Phase Uniqueness for the Mallows Measure on Permutations

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Abstract

For a positive number $q$ the Mallows measure on the symmetric group is the probability measure $P_{n,q}(\pi)$ proportional to $q^{-\text{inv}(\pi)}$ where $\text{inv}(\pi)$ equals the number of inversions: $\text{inv}(\pi)$ equals the number of pairs $i < j$ such that $\pi_i > \pi_j$. One may consider this as a mean-field model from statistical mechanics. The weak large deviation principle may replace the Gibbs variational principle for characterizing equilibrium measures. In this sense, we prove absence of phase transition, i.e., phase uniqueness.

1 Introduction

The Mallows measure on permutations is a non-uniform measure which may be motivated in various ways. It arises in non-parametric statistics [17]

$$\forall \pi \in S_n, \quad P_{n,q}(\pi) = Z_{n,q}^{-1} q^{\text{inv}(\pi)}, \quad \text{where} \quad \text{inv}(\pi) \overset{\text{def}}{=} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} 1_{(-\infty,0)}(\pi_j - \pi_i),$$

for some parameter $q \in (0, \infty)$.

A good recent review of several important examples of non-uniform measures is [21]. In addition, in that reference, Mukherjee considered thermodynamic limits, and he derived large deviation principles. That is the starting point for us.

The Mallows model has also been studied for other reasons. Diaconis and Ram showed a connection to the Hecke algebra [9]. The Mallows measure is a measure on permutations. But it is also closely related to the “blocking measure” which are invariant measures of the asymmetric exclusion process (ASEP). In fact the ASEP may be viewed as a projection of a biased card shuffling algorithm introduced by Diaconis and Ram. This was exploited by Benjamini, Berger, Hoffman and Mossel [5], using David Bruce Wilson’s height functions [32] to bound the mixing time for the card shuffling model, starting from the mixing time for the ASEP.

At a simpler level, one may try to use information about the ASEP invariant measures to gain information about the Mallows measure. The ASEP invariant measures are well-known. See, for example, Chapter VIII, Section 5 of [16]. This is a well-known approach, following Wilson [32].

In the present note, we consider the large deviation principle for a continuous version of the Mallows model, $\mu_{n,\beta}$ on $([0,1]^2)^n$ such that

$$d\mu_{n,\beta}((x_1, y_1), \ldots, (x_n, y_n)) = Z_n(\beta)^{-1} e^{-\beta H_n((x_1, y_1), \ldots, (x_n, y_n))},$$

$$H_n((x_1, y_1), \ldots, (x_n, y_n)) = \frac{1}{n-1} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} h((x_i, x_j), (y_i, y_j)) \quad (1)$$

$$h((x_1, y_1), (x_2, y_2)) = 1_{(-\infty,0)}((x_1 - x_2)(y_1 - y_2)).$$
Mukherjee found