is somewhat better than the method of NPS.

The bound we obtain in the standard model is 4.500; this is not better than the bound of 4.490 obtained by Diaz et al. in [11]. Their calculation adds 2 ingredients to the method of [12]: typicality of clauses and elimination of pure literals. These 2 ingredients might be combined to our approach to improve on the 4.490, but this would involve too complicated calculations with respect to the expected improvement. However in models where signs are balanced it is irrelevant to eliminate pure literals.

### 4 The First Moment Method

#### 4.1 Types of variables

We split the set of variables into several sets and subsets of variables. In order to be able to match the original random 3-CNF model of formulas where all literals are drawn independently, we should consider $p$ and $q$ to range in $\mathbb{N}$. For convenience of our forthcoming maximization, we only take into account bounded values of $p$ and $q$. So we are going to consider 2 kinds of variables, according to their numbers of occurrences. We follow the notations of [11]. We denote by $M$ some integer whose value will be determined according to the required accuracy of the calculations; in practice we shall take $M = 21$. $M$ enables us to define 2 kinds of variables:

1. the set of light variables, that is variables which indices are in the set

$$\mathcal{L} = \{(p, q) \in \mathbb{N}^2, p \leq M \land q \leq M \land d_{p,q} > 0\}; \quad (2)$$
they are the most important variables since almost all variables are light in the models we consider; we call \( \delta_{p,q} \) the proportion of light variables having \( p \) positive occurrences, \( q \) negative occurrences, and assigned 1. As a further refinement, we call \( \pi_{i,j,k,l,m,v} \) the proportion of variables of type \((i,j,k,l,m,v)\) whose corresponding weight \( \omega_{i,j,k,l,m,v} \) is non zero, and omit the other ones because we shall need all active \( \pi_{i,j,k,l,m,v} \) to be non zero. To connect \( \pi_{i,j,k,l,m,v} \)'s with \( \delta_{p,q} \)'s we introduce the following set of tuples of integers: \( Q_{p,q} = \{(i,j,k,l,m) \in N^5, i + j + k = p \land l + m = q \} \); thus we have

\[
\sum_{(i,j,k,l,m) \in Q_{p,q}} \pi_{i,j,k,l,m,1} = \delta_{p,q} ;
\]

\[
\sum_{(i,j,k,l,m) \in Q_{p,q}} \pi_{i,j,k,l,m,0} = d_{p,q} - \delta_{p,q} .
\]

Note that equality \(4\) involves \( Q_{q,p} \) whereas equality \(3\) involves \( Q_{p,q} \).

2. the set of heavy variables, that is all other variables; their indices are thus in the set

\[
\mathcal{H} = \{(p,q) \in N^2, p > M \lor q > M \lor d_{p,q} = 0 \} ;
\]

we weaken the notion of satisfiability by considering that heavy variables are always satisfied, regardless of their signs and values. Doing so is harmless for the validity of the first moment method because we can only increase the number of solutions. In other words we are going to consider heavy variables as indistinguishable members of a tote bag. We call \( \tau \) the global scaled number of heavy variables: \( \tau = \sum_{(p,q) \in \mathcal{H}} d_{p,q} \).

We also need to distinguish some types of occurrences of heavy variables. We call \( H \) the global scaled number of occurrences of heavy variables:

\[
H = \sum_{(p,q) \in \mathcal{H}} (p+q)d_{p,q} = 3c - \sum_{(p,q) \in \mathcal{L}} (p+q)d_{p,q} .
\]

According to the types of clauses where occurrences appear, \( H \) is divided into \( H_t \)'s, where \( H_t \) is the scaled number of occurrences of heavy variables in clauses of type \( t \).

We are now ready to write down the expression of the first moment of \( X \), the weight of all solutions.

### 4.2 Expression of the First Moment and its Constraints

We recall that all occurrences of literals are drawn according to the distribution \( d_{p,q} \) (see section \(2\)). Thus the sample space we consider consists in the \((3cn)!\) permutations of labelled occurrences of literals, and our parameters are \( n, c, d_{t,p}, \tau, H \) and \( \omega_{i,j,k,l,m,v} \)'s (although we must carefully choose the weights \( \omega_{i,j,k,l,m,v} \), as explained below in section \(13\)).

All other quantities: \( \beta_1, H_t, \delta_{t,p} \) and \( \pi_{i,j,k,l,m,v} \) are variables, and the first moment of \( X \) can be split up into a big sum over all variables of the product of the following factors depending on variables: number of assignments, weight of an assignment and probability for an assignment to be a solution.

1. number of assignments: each variable is assigned 0 or 1: \( 2^\tau \prod_{(p,q) \in \mathcal{L}} \left( d_{p,q}^{n} \right) \).
2. weight of an assignment: \( \prod_{(p,q) \in \mathcal{L}} \prod_{(i,j,k,l,m) \in Q_{p,q}} \omega_{i,j,k,l,m,v}^{\pi_{i,j,k,l,m,v}} ; \):
3. probability for an assignment to be a solution: quotient of the number of satisfied configurations by the total number of configurations:

   (a) number of satisfied configurations: a configuration can be seen as a set of bins filled with occurrences of literals:

   i. each of the \((3cn)!\) bins is first given a truth value:

   there are \( (\beta_1c,n,\beta_2c,n,\beta_3c,n)^{3(\beta_1+\beta_2)c} \) possibilities, and the following constraint appears:

   \[
   \beta_1 + \beta_2 + \beta_3 = 1 .
   \]

   ii. each light literal is given a tuple \((i,j,k,l,m)\) consistently with \( d_{p,q} \) and \( \delta_{p,q} \). This gives a series of constraints:

   \[
   \sum_{(i,j,k,l,m) \in Q_{p,q}} \pi_{i,j,k,l,m,1} + \sum_{(i,j,k,l,m) \in Q_{p,q}} \pi_{i,j,k,l,m,0} = d_{p,q} .
   \]
Note that \( \delta_{p,q} = \sum_{(i,j,k,l,m) \in Q_{p,q}} \pi_{i,j,k,l,m,1} \). Thus, given a family \((\pi_{i,j,k,l,m,v})\), there are

\[
\prod_{(p,q) \in L} \left( \frac{\delta_{p,q} n}{\pi_{i,j,k,l,m,1,n \ldots, (i,j,k,l,m)_{Q_{p,q}}} \pi_{i,j,k,l,m,0 n \ldots, (i,j,k,l,m)_{Q_{p,q}}}}\right)
\]

possible allocations. Moreover the following constraints appear, so that all occurrences of literals can fit into the destined types of clauses:

\[
\sum_{(p,q) \in L} \left( \sum_{v \in \{0,1\}} \pi_{i,j,k,l,m,v} + H_1 = \beta_1 c \right); \tag{8}
\]

\[
\sum_{(p,q) \in L} \left( \sum_{v \in \{0,1\}} \pi_{i,j,k,l,m,v} + H_2 = 2\beta_2 c \right); \tag{9}
\]

\[
\sum_{(p,q) \in L} \left( \sum_{v \in \{0,1\}} \pi_{i,j,k,l,m,v} + H_3 = 3\beta_3 c \right); \tag{10}
\]

\[
\sum_{(p,q) \in L} \left( \sum_{v \in \{0,1\}} \pi_{i,j,k,l,m,v} = 2\beta_1 c \right); \tag{11}
\]

\[
\sum_{(p,q) \in L} \left( \sum_{v \in \{0,1\}} \pi_{i,j,k,l,m,v} = \beta_2 c \right). \tag{12}
\]

iii. all occurrences of light variables are allocated to the 5 regions:

\[
\prod_{(i,j,k,l,m) \in Q_{p,q}} \left( \alpha_{i,j,k,l,m,v} \right) \pi_{i,j,k,l,m,0} \text{ allocations are possible;}
\]

iv. all occurrences of heavy variables are allocated to the 3 satisfied regions, which yields \((H_{1n}, H_{2n}, H_{3n})\) possible allocations; and we must add the following constraint:

\[
H_1 + H_2 + H_3 = H. \tag{13}
\]

v. all permutations of occurrences of literals are possible inside the 5 regions:

their number is \((\beta_1 cn)! (2\beta_2 cn)! (3\beta_3 cn)! (2\beta_1 cn)! (\beta_2 cn)!\);

(b) total number of configurations: the occurrences of literals can be in any order: \((3cn)!\) permutations are possible.

We denote by \(\mathcal{P}\) the set of all families \(\zeta\) of non negative numbers

\[
\left( \sum_{(p,q) \in L} \left( \sum_{(i,j,k,l,m) \in Q_{p,q}} \pi_{i,j,k,l,m,v} \right), (H_1, H_2, H_3), (\beta_1, \beta_2, \beta_3) \right) \tag{14}
\]

satisfying the above constraints; note that \(\mathcal{P}\) is convex (by linearity of constraints). We denote by \(\mathcal{I}(n)\) the intersection of \(\mathcal{P}\) with the multiples of \(\frac{1}{n}\); we get the following expression of the first moment: \(E_X = \sum_{\zeta \in \mathcal{I}(n)} T(n)\) where
\[ T(n) = 2^{\gamma n} \left( \frac{H_n}{H_{1n} H_{2n} H_{3n}} \right)^{\frac{\gamma n}{(3\gamma n)!}} \frac{\beta_1 \gamma n}{(2\beta_2 \gamma n)! (3\beta_3 \gamma n)! (2\beta_1 \gamma n)! (\beta_2 \gamma n)!} \]

\[ \prod_{(p,q) \in \mathcal{L}} \left( \frac{d_{p,q} \gamma n}{\beta_{p,q} \gamma n} \right) \prod_{(p,q) \in \mathcal{L}} \left( \frac{\beta_{p,q} \gamma n}{\pi_{i,j,k,l,m,1} n, \ldots} \right) (i,j,k,l,m) \in Q_{p,q} \]

\[ \prod_{(p,q) \in \mathcal{L}} \left( \frac{C_{p,q} \gamma n}{\pi_{i,j,k,l,m,0} n, \ldots} \right) (i,j,k,l,m) \in Q_{p,q} \]

\[ \prod_{(p,q) \in \mathcal{L}} \left( \frac{\omega_{i,j,k,l,m,v} (i + j + k) (l + m)}{\pi_{i,j,k,l,m,v}} \right)^{\pi_{i,j,k,l,m,v}} \cdot \tau_{i,j,k,l,m,v} \cdot \tau_{i,j,k,l,m} \cdot \tau_{i,j,k,l,m,0} \].

We get rid of all factorials thanks to the following Stirling’s inequalities due to Batir [14]: \( (\frac{k}{e})^k \sqrt{2\pi (k + \frac{1}{4})} < k! < (\frac{k}{e})^k \sqrt{2\pi (k + \frac{e^2}{4} - \frac{1}{4})} \).

The boundedness of the set \( \mathcal{L} \) of light variables (and thus the boundedness of the sets \( Q_{p,q} \)) allows to write that \( T(n) \leq \text{poly}_1(n) F^n \).

### 4.3 Maximization of \( \ln F \)

This is the technical part of our work. We mainly use the same techniques as [11].

1. In order to maximize \( \ln F \) under our constraints, we use the standard Lagrange multipliers technique. This is appendix [A]. The following equations come from the Lagrange derivations and are important for our study:

\[ \pi_{i,j,k,l,m,1} = \omega_{i,j,k,l,m,1} \left( \frac{i + j + k}{i,j,k} \right) \left( \frac{l + m}{l,m} \right)^{r_{i+j+k,l+m} x_1^{2j} y_1^{2m}} \]

\[ \pi_{i,j,k,l,m,0} = \omega_{i,j,k,l,m,0} \left( \frac{i + j + k}{i,j,k} \right) \left( \frac{l + m}{l,m} \right)^{r_{l+m,i+j+k} x_1^{2j} y_1^{2m}} \]

\( x_1, x_2, y_1 \) and \( y_2 \) are Lagrange multipliers, that is positive numbers; moreover \( r_{p,q} \) is defined as follows:

\[ r_{p,q} = \frac{A_{p,q}}{A_{q,p}} \]

\[ A_{p,q} = \sum_{(i,j,k,l,m) \in Q_{p,q}} \omega_{i,j,k,l,m,1} \left( \frac{p}{i,j,k} \right) \left( \frac{q}{l,m} \right)^{x_1^{2j} y_1^{2m}} \]

\[ + \sum_{(i,j,k,l,m) \in Q_{q,p}} \omega_{i,j,k,l,m,0} \left( \frac{q}{i,j,k} \right) \left( \frac{p}{l,m} \right)^{x_1^{2j} y_1^{2m}} \]
2. In order to justify the use of this technique we must show that the function $\ln F$ does not maximize on the boundary of the polytope of constraints; to do so we show that starting at a boundary point there is always a “good” direction inside the polytope which makes $\ln F$ greater. This is appendix B.

3. Finally we must ensure that the solution we found by the Lagrange multiplier technique is indeed a global maximum; to do so we make a sweep over different values of the parameters $\beta_i$; indeed when these $\beta_i$ are fixed the function $\ln F$ is strictly concave relative to the remaining variables, thus easier to maximize. This is appendix C.

### 4.4 Minimization of Global Weight

Let us see how one can minimize $F$ (or equivalently $\ln F$) by a good choice of the weights. The following reasoning is not rigorous; we only aim at giving some hints to explain the choice of the weights we made in section 3.

Remember that $F$ is given by equation 16. We want to minimize $\ln F$ by tuning the weights $\omega_{0,j,k,l,m,v}$, so we are going to differentiate $\ln F$ with respect to an individual $\omega_{0,j,k,l,m,1}$. Of course due to the constraints every variable depend on $\omega_{0,j,k,l,m,1}$ in the process of maximizing $\ln F$ under these constraints. But we consider that the variations on all variables are negligible except for $\pi_{0,j,k,l,m,1}$ (because of equation 17) and $\pi_{0,l,m,j,k,0}$ (because of equations 18 and 1), so we can write:

$$
\frac{\partial (\ln F)}{\partial \omega_{0,j,k,l,m,1}} \approx \left( \frac{\partial (\ln F)}{\partial \pi_{0,j,k,l,m,1}} \frac{\partial \pi_{0,j,k,l,m,1}}{\partial \omega_{0,j,k,l,m,1}} + \frac{\partial (\ln F)}{\partial \pi_{0,l,m,j,k,0}} \frac{\partial \pi_{0,l,m,j,k,0}}{\partial \omega_{0,j,k,l,m,1}} \right). \tag{21}
$$

Using equations 17, 18 and 1 we find that:

$$
\frac{\partial (\ln F)}{\partial \omega_{0,j,k,l,m,1}} \approx -\left( \frac{\partial (\ln F)}{\partial \pi_{0,j,k,l,m,1}} \frac{\partial \pi_{0,j,k,l,m,1}}{\partial \omega_{0,j,k,l,m,1}} + \frac{\partial (\ln F)}{\partial \pi_{0,l,m,j,k,0}} \frac{\partial \pi_{0,l,m,j,k,0}}{\partial \omega_{0,j,k,l,m,1}} \right).
$$

Now due to equations 19 and 20 and numerical experiments we make the following approximations:

$$r_{j+k,l+m}x_{2j}y_{1j}y_{2k} \ll 1 \text{ and } r_{j+k,l+m}x_{2j}y_{1j}y_{2k} \ll 1. \text{ As the function } x \rightarrow x \ln(ax) \text{ is strictly decreasing between 0 and } \frac{1}{ax}, \text{ we can infer the following property: } \frac{\partial (\ln F)}{\partial \omega_{0,j,k,l,m,1}} > 0 \text{ iff } x_{2j}y_{1j}y_{2k} < x_{2j}y_{1j}y_{2k}, \text{ i.e. } \left( \frac{x_{2j}}{y_{1j}} \right)^{j-l} \left( \frac{y_{1j}}{y_{2k}} \right)^{k-m} < 1.
$$

Now let us consider we are at the minimum point of $\ln F$. If $\frac{\partial (\ln F)}{\partial \omega_{0,j,k,l,m,1}} \neq 0$, then $\omega_{0,j,k,l,m,1}$ must be at the boundary, i.e. 0 or 1.

$$\frac{\partial (\ln F)}{\partial \omega_{0,j,k,l,m,1}} > 0 \text{ iff } \alpha_1 \omega_{0,j,l} + \alpha_3 \rho_{k,m} < 0, \text{ where } \alpha_1 = \ln \frac{x_{2j}}{y_{1j}} \text{ and } \alpha_3 = \ln \left( \frac{y_{1j}}{y_{2k}} \right). \text{ Thus:}
$$

1. If $\alpha_1 \rho_{j,l} + \alpha_3 \rho_{k,m} < 0$, then $\omega_{0,j,k,l,m,1} = 0$;
2. If $\alpha_1 \rho_{j,l} + \alpha_3 \rho_{k,m} > 0$, then $\omega_{0,j,k,l,m,1} = 1$;
3. If $\alpha_1 \rho_{j,l} + \alpha_3 \rho_{k,m} = 0$, nothing can be said about $\omega_{0,j,k,l,m,1}$.

What about $\omega_{0,j,k,l,m,0}$?

1. If $\alpha_1 \rho_{j,l} + \alpha_3 \rho_{k,m} < 0$, then $\alpha_1 \rho_{j,l} + \alpha_3 \rho_{m,k} > 0$, thus $\omega_{0,l,m,j,k,1} = 1$, so $\omega_{0,j,k,l,m,0} = 0$;
2. If $\alpha_1 \rho_{j,l} + \alpha_3 \rho_{m,k} > 0$, then by the same argument, $\omega_{0,j,k,l,m,0} = 1$;
3. If $\alpha_1 \rho_{j,l} + \alpha_3 \rho_{m,k} = 0$, nothing can be said about $\omega_{0,j,k,l,m,0}$.

5 Conclusion

We hope that the new track we opened will help gain some more insight and some more decimals in the quest of the 3-SAT threshold. In particular note that we required the relation $>$ between solutions to be circuit-free although this might not be necessary; indeed we only used the fact that this relation had at least one minimal element. The same remark holds for the constraints we put on the weights of two neighboring solutions as introduced in equation 4 since this might be too strong. Thus there may be better orientations or weighting schemes than ours.
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Appendices

Let us recall that we want to maximize the function:

$$F = 2^\tau \frac{H^H}{H_1^H \cdot H_2^H \cdot H_3^H} \left( \frac{1}{3} (2\beta_1)^{\beta_1} (2\beta_2)^{\beta_2} (3\beta_3)^{\beta_3} \right)^{2\tau} \prod_{(p,q) \in \mathcal{L}} D_{p,q} \prod_{(p,q) \in \mathcal{L}} \prod_{(i,j,k,l,m,v) \in \mathcal{Q}_{p,q}} \left( \omega_{i,j,k,l,m,v} \left( \frac{i+j+k}{i,j,k} \cdot \frac{l+m}{l,m} \right) \pi_{i,j,k,l,m,v} \right).$$

(23)
on variables \((\pi_{i,j,k,l,m,v})_{(p,q)\in \mathcal{L}, (i,j,k,l,m)\in \mathcal{Q}_{p,q}, v \in \{0,1\}})\), \((H_1, H_2, H_3)\), \((\beta_1, \beta_2, \beta_3)\) subject to the following constraints:

\[
\sum_{(i,j,k,l,m)\in \mathcal{Q}_{p,q}} \beta_1 + \beta_2 + \beta_3 = 1
\] (24)

\[
\sum_{(i,j,k,l,m)\in \mathcal{Q}_{p,q}} \pi_{i,j,k,l,m,1} + \sum_{(i,j,k,l,m)\in \mathcal{Q}_{q,p}} \pi_{i,j,k,l,m,0} = d_{p,q}
\] (25)

\[
H_1 + H_2 + H_3 = \sum_{(p,q)\in \mathcal{H}} (p + q) d_{p,q}
\] (26)

\[
\sum_{(p,q)\in \mathcal{L}, (i,j,k,l,m)\in \mathcal{Q}_{p,q}, v \in \{0,1\}} \pi_{i,j,k,l,m,v} + H_1 = \beta_1 c
\] (27)

\[
\sum_{(p,q)\in \mathcal{L}, (i,j,k,l,m)\in \mathcal{Q}_{p,q}, v \in \{0,1\}} \pi_{i,j,k,l,m,v} + H_2 = 2\beta_2 c
\] (28)

\[
\sum_{(p,q)\in \mathcal{L}, (i,j,k,l,m)\in \mathcal{Q}_{p,q}, v \in \{0,1\}} \pi_{i,j,k,l,m,v} + H_3 = 3\beta_3 c
\] (29)

\[
\sum_{(p,q)\in \mathcal{L}, (i,j,k,l,m)\in \mathcal{Q}_{p,q}, v \in \{0,1\}} \pi_{i,j,k,l,m,v} = 2\beta_1 c
\] (30)

\[
\sum_{(p,q)\in \mathcal{L}, (i,j,k,l,m)\in \mathcal{Q}_{p,q}, v \in \{0,1\}} \pi_{i,j,k,l,m,v} = \beta_2 c
\] (31)

To perform such a maximization we use the standard technique of Lagrange multipliers.

A Resolution of the Global Lagrange Multipliers Problem

A.1 Elimination of redundant constraints

The first thing to do is to remove redundant constraints. It appears that e.g. constraint (29) is redundant with constraints (27), (29), (30), (31), because summing these 5 equations and using the previous ones (24), (26), (25) gives a tautology:

\[
\sum_{(i,j,k,l,m)\in \mathcal{Q}_{p,q}, v \in \{0,1\}} ((i + k) \pi_{i,j,k,l,m,1} + (l + m) \pi_{i,j,k,l,m,1} + (i + k) \pi_{i,j,k,l,m,0} + (l + m) \pi_{i,j,k,l,m,0}) + H = 3c
\]

\[
\sum_{(i,j,k,l,m)\in \mathcal{Q}_{p,q}, v \in \{0,1\}} ((i + k) \pi_{i,j,k,l,m,1} + (l + m) \pi_{i,j,k,l,m,1}) + H = 3c
\]

\[
\sum_{(p,q)\in \mathcal{L}, (i,j,k,l,m)\in \mathcal{Q}_{p,q}, v \in \{0,1\}} p \pi_{i,j,k,l,m,1} + q \pi_{i,j,k,l,m,1} + p \pi_{i,j,k,l,m,0} + q \pi_{i,j,k,l,m,0} + H = 3c
\]
\[
\sum_{(p,q) \in \mathcal{L}} (p + q) \left( \sum_{(i,j,k,l,m) \in Q_{p,q}} \pi_{i,j,k,l,m,1} + \sum_{(i,j,k,l,m) \in Q_{q,p}} \pi_{i,j,k,l,m,0} \right) + H = 3c
\]

which was a requirement we made on \( (d_{p,q}) \).
Thus we get rid of constraint \([\text{31}]\) and there remain 7 constraints.

### A.2 Definition of the Lagrangian

\[
A = \tau \ln 2 + H \ln H - H_1 \ln \left( \frac{H_1}{e} \right) - H_2 \ln \left( \frac{H_2}{e} \right) - H_3 \ln \left( \frac{H_3}{e} \right) - H
\]

\[+ \sum_{(p,q) \in \mathcal{L}} d_{p,q} \ln d_{p,q} + \sum_{(p,q) \in \mathcal{L}} \pi_{i,j,k,l,m,v} \ln \left( \omega_{i,j,k,l,m,v} e^{(i+j+k)(l+m)} \pi_{i,j,k,l,m,v} \right) - 1 \]

\[-2c \ln 3 + 2c \ln \left( \frac{2 \beta_1}{e} \right) + 2c \ln \left( \frac{2 \beta_2}{e} \right) + 2c \ln \left( \frac{3 \beta_1}{e} \right) + 2c \]

\[+ (2 \ln b) (\beta_1 + \beta_2 + \beta_3 - 1) \]

\[+ \sum_{(p,q) \in \mathcal{L}} \ln r_{p,q} \left( \sum_{(i,j,k,l,m) \in Q_{p,q}} \pi_{i,j,k,l,m,1} + \sum_{(i,j,k,l,m) \in Q_{q,p}} \pi_{i,j,k,l,m,0} - d_{p,q} \right) \]

\[+ (\ln \beta_1) \left( H_1 + H_2 + H_3 - \sum_{(p,q) \in \mathcal{H}} (p + q) d_{p,q} \right) \]

\[+ (2 \ln x_1) \left( \sum_{(p,q) \in \mathcal{L}} i \pi_{i,j,k,l,m,v} + H_1 - \beta_1 c \right) + (\ln x_2) \left( \sum_{(p,q) \in \mathcal{L}} j \pi_{i,j,k,l,m,v} + H_2 - 2 \beta_2 c \right) \]

\[+ (\ln y_1) \left( \sum_{(p,q) \in \mathcal{L}} l \pi_{i,j,k,l,m,v} - 2 \beta_1 c \right) + (2 \ln y_2) \left( \sum_{(p,q) \in \mathcal{L}} m \pi_{i,j,k,l,m,v} - \beta_2 c \right) \]

### A.3 Derivatives with Respect to \( \pi_{i,j,k,l,m,v} \)

\[
\frac{\partial A}{\partial \pi_{i,j,k,l,m,1}} = \ln \omega_{i,j,k,l,m,1} + \ln \left( \frac{i}{i,j,k}(l+m) \right) - \ln \pi_{i,j,k,l,m,1} + \ln r_{i+j+k,l+m}
\]

\[+ 2i \ln x_1 + j \ln x_2 + l \ln y_1 + 2m \ln y_2 \]

\[
\frac{\partial A}{\partial \pi_{i,j,k,l,m,0}} = \ln \omega_{i,j,k,l,m,0} + \ln \left( \frac{i+j+k}{i,j,k}(l+m) \right) - \ln \pi_{i,j,k,l,m,0} + \ln r_{l+m,i+j+k}
\]

\[+ 2i \ln x_1 + j \ln x_2 + l \ln y_1 + 2m \ln y_2 \]

\[
\pi_{i,j,k,l,m,1} = \omega_{i,j,k,l,m,1} \left( \frac{i+j+k}{i,j,k}(l+m) \right) r_{i+j+k,l+m} x_{1}^{2i} y_{2}^{2m}
\]

\[
\pi_{i,j,k,l,m,0} = \omega_{i,j,k,l,m,0} \left( \frac{i+j+k}{i,j,k}(l+m) \right) r_{l+m,i+j+k} x_{1}^{2i} y_{2}^{2m}
\]
The $r_{p,q}$ contraints become:

$$
\sum_{(i,j,k,l,m) \in Q_{p,q}} \omega_{i,j,k,l,m,1} (i + j + k) \binom{l + m}{l,m} r_{i+j+k,l+m} x_{i,j,k,l,m}^{2i+j} y_{1}^{2m} + \sum_{(i,j,k,l,m) \in Q_{q,p}} \omega_{i,j,k,l,m,0} (i + j + k) \binom{l + m}{l,m} r_{i+m,i+j+k} x_{i,j,k,l,m}^{2i+j} y_{1}^{2m} = d_{p,q}
$$

Let us introduce

$$
A_{p,q} = \sum_{(i,j,k,l,m) \in Q_{p,q}} \omega_{i,j,k,l,m,1} (i,j,k,l,m) \binom{l + m}{l,m} d_{i,j+k,l+m} x_{i,j,k,l,m}^{2i+j} y_{1}^{2m} + \sum_{(i,j,k,l,m) \in Q_{q,p}} \omega_{i,j,k,l,m,0} (i,j,k,l,m) \binom{l + m}{l,m} d_{i+m,i+j+k} x_{i,j,k,l,m}^{2i+j} y_{1}^{2m}
$$

We have:

$$
r_{p,q} A_{p,q} = d_{p,q}
$$

$$
r_{p,q} = \frac{d_{p,q}}{A_{p,q}}
$$

Thus

$$
\pi_{i,j,k,l,m,1} = \omega_{i,j,k,l,m,1} (i,j,k,l,m) \binom{l + m}{l,m} d_{i+j+k,l+m} x_{i,j,k,l,m}^{2i+j} y_{1}^{2m} A_{i+j+k,l+m}
$$

$$
\pi_{i,j,k,l,m,0} = \omega_{i,j,k,l,m,0} (i,j,k,l,m) \binom{l + m}{l,m} d_{i+m,i+j+k} x_{i,j,k,l,m}^{2i+j} y_{1}^{2m} A_{i+m,i+j+k}
$$

### A.4 Derivatives with Respect to $\beta_t$

$$
\frac{\partial A}{\partial \beta_1} = 2c \ln 2 + 2c \ln \beta_1 + 2c \ln b - 2c \ln x_1 - 2c \ln y_1
$$

$$
\frac{\partial A}{\partial \beta_2} = 2c \ln 2 + 2c \ln \beta_2 + 2c \ln b - 2c \ln x_2 - 2c \ln y_2
$$

$$
\frac{\partial A}{\partial \beta_3} = 2c \ln 3 + 2c \ln \beta_3 + 2c \ln b
$$

$$
\beta_1 = \frac{x_1 y_1}{2b}
$$

$$
\beta_2 = \frac{x_2 y_2}{2b}
$$

$$
\beta_3 = \frac{1}{3b}
$$

The $b$ constraint becomes:

$$
b = \frac{x_1 y_1}{2} + \frac{x_2 y_2}{2} + \frac{1}{3}
$$

### A.5 Derivatives with Respect to $H_t$

$$
\frac{\partial A}{\partial H_1} = -\ln H_1 + \ln h + 2 \ln x_1
$$

$$
\frac{\partial A}{\partial H_2} = -\ln H_2 + \ln h + \ln x_2
$$

$$
\frac{\partial A}{\partial H_3} = -\ln H_3 + \ln h
$$
A.6 Further Simplifications

1st Moment:

Thus:

The \( h \) constraint becomes then:

\[
H(x_1^2 + x_2 + 1) = H
\]

\[
h = \frac{H}{x_1^2 + x_2 + 1}
\]

Thus:

\[
H_1 = \frac{Hx_1^2}{x_1^2 + x_2 + 1}
\]

\[
H_2 = \frac{Hx_2}{x_1^2 + x_2 + 1}
\]

\[
H_3 = \frac{H}{x_1^2 + x_2 + 1}
\]
\[ F = 2^T \left( \frac{H}{h} \right)^N \prod_{(p,q) \in L} \left( \frac{A_{p,q}}{d_{p,q}} \right)^{d_{p,q}} \delta^{2c} \left( x_1^{2\beta_1 c} x_2^{2\beta_2 c} y_1^{2\beta_1 c} y_2^{2\beta_2 c} \right)^{2c} \]

\[ F = 2^T \left( x_1^2 + x_2 + 1 \right)^N \prod_{(p,q) \in L} \left( \frac{A_{p,q}}{d_{p,q}} \right)^{d_{p,q}} \left( \frac{3x_1^2 y_1}{2} + \frac{3x_2^2 y_2}{2} + 1 \right)^{2c} \]

Remaining constraints:

\[ \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,j,k,l,m) \in Q_{p,q}} i \left( \frac{p}{i,j,k} \right) \left( \frac{q}{l,m} \right) x_1^{2\beta_1 c} x_2^{2\beta_2 c} y_1^{2\beta_1 c} y_2^{2\beta_2 c} \omega_{i,j,k,l,m} = \frac{x_1 y_1 c}{\frac{x_1^2}{2} + x_2 + 1} \]

\[ + \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,j,k,l,m) \in Q_{p,q}} j \left( \frac{p}{i,j,k} \right) \left( \frac{q}{l,m} \right) x_1^{2\beta_1 c} x_2^{2\beta_2 c} y_1^{2\beta_1 c} y_2^{2\beta_2 c} \omega_{i,j,k,l,m} = \frac{x_2 y_2 c}{\frac{x_1^2}{2} + x_2 + 1} \]

\[ + \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,j,k,l,m) \in Q_{p,q}} l \left( \frac{p}{i,j,k} \right) \left( \frac{q}{l,m} \right) x_1^{2\beta_1 c} x_2^{2\beta_2 c} y_1^{2\beta_1 c} y_2^{2\beta_2 c} \omega_{i,j,k,l,m} = \frac{x_1 y_1 c}{\frac{x_1^2}{2} + x_2 + 1} \]

\[ + \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,j,k,l,m) \in Q_{p,q}} m \left( \frac{p}{i,j,k} \right) \left( \frac{q}{l,m} \right) x_1^{2\beta_1 c} x_2^{2\beta_2 c} y_1^{2\beta_1 c} y_2^{2\beta_2 c} \omega_{i,j,k,l,m} = \frac{x_2 y_2 c}{\frac{x_1^2}{2} + x_2 + 1} \]

\[ \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \frac{x_1}{2} \frac{\partial A_{p,q}}{\partial x_1} + \frac{H x_1^2}{x_1^2 + x_2 + 1} = \frac{x_1 y_1 c}{\frac{x_1^2}{2} + x_2 + 1} \]

\[ \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \frac{x_2}{2} \frac{\partial A_{p,q}}{\partial x_2} + \frac{H x_2^2}{x_2^2 + x_2 + 1} = \frac{x_2 y_2 c}{\frac{x_1^2}{2} + x_2 + 1} \]

\[ \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \frac{y_1}{2} \frac{\partial A_{p,q}}{\partial y_1} = \frac{x_1 y_1 c}{\frac{x_1^2}{2} + x_2 + 1} \]

\[ \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \frac{y_2}{2} \frac{\partial A_{p,q}}{\partial y_2} = \frac{x_2 y_2 c}{\frac{x_1^2}{2} + x_2 + 1} \]

Then we introduce \( Z = \prod_{(p,q) \in L} A_{p,q} \) and \( Y = \ln Z \):

\[ \frac{\partial Y}{\partial x_1} = \frac{2H x_1}{x_1^2 + x_2 + 1} = \frac{y_1 c}{\frac{x_1^2}{2} + x_2 + 1} \]

\[ \frac{\partial Y}{\partial x_2} = \frac{H}{x_1^2 + x_2 + 1} = \frac{y_2 c}{\frac{x_1^2}{2} + x_2 + 1} \]

\[ \frac{\partial Y}{\partial y_1} = \frac{x_1 c}{\frac{x_1^2}{2} + x_2 + 1} \]

\[ \frac{\partial Y}{\partial y_2} = \frac{x_2 c}{\frac{x_1^2}{2} + x_2 + 1} \]

To solve these equations we used Mathematica™. The bound we obtained for \( c \) are summed up in table G.
Table 2. Summary of results obtained by Lagrange’s method.

| model                                                                 | standard | balanced signs | balanced occurrences | balanced signs and occurrences |
|----------------------------------------------------------------------|----------|----------------|----------------------|---------------------------------|
| our method \((\alpha p_{x,t} + p_{y,m,v}) > (0,0)\)                 | 4.500    | 3.509          | 4.623                | 3.546                           |
| \(x_1\)                                                             | 2.00     | 1.01           | 2.01                 | 1.01                            |
| \(x_2\)                                                             | 2.06625  | 3.09005        | 2.08256              | 3.38506                         |
| \(y_1\)                                                             | 2.18256  | 3.27457        | 2.19038              | 3.51076                         |
| \(y_2\)                                                             | 1.01253  | 1.02742        | 1.01221              | 1.045                           |
| \(\beta_1\)                                                         | 0.44373  | 0.55749        | 0.445306             | 0.568436                        |
| \(\beta_2\)                                                         | 0.421847 | 0.365723       | 0.421418             | 0.363128                        |
| \(\beta_3\)                                                         | 0.134422 | 0.0767974      | 0.133276             | 0.0684362                       |

B Inspection of the Boundary of \(\mathcal{P}\)

The boundary of \(\mathcal{P}\) is reached when one of the variables is at 0. We want to be sure that \(F\) cannot be maximized by such a configuration. Remember that

\[
\ln F = \tau \ln 2 + H \ln H - H_1 \ln \left(\frac{H_1}{e}\right) - H_2 \ln \left(\frac{H_2}{e}\right) - H_3 \ln \left(\frac{H_3}{e}\right) - H \\
+ \sum_{(p,q)\in \mathcal{E}} d_{p,q} \ln d_{p,q} + \sum_{(i,j,k,l,m,v)\in \mathcal{Q}_{p,q}} \pi_{i,j,k,l,m,v} \ln \left(\omega_{i,j,k,l,m,v}(\frac{i+j+k}{i,j,k,l,m,v} + 1)\right) + 1 \\
-2c\ln 3 + 2c\beta_1 \ln \left(\frac{2\beta_1}{e}\right) + 2c\beta_2 \ln \left(\frac{2\beta_2}{e}\right) + 2c\beta_3 \ln \left(\frac{3\beta_3}{e}\right) + 2c
\]

If we increase an \(H_t\) or a \(\pi_{i,j,k,l,m,v}\) from 0 to a small \(\xi > 0\) and we change any other non zero variables, then the variation of \(\ln F\) is \(f = -\xi \ln \xi + \Theta(\xi)\) is such that \(\frac{d}{d\xi} = -\ln \xi + \Theta(1) \rightarrow +\infty\), so \(\ln F\) must increase; but what if we increase a \(\beta_i\) from 0 to a \(\xi > 0\)? Then \(\frac{d}{d\xi} = +\ln \xi + \Theta(1) \rightarrow -\infty\). Thus the problem at the boundary of \(\mathcal{P}\) comes from the \(\beta_i\). The technique will be, as in [1211], to make a small move in a well chosen direction in order to circumvent the negative side-effect of increasing a \(\beta_i\) which is at 0. Such a direction will be referred to as an increasing direction. However we must ensure that such a direction is indeed in the polytope \(\mathcal{P}\). Note that in case we find the direction by pointing towards another point in \(\mathcal{P}\), this property results from the convexity of \(\mathcal{P}\).

We used Mathematica™ to minimize and maximize \(\beta_1\) under the above constraints in each model and our corresponding weighting scheme; the precise bounds we obtained for \(\beta_1\) in each model are summed up in table [4]. Noteworthy is the fact that \(\beta_1\) can be neither 0 nor 1 (thus we can have neither \(\beta_1 = 0\) nor \(\beta_2 = \beta_3 = 0\).

| model                                                                  | standard | balanced signs | balanced occurrences | balanced signs and occurrences |
|----------------------------------------------------------------------|----------|----------------|----------------------|---------------------------------|
| our method \((\alpha p_{x,t} + p_{y,m,v}) > (0,0)\)                 | 4.500    | 3.509          | 4.623                | 3.546                           |
| \(\beta_1\)                                                         | 0.1772   | 0.912          | 0.428                | 0.786                           |
| \(\beta_2\)                                                         | 0.1828   | 0.9009         | 0.5206               | 0.755                           |
| \(\beta_3\)                                                         | 0.409    | 0.2501         | 0.4354               | 0.2501                          |

Table 3. Summary of bounds on \(\beta_t\).
1. case where \( \beta_2 = 0 \): then \( H_2 = 0 \) and \( \pi_{i,j,k,l,m,v} = 0 \) unless \( j = m = 0 \); we call these variables forced as did [11]; moreover in the models where there are no heavy variables we consider variables \( H_q \) to be forced to 0 as well.

- subcase where there is an unforced variable at zero: we find a feasible point where \( \beta \) variables are non zero. Then a move towards this point gives an increasing direction (because \( \beta_1 > 0 \) and \( \beta_3 > 0 \)). To find such a point, we use the Lagrange multipliers method, as follows:

* Definition of the lagrangian

\[
A = \tau \ln 2 + H \ln H - H_1 \ln \left( \frac{H_1}{e} \right) - H_3 \ln \left( \frac{H_3}{e} \right) - H
\]

\[
+ \sum_{(p,q) \in \mathcal{L}} d_{p,q} \ln d_{p,q} + \sum_{(i,o,k,l,0) \in Q_{p,q}, v \in \{0,1\}} \pi_{i,0,k,l,0,v} \ln \left( \omega_{i,0,k,l,0,v} \frac{e^{(i+k)}}{\pi_{i,0,k,l,0,v}} \right) + 1
\]

\[
- 2c \ln 3 + 2c \beta_1 \ln \left( \frac{2 \beta_1}{e} \right) + 2c \beta_3 \ln \left( \frac{3 \beta_3}{e} \right) + 2c
\]

\[
+ (2c \ln b)(\beta_1 + \beta_3 - 1)
\]

\[
+ \sum_{(p,q) \in \mathcal{L}} (\ln r_{p,q}) \left( \sum_{(i,o,k,l,0) \in Q_{p,q}} \pi_{i,j,k,l,m,1} + \sum_{(i,o,k,l,0) \in Q_{q,p}} \pi_{i,j,k,l,m,0} - d_{p,q} \right)
\]

\[
+ (\ln h)(H_1 + H_3 - H)
\]

\[
+ (2 \ln x_1) \left( \sum_{(p,q) \in \mathcal{L}} (\ln \pi_{i,0,k,l,0,v} + H_1 - \beta_1 c) \right) + (\ln y_1) \left( \sum_{(p,q) \in \mathcal{L}} (\ln \pi_{i,0,k,l,0,v} - 2 \beta_1 c) \right)
\]

* Derivatives with respect to \( \pi_{i,0,k,l,0,v} \)

\[
\frac{\partial A}{\partial \pi_{i,0,k,l,0,1}} = \ln \omega_{i,0,k,l,0,1} + \ln \left( \frac{i + k}{i, k} \right) - \ln \pi_{i,0,k,l,0,v} + \ln r_{i+k,l} + 2 \ln x_1 + l \ln y_1
\]

\[
\frac{\partial A}{\partial \pi_{i,0,k,l,0,0}} = \ln \omega_{i,0,k,l,0,0} + \ln \left( \frac{i + k}{i, k} \right) - \ln \pi_{i,0,k,l,0,v} + \ln r_{i+k,l} + 2 \ln x_1 + l \ln y_1
\]

\[
\pi_{i,0,k,l,0,1} = \omega_{i,0,k,l,0,1} \left( \frac{i + k}{i, k} \right) r_{i+k,l} x_1^2 y_1^l
\]

\[
\pi_{i,0,k,l,0,0} = \omega_{i,0,k,l,0,0} \left( \frac{i + k}{i, k} \right) r_{i+k,l} x_1^2 y_1^l
\]

The \( r_{p,q} \) contraints become:

\[
\sum_{(i,o,k,q,0) \in \mathcal{Q}_{p,q}} \omega_{i,0,k,q,0,1} \left( \frac{i + k}{i, k} \right) r_{i+k,q,0,1} x_1^2 y_1^q = d_{p,q}
\]

\[
+ \sum_{(i,o,k,p,0) \in \mathcal{Q}_{q,p}} \omega_{i,0,k,p,0,0} \left( \frac{i + k}{i, k} \right) r_{i+k,p,0,0} x_1^2 y_1^p = d_{p,q}
\]

Let us introduce \( A_{p,q} = \sum_{(i,o,k,q,0) \in \mathcal{Q}_{p,q}} \omega_{i,0,k,q,0,1} \left( \frac{i + k}{i, k} \right) x_1^2 y_1^q + \sum_{(i,o,k,l,0) \in \mathcal{Q}_{q,p}} \omega_{i,0,k,p,0,0} \left( \frac{i + k}{i, k} \right) x_1^2 y_1^p \):

\[
r_{p,q} A_{p,q} = d_{p,q}
\]

\[
r_{p,q} = \frac{d_{p,q}}{A_{p,q}}
\]
Thus
\[
\pi_{i,0,k,l,0} = \omega_{i,0,k,l,0} \left( i + k \right) \frac{d_{i,k,l}}{A_{i,k,l}}_1 y_1^{2i}
\]
\[
\pi_{i,0,k,l,1} = \omega_{i,0,k,l,0} \left( i + k \right) \frac{d_{i,k,l}}{A_{i,k,l}}_1 y_1^{2i}
\]

- Derivatives with respect to $\beta_t$
  \[
  \frac{\partial A}{\partial \beta_1} = 2c \ln 2 + 2c \ln \beta_1 + 2c \ln b - 2c \ln x_1 - 2c \ln y_1
  \]
  \[
  \frac{\partial A}{\partial \beta_3} = 2c \ln 3 + 2c \ln \beta_3 + 2c \ln b
  \]
  \[
  \beta_1 = \frac{x_1 y_1}{2b}
  \]
  \[
  \beta_3 = \frac{1}{3b}
  \]
  The $b$ constraint becomes:
  \[
  \frac{x_1 y_1}{2b} + \frac{1}{3b} = 1
  \]
  \[
  b = \frac{x_1 y_1}{2} + \frac{1}{3}
  \]

- Derivatives with respect to $H_t$
  \[
  \frac{\partial A}{\partial H_1} = -\ln H_1 + \ln h + 2 \ln x_1
  \]
  \[
  \frac{\partial A}{\partial H_3} = -\ln H_3 + \ln h
  \]
  \[
  H_1 = h x_1^2
  \]
  \[
  H_3 = h
  \]
  The $h$ constraint becomes then:
  \[
  h \left( x_1^2 + 1 \right) = H
  \]
  \[
  h = \frac{H}{x_1^2 + 1}
  \]

- Remaining constraints:
  \[
  \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,k,q,0) \in Q_{p,q}} \left( i \left( p \right) \right) x_1^{2i} y_1^q \omega_{i,0,k,q,0,1}
  \]
  \[
  \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,k,p,0) \in Q_{p,q}} \left( q \left( i, k \right) \right) x_1^{2i} y_1^q \omega_{i,0,k,p,0,0} + \frac{H x_1^2}{x_1^2 + 1} = \frac{x_1 y_1 c}{2 \left( \frac{x_1 y_1}{2} + \frac{1}{3} \right)}
  \]
  \[
  \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,k,q,0) \in Q_{p,q}} \left( p \left( i, k \right) \right) x_1^{2i} y_1^q \omega_{i,0,k,q,0,1}
  \]
  \[
  + \sum_{(p,q) \in L} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,k,p,0) \in Q_{p,q}} \left( q \left( i, k \right) \right) x_1^{2i} y_1^q \omega_{i,0,k,p,0,0} = \frac{x_1 y_1 c}{2 \left( \frac{x_1 y_1}{2} + \frac{1}{3} \right)}
  \]
Then we introduce \( Z = \prod_{(p,q) \in \mathcal{C}} A_{p,q}^{d_{p,q}} \) and \( Y = \ln Z \):

\[
\frac{\partial Y}{\partial x_1} + \frac{2Hx_1}{x_1^2 + 1} = \frac{y_1c}{\left( \frac{x_1y_2}{2} + \frac{j}{3} \right)} \quad \frac{\partial Y}{\partial y_1} = \frac{x_1c}{\left( \frac{x_1y_2}{2} + \frac{j}{3} \right)}
\]

With Mathematica\( ^{\text{TM}} \) we found the following solutions (and the corresponding values of \( \ln F \)):

| \( p \) | \( q \) | \( c \) | \( x_1 \) | \( y_1 \) | \( \ln F \) |
|------|------|------|------|------|------|
| \( 1 \) | \( 1 \) | 4.500 | 0.997334 | 2.07123 | -2.463 |
| \( 2 \) | \( 2 \) | 3.500 | 0.96803 | 2.06284 | -1.78313 |

So all unforced variables are non zero.

- subcase where all unforced variables are non zero: we define a function \( f(\xi) \) representing the variation of \( \ln F \) under a small positive variation \( \xi \) in the following direction; remember that \( \omega_{i,j,k,l,m,v} = 1 \) as soon as \( i \geq 1 \) thus the corresponding variable \( \pi_{i,j,k,l,m,v} \) exists. Let us take some \( p \geq 3 \) and \( q \geq 2 \) such that \( d_{p,q} > 0 \). We make the following move:

\[
\begin{align*}
\beta_1 & \rightarrow \beta_1 - \frac{\xi}{c} \\
\beta_2 & \rightarrow \beta_2 + \frac{2\xi}{c} \\
\beta_3 & \rightarrow \beta_3 - \frac{\xi}{c} \\
\pi_{p-1,0,1,q,0,1} & \rightarrow \pi_{p-1,0,1,q,0,1} - 5\xi \\
\pi_{p-2,1,1,q,0,1} & \rightarrow \pi_{p-2,1,1,q,0,1} + \xi \\
\pi_{p-1,0,1,q-2,2,1} & \rightarrow \pi_{p-1,0,1,q-2,2,1} + \xi \\
\pi_{p-1,1,0,q,0,1} & \rightarrow \pi_{p-1,1,0,q,0,1} + 3\xi
\end{align*}
\]

so that all constraints remain satisfied; in fact we are performing a small move inside the polytope \( \mathcal{P} \) and we would like to show that along this direction \( \ln F \) is increasing. Note that \( \beta_2 = \pi_{p-2,1,1,q,0,1} = \pi_{p-1,0,1,q-2,2,1} = \pi_{p-1,1,0,q,0,1} = 0 \) and all other variables here are non zero, so we have:

\[
f(\xi) = 2c \left( \beta_1 - \frac{\xi}{c} \right) \ln \left( \frac{2}{c} \left( \beta_1 - \frac{\xi}{c} \right) \right) - 2c\beta_1 \ln \left( \frac{2}{c}\beta_1 \right) + 2c \left( \beta_2 + \frac{2\xi}{c} \right) \ln \left( \frac{2}{c} \left( \beta_2 + \frac{2\xi}{c} \right) \right) + 2c \left( \beta_3 - \frac{\xi}{c} \right) \ln \left( \frac{2}{c} \left( \beta_3 - \frac{\xi}{c} \right) \right) - 2c\beta_3 \ln \left( \frac{2}{c}\beta_3 \right) - (\pi_{p-1,0,1,q,0,1} - 5\xi) \ln (\pi_{p-1,0,1,q,0,1} - 5\xi) + \pi_{p-1,0,1,q,0,1} \ln \pi_{p-1,0,1,q,0,1} - (\pi_{p-2,1,1,q,0,1} + \xi) \ln (\pi_{p-2,1,1,q,0,1} + \xi) - (\pi_{p-1,0,1,q-2,2,1} + \xi) \ln (\pi_{p-1,0,1,q-2,2,1} + \xi) - (\pi_{p-1,1,0,q,0,1} + 3\xi) \ln (\pi_{p-1,1,0,q,0,1} + 3\xi) + \Theta(\xi)
\]
\[ f(\xi) = 2c \left( \beta_1 - \frac{\xi}{e} \right) \ln \left( \frac{2}{e} \left( \beta_1 - \frac{\xi}{e} \right) \right) - 2c\beta_1 \ln \left( \frac{2}{e} \beta_1 \right) + 4\xi \ln \left( 4\xi \right) + \frac{2c}{e}, \]
\[ + 2c \left( \beta_3 - \frac{\xi}{e} \right) \ln \left( \frac{3}{e} \left( \beta_3 - \frac{\xi}{e} \right) \right) - 2c\beta_3 \ln \left( \frac{3}{e} \beta_3 \right) - (\pi_{p-1,0,1,q,0,1} - 5\xi) \ln (\pi_{p-1,0,1,q,0,1} + \pi_{p-1,0,1,q,0,1} \ln \pi_{p-1,0,1,q,0,1} - 2\xi \ln \xi - 3\xi \ln (3\xi) + \Theta(\xi)) \]

and thus:
\[ \lim_{\xi \to 0} \frac{f(\xi)}{\xi} = \lim_{\xi \to 0} (-\ln \xi) + \Theta(1) \]

Since \( \lim_{\xi \to 0} \frac{f(\xi)}{\xi} = +\infty \), we have found an increasing direction.

2. case where \( \beta_3 = 0 \): then \( H_3 = 0 \) and \( \pi_{i,j,k,l,m,v} = 0 \) unless \( k = 0 \); again we call these variables \textit{forced}.

- subcase where there is an unforced variable at zero: we find a feasible point where \( \beta_3 = 0 \) and all unforced variables are non zero. Then a move towards this point gives an increasing direction (because \( \beta_1 > 0 \) and \( \beta_2 > 0 \)). To find such a point we use again the Lagrange multipliers method, as follows:

- **Definition of the lagrangian**

\[
A = \tau \ln 2 + H \ln H - H_1 \ln \left( \frac{H_1}{e} \right) - H_2 \ln \left( \frac{H_2}{e} \right) - H
\]
\[
+ \sum_{(p,q) \in L} d_{p,q} \ln d_{p,q} + \sum_{(p,q) \in L \atop (i,j,0,l,m,v) \in Q_{p,q} \atop v \in \{0,1\}} \pi_{i,j,0,l,m,v} \ln \left( \omega_{i,j,0,l,m,v} \right) + 1
\]
\[
- 2c \ln 3 + 2c\beta_1 \ln \left( \frac{\beta_1}{e} \right) + 2c\beta_2 \ln \left( \frac{\beta_2}{e} \right) + 2c
\]
\[
+ (2c \ln b) (\beta_1 + \beta_2 - 1)
\]
\[
+ \sum_{(p,q) \in L \atop (i,j,0,l,m) \in Q_{p,q} \atop v \in \{0,1\}} \pi_{i,j,0,l,m,1} + \sum_{(i,j,0,l,m) \in Q_{v,p}, v \in \{0,1\}} \pi_{i,j,0,l,m,0} - d_{p,q}
\]
\[
+ (\ln h) (H_1 + H_2 - H)
\]
\[
+ (2 \ln x_1) \left( \sum_{(p,q) \in L \atop (i,j,0,l,m) \in Q_{p,q} \atop v \in \{0,1\}} i \pi_{i,j,0,l,m,v} + H_1 - \beta_1 c \right)
\]
\[
+ (\ln x_2) \left( \sum_{(p,q) \in L \atop (i,j,0,l,m) \in Q_{p,q} \atop v \in \{0,1\}} j \pi_{i,j,0,l,m,v} + H_2 - 2\beta_2 c \right)
\]
\[
+ (\ln y_1) \left( \sum_{(p,q) \in L \atop (i,j,0,l,m) \in Q_{p,q} \atop v \in \{0,1\}} l \pi_{i,j,0,l,m,v} - 2\beta_1 c \right)
\]
\[
+ (2 \ln y_2) \left( \sum_{(p,q) \in L \atop (i,j,0,l,m) \in Q_{p,q} \atop v \in \{0,1\}} m \pi_{i,j,0,l,m,v} - \beta_2 c \right)
\]

- **Derivatives with respect to \( \pi_{i,j,0,l,m,v} \)**

\[
\frac{\partial A}{\partial \pi_{i,j,0,l,m,1}} = \ln \omega_{i,j,0,l,m,1} + \ln \left( \frac{i+j}{i,j} \right) \left( \frac{l+m}{l,m} \right) - \ln \pi_{i,j,0,l,m,v} + \ln r_{i+j,l+m}
\]
\[
+ 2i \ln x_1 + j \ln x_2 + l \ln y_1 + 2m \ln y_2
\]
\[
\frac{\partial A}{\partial \pi_{i,j,0,l,m,0}} = \ln \omega_{i,j,0,l,m,0} + \ln \left( \frac{i+j}{i,j} \right) \left( \frac{l+m}{l,m} \right) - \ln \pi_{i,j,0,l,m,v} + \ln r_{l+m,i+j}
\]
\[
+ 2i \ln x_1 + j \ln x_2 + l \ln y_1 + 2m \ln y_2
\]
\[
\begin{align*}
\pi_{i,j,0,l,m,1} &= \omega_{i,j,0,l,m,1} \left(\frac{i+j}{i,j} \right) \left(\frac{l+m}{l,m} \right) r_{i+j,l+m,x_1^2 y_1^2 y_2^2}^2 \\
\pi_{i,j,0,l,m,0} &= \omega_{i,j,0,l,m,0} \left(\frac{i+j}{i,j} \right) \left(\frac{l+m}{l,m} \right) r_{i+j,l+m,x_1^2 y_1^2 y_2^2}^2
\end{align*}
\]

The \(r_{p,q}\) constraints become:

\[
\sum_{(i,j,0,l,m) \in Q_{p,q}} \omega_{i,j,0,l,m,1} \left(\frac{i+j}{i,j} \right) \left(\frac{l+m}{l,m} \right) r_{i+j,l+m,x_1^2 y_1^2 y_2^2}^2 + \sum_{(i,j,0,l,m) \in Q_{q,p}} \omega_{i,j,0,l,m,0} \left(\frac{i+j}{i,j} \right) \left(\frac{l+m}{l,m} \right) r_{i+j,l+m,x_1^2 y_1^2 y_2^2}^2 = d_{p,q}
\]

Let us introduce

\[
A_{p,q} = \sum_{(i,j,0,l,m) \in Q_{p,q}} \omega_{i,j,0,l,m,1} \left(\frac{p}{i,j} \right) \left(\frac{q}{l,m} \right) x_1^2 x_2^2 y_1^2 y_2^2 + \sum_{(i,j,0,l,m) \in Q_{q,p}} \omega_{i,j,0,l,m,0} \left(\frac{q}{i,j} \right) \left(\frac{p}{l,m} \right) x_1^2 x_2^2 y_1^2 y_2^2
\]

We have:

\[
r_{p,q} A_{p,q} = d_{p,q}
\]

\[
r_{p,q} = \frac{d_{p,q}}{A_{p,q}}
\]

Thus

\[
\begin{align*}
\pi_{i,j,0,l,m,1} &= \omega_{i,j,0,l,m,1} \left(\frac{i+j}{i,j} \right) \left(\frac{l+m}{l,m} \right) \frac{d_{i+j,l+m}}{A_{i+j,l+m}} x_1^2 x_2^2 y_1^2 y_2^2 \\
\pi_{i,j,0,l,m,0} &= \omega_{i,j,0,l,m,0} \left(\frac{i+j}{i,j} \right) \left(\frac{l+m}{l,m} \right) \frac{d_{l+m,i+j}}{A_{l+m,i+j}} x_1^2 x_2^2 y_1^2 y_2^2
\end{align*}
\]

- Derivatives with respect to \(\beta_t\)

\[
\frac{\partial A}{\partial \beta_1} = 2c \ln 2 + 2c \ln \beta_1 + 2c \ln b - 2c \ln x_1 - 2c \ln y_1
\]

\[
\frac{\partial A}{\partial \beta_2} = 2c \ln 2 + 2c \ln \beta_2 + 2c \ln b - 2c \ln x_2 - 2c \ln y_2
\]

\[
\beta_1 = \frac{x_1 y_1}{2b}
\]

\[
\beta_2 = \frac{x_2 y_2}{2b}
\]

The \(b\) constraint becomes:

\[
\frac{x_1 y_1}{2b} + \frac{x_2 y_2}{2b} = 1
\]

\[
b = \frac{x_1 y_1}{2} + \frac{x_2 y_2}{2}
\]

- Derivatives with respect to \(H_t\)
With Mathematica

So all unforced variables are non zero.

Then we introduce

\[
\frac{\partial A}{\partial H_1} = -\ln H_1 + \ln h + 2 \ln x_1
\]

\[
\frac{\partial A}{\partial H_2} = -\ln H_2 + \ln h + \ln x_2
\]

\[
H_1 = hx_1^2
\]

\[
H_2 = hx_2
\]

The \( h \) constraint becomes then:

\[
h \left( x_1^2 + x_2 \right) = H
\]

\[
h = \frac{H}{x_1^2 + x_2}
\]

- Remaining constraints:

\[
\sum_{(p,q) \in \mathcal{L}} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,j,0,l,m) \in Q_{p,q}} i \left( \frac{p}{i,j} \right) \left( \frac{q}{l,m} \right) x_1^{2i} x_2^{2j} y_1^{2m} y_2^m \omega_{i,j,0,l,m,1}
\]

\[
+ \sum_{(p,q) \in \mathcal{L}} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,j,0,l,m) \in Q_{p,q}} j \left( \frac{p}{i,j} \right) \left( \frac{q}{l,m} \right) x_1^{2i} x_2^{2j} y_1^{2m} y_2^m \omega_{i,j,0,l,m,1}
\]

\[
+ \sum_{(p,q) \in \mathcal{L}} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,j,0,l,m) \in Q_{p,q}} l \left( \frac{p}{i,j} \right) \left( \frac{q}{l,m} \right) x_1^{2i} x_2^{2j} y_1^{2m} y_2^m \omega_{i,j,0,l,m,1}
\]

\[
+ \sum_{(p,q) \in \mathcal{L}} \frac{d_{p,q}}{A_{p,q}} \sum_{(i,j,0,l,m) \in Q_{p,q}} m \left( \frac{p}{i,j} \right) \left( \frac{q}{l,m} \right) x_1^{2i} x_2^{2j} y_1^{2m} y_2^m \omega_{i,j,0,l,m,1}
\]

Then we introduce \( Z = \prod_{(p,q) \in \mathcal{L}} A_{p,q}^{d_{p,q}} \) and \( Y = \ln Z \):

\[
\frac{\partial Y}{\partial x_1} + \frac{2Hx_1}{x_1^2 + x_2} = \frac{y_1c}{\left( \frac{x_1 y_1}{2} + \frac{x_2 y_2}{2} \right)}
\]

\[
\frac{\partial Y}{\partial x_2} + \frac{H}{x_1^2 + x_2} = \frac{y_2c}{\left( \frac{x_1 y_1}{2} + \frac{x_2 y_2}{2} \right)}
\]

\[
\frac{\partial Y}{\partial y_1} = \frac{x_1 c}{\left( \frac{x_1 y_1}{2} + \frac{x_2 y_2}{2} \right)}
\]

\[
\frac{\partial Y}{\partial y_2} = \frac{x_2 c}{\left( \frac{x_1 y_1}{2} + \frac{x_2 y_2}{2} \right)}
\]

With Mathematica\textsuperscript{TM} we found the following solutions (and the corresponding values of \( \ln F \)):

So all unforced variables are non zero.
balanced occurrences

| model | standard | balanced signs | balanced signs and occurrences |
|-------|----------|----------------|-------------------------------|
| c     | 4.500    | 3.509          | 4.623                         |
| x₁    | 0.512382 | 0.473066       | 0.493115                      | 0.494614 |
| x₂    | 0.546014 | 0.489687       | 0.501307                      | 0.494614 |
| y₁    | 0.583465 | 0.520769       | 0.531045                      | 0.494614 |
| y₂    | 0.529328 | 0.513117       | 0.505216                      | 0.494614 |
| ln P  | −0.682149| −0.375917      | −0.695819                     | −0.33427 |

Table 5. Interior point when \( \beta_3 = 0 \).

| model | standard | balanced signs | balanced signs and occurrences |
|-------|----------|----------------|-------------------------------|
| c     | 4.500    | 3.509          | 4.623                         |
| x₁    | 0.512382 | 0.473066       | 0.493115                      | 0.494614 |
| x₂    | 0.546014 | 0.489687       | 0.501307                      | 0.494614 |
| y₁    | 0.583465 | 0.520769       | 0.531045                      | 0.494614 |
| y₂    | 0.529328 | 0.513117       | 0.505216                      | 0.494614 |
| ln P  | −0.682149| −0.375917      | −0.695819                     | −0.33427 |

− subcase where all unforced variables are non zero: we define a function \( f(\xi) \) representing the variation of \( \ln F \) under a small positive variation \( \xi \) in the following direction; remember that \( \omega_{i,j,k,l,m,v} = 1 \) as soon as \( i \geq 1 \) thus the corresponding variable \( \pi_{i,j,k,l,m,v} \) exists. Let us take some \( p \geq 3 \) and \( q \geq 2 \) such that \( d_{p,q} > 0 \). We make the following move:

\[
\begin{align*}
\beta_1 & \rightarrow \beta_1 + \frac{\xi}{c} \\
\beta_2 & \rightarrow \beta_2 - \frac{2\xi}{c} \\
\beta_3 & \rightarrow \beta_3 + \frac{\xi}{c} \\
\pi_{p-2,2,0,q-1,1,1} & \rightarrow \pi_{p-2,2,0,q-1,1,1} - 3\xi \\
\pi_{p-1,0,1,q-1,1,1} & \rightarrow \pi_{p-1,0,1,q-1,1,1} + \xi \\
\pi_{p-2,1,1,q,0,1} & \rightarrow \pi_{p-2,1,1,q,0,1} + 2\xi
\end{align*}
\]

so that all constraints remain satisfied; in fact we are performing a small move inside the polytope \( \mathcal{P} \) and we would like to show that along this direction \( \ln F \) is increasing. Note that \( \beta_3 = \pi_{p-1,0,1,q-1,1,1} = \pi_{p-2,1,1,q,0,1} = 0 \) and all other variables here are non zero, so we have:

\[
\begin{align*}
f(\xi) &= 2c \left( \beta_1 + \frac{\xi}{c} \right) \ln \left( \frac{2}{e} \left( \beta_1 + \frac{\xi}{c} \right) \right) - 2c\beta_1 \ln \left( \frac{2}{e} \beta_1 \right) \\
&\quad + 2c \left( \beta_2 - \frac{2\xi}{c} \right) \ln \left( \frac{2}{e} \left( \beta_2 - \frac{2\xi}{c} \right) \right) - 2c\beta_2 \ln \left( \frac{2}{e} \beta_2 \right) \\
&\quad + 2c \left( \beta_3 + \frac{\xi}{c} \right) \ln \left( \frac{3}{e} \left( \beta_3 + \frac{\xi}{c} \right) \right) \\
&\quad - (\pi_{p-2,2,0,q-1,1,1} - 3\xi) \ln \left( \pi_{p-2,2,0,q-1,1,1} - 3\xi \right) + \pi_{p-2,2,0,q-1,1,1} \ln \pi_{p-2,2,0,q-1,1,1} \\
&\quad - (\pi_{p-1,0,1,q-1,1,1} + \xi) \ln \left( \pi_{p-1,0,1,q-1,1,1} + \xi \right) - (\pi_{p-2,1,1,q,0,1} + 2\xi) \ln \left( \pi_{p-2,1,1,q,0,1} + 2\xi \right) + \Theta(\xi) \\
\end{align*}
\]

\[
\begin{align*}
f(\xi) &= +2c \left( \beta_1 + \frac{\xi}{c} \right) \ln \left( \frac{2}{e} \left( \beta_1 + \frac{\xi}{c} \right) \right) - 2c\beta_1 \ln \left( \frac{2}{e} \beta_1 \right) \\
&\quad + 2c \left( \beta_2 - \frac{2\xi}{c} \right) \ln \left( \frac{2}{e} \left( \beta_2 - \frac{2\xi}{c} \right) \right) - 2c\beta_2 \ln \left( \frac{2}{e} \beta_2 \right) \\
&\quad + 2c \ln \left( \frac{3\xi}{ec} \right) \\
&\quad - (\pi_{p-2,2,0,q-1,1,1} - 3\xi) \ln \left( \pi_{p-2,2,0,q-1,1,1} - 3\xi \right) + \pi_{p-2,2,0,q-1,1,1} \ln \pi_{p-2,2,0,q-1,1,1} \\
&\quad - \xi \ln \xi + 2\xi \ln (2\xi) + \Theta(\xi)
\end{align*}
\]

and thus:

\[
\lim_{\xi \to 0} \frac{f(\xi)}{\xi} = \lim_{\xi \to 0} (-\ln \xi) + \Theta(1)
\]

Since \( \lim_{\xi \to 0} \frac{dF}{\xi} = +\infty \), we have found an increasing direction.

3. case where all \( \beta_i > 0 \); suppose there is another variable at zero; we move towards the general solution we found in appendix A, where all variables are non zero. Then again \( \lim_{\xi \to 0} \frac{f(\xi)}{\xi} = +\infty \); so this is an increasing direction.
C Inspection of the Interior of $\mathcal{P}$

As Equation noticed in their calculation, we can perform a sweep over some coordinates in order to check that the solution of the Lagrange multipliers problem is indeed a global maximum. Namely when we fix all $\beta_1$, $\beta_2$ (and $\beta_3 = 1 - \beta_1 - \beta_2$), the function $\ln F$ is strictly concave in the other variables. Let $\mathcal{P}_{\beta_1, \beta_2}$ the polytope where the remaining variables are allowed to move; remember that the function to maximize is:

\[
\ln F = \tau \ln 2 + H \ln H - H_1 \ln \left(\frac{H_1}{e}\right) - H_2 \ln \left(\frac{H_2}{e}\right) - H_3 \ln \left(\frac{H_3}{e}\right) - H
\]

\[
= \sum_{(p,q) \in \mathcal{L}} d_{p,q} \ln d_{p,q} + \sum_{(p,q) \in \mathcal{L}, (i,j,k,l,m) \in \mathcal{Q}_{p,q}} \pi_{i,j,k,l,m,v} \ln \left(\omega_{i,j,k,l,m,v} \frac{\sum_{i,j,k} (i+j+k)}{e^{\pi_{i,j,k,l,m,v}}} \right) + 1
\]

\[-2c \ln 3 + 2c \beta_1 \ln \left(\frac{2 \beta_1}{e}\right) + 2c \beta_2 \ln \left(\frac{2 \beta_2}{e}\right) + 2c \beta_3 \ln \left(\frac{2 \beta_3}{e}\right) + 2c
\]

If we increase an $H_i$ or a $\pi_{i,j,k,l,m,v}$ from 0 to a small $\xi > 0$ and we change any other non-zero variables, then the variation $f$ of $\ln F$: $f = -\xi \ln \xi + \Theta(\xi)$ is such that $\frac{f}{\xi} = -\ln \xi + \Theta(1) \to +\infty$, so $\ln F$ must increase; thus the function cannot maximize on the boundary of $\mathcal{P}_{\beta_1, \beta_2}$ and we can apply the Lagrange multiplier technique again.

But now by strict concavity of the objective function, we know that the solution we find corresponds to a global maximum.

- **Definition of the lagrangian**

\[
A = \tau \ln 2 + H \ln H - H_1 \ln \left(\frac{H_1}{e}\right) - H_2 \ln \left(\frac{H_2}{e}\right) - H_3 \ln \left(\frac{H_3}{e}\right) - H
\]

\[
+ \sum_{(p,q) \in \mathcal{L}} d_{p,q} \ln d_{p,q} + \sum_{(p,q) \in \mathcal{L}, (i,j,k,l,m) \in \mathcal{Q}_{p,q}} \pi_{i,j,k,l,m,v} \ln \left(\omega_{i,j,k,l,m,v} \frac{\sum_{i,j,k} (i+j+k)}{e^{\pi_{i,j,k,l,m,v}}} \right) + 1
\]

\[-2c \ln 3 + 2c \beta_1 \ln \left(\frac{2 \beta_1}{e}\right) + 2c \beta_2 \ln \left(\frac{2 \beta_2}{e}\right) + 2c \beta_3 \ln \left(\frac{2 \beta_3}{e}\right) + 2c
\]

\[
+ \sum_{(p,q) \in \mathcal{L}} (\ln r_{p,q}) \left( \sum_{(i,j,k,l,m) \in \mathcal{Q}_{p,q}} \pi_{i,j,k,l,m,1} + \sum_{(i,j,k,l,m) \in \mathcal{Q}_{q,p}} \pi_{i,j,k,l,m,0} - d_{p,q} \right)
\]

\[+ (\ln h) \left( H_1 + H_2 + H_3 - \sum_{(p,q) \in \mathcal{H}} (p+q) d_{p,q} \right)
\]

\[+ (2 \ln x_1) \left( \sum_{(p,q) \in \mathcal{L}, (i,j,k,l,m) \in \mathcal{Q}_{p,q}} i \pi_{i,j,k,l,m,v} + H_1 - \beta_1 c \right) + (\ln x_2) \left( \sum_{(p,q) \in \mathcal{L}, (i,j,k,l,m) \in \mathcal{Q}_{p,q}} j \pi_{i,j,k,l,m,v} + H_2 - 2 \beta_2 c \right)
\]

\[+ (\ln y_1) \left( \sum_{(p,q) \in \mathcal{L}, (i,j,k,l,m) \in \mathcal{Q}_{p,q}} l \pi_{i,j,k,l,m,v} - 2 \beta_1 c \right) + (2 \ln y_2) \left( \sum_{(p,q) \in \mathcal{L}, (i,j,k,l,m) \in \mathcal{Q}_{p,q}} m \pi_{i,j,k,l,m,v} - \beta_2 c \right)
\]

- **Derivatives with respect to $\pi_{i,j,k,l,m,v}$**
As in the general case we find that

\[ \pi_{i,j,k,l,m,1} = \omega_{i,j,k,l,m,1}(i + j + k)(l + m) \frac{d_{i+m,i+j+k}}{A_{i+m,i+j+k}} x_1 y_1 y_2 \]

\[ \pi_{i,j,k,l,m,0} = \omega_{i,j,k,l,m,0}(i + j + k)(l + m) \frac{d_{i+m,i+j+k}}{A_{i+m,i+j+k}} x_1 y_1 y_2 \]

- Derivatives with respect to \( H \)

As in the general case we find that

\[ H_1 = \frac{Hx_1^2}{x_1^2 + x_2 + 1} \]

\[ H_2 = \frac{Hx_2}{x_1^2 + x_2 + 1} \]

\[ H_3 = \frac{H}{x_1^2 + x_2 + 1} \]

- Remaining constraints:

\[
\begin{align*}
\frac{\partial Y}{\partial x_1} + \frac{2Hx_1}{x_1^2 + x_2 + 1} &= \frac{2\beta_1 c}{x_1} \\
\frac{\partial Y}{\partial x_2} + \frac{H}{x_1^2 + x_2 + 1} &= \frac{2\beta_2 c}{x_2} \\
\frac{\partial Y}{\partial y_1} &= \frac{2\beta_1 c}{y_1} \\
\frac{\partial Y}{\partial y_2} &= \frac{2\beta_2 c}{y_2}
\end{align*}
\]

- Objective function:

\[
F = 2^r \left( x_1^2 + x_2 + 1 \right)^H \prod_{(p,q) \in \mathcal{L}} d_{p,q}^{d_{p,q}} \prod_{(p,q) \in \mathcal{L}} \left( \omega_{i,j,k,l,m,v}(i + j + k)(l + m) \pi_{i,j,k,l,m,v} \right) \left( \frac{1}{3} \left( x_1 y_1 \right)^\beta_1 \left( x_2 y_2 \right)^\beta_2 \left( 3 \beta_3 \right)^\beta_3 \right)^2c
\]

\[
F = 2^r \left( x_1^2 + x_2 + 1 \right)^H \prod_{(p,q) \in \mathcal{L}} \left( A_{p,q}^{d_{p,q}} \right) \left( \frac{1}{3} \left( \frac{2\beta_1}{x_1 y_1} \right)^\beta_1 \left( \frac{2\beta_2}{x_2 y_2} \right)^\beta_2 \left( 3 \beta_3 \right)^\beta_3 \right)^2c
\]

So we made a sweep over \( \beta_1 \) and \( \beta_2 \) in the feasible region and plotted the maximum point given as the solution of these equations, which confirmed the fact that the solutions to the global Lagrange system are indeed global maxima.

**Table 6.** Summary of results obtained by Lagrange’s method.

| model | standard | balanced signs | balanced occurrences | balanced signs and occurrences |
|-------|----------|----------------|----------------------|-------------------------------|
| our method \((\alpha p_i, l + \rho_h, m, v) > (0, 0)\) | 4.500 | 3.509 | 4.623 | 3.546 |
| \( \beta_1 \) | 0.44373 | 0.557479 | 0.445396 | 0.568436 |
| \( \beta_2 \) | 0.421847 | 0.365723 | 0.421418 | 0.363128 |
| \( \beta_3 \) | 0.134422 | 0.0767747 | 0.133270 | 0.0684362 |
Fig. 3. Maximum of $\ln F$ for different values of $\beta_1$ and $\beta_2$ in the standard model at $c = 4.500$. Numerically we found that the maximum is at $\beta_1 \simeq 0.44313$ and $\beta_2 \simeq 0.421847$. 
Fig. 4. Maximum of $\ln F$ for different values of $\beta_1$ and $\beta_2$ in the model with balanced signs at $c = 3.509$. Numerically we found that the maximum is at $\beta_1 \simeq 0.557479$ and $\beta_2 \simeq 0.365723$. 
Fig. 5. Maximum of $\ln F$ for different values of $\beta_1$ and $\beta_2$ in the model with balanced occurrences at $c = 4.623$. Numerically we found that the maximum is at $\beta_1 \simeq 0.445306$ and $\beta_2 \simeq 0.421418$.

Fig. 6. Maximum of $\ln F$ for different values of $\beta_1$ in the model with balanced signs and occurrences at $c = 3.546$. In this particular model where each variable has as many positive occurrences as negative ones, true and false surfaces are equal: $\beta_1 + 2\beta_2 + 3\beta_3 = 2\beta_1 + \beta_2$, thus $\beta_2 = 1.5 - 2\beta_1$. Numerically we found that the maximum is at $\beta_1 \simeq 0.568436$ and $\beta_2 \simeq 0.363128$. 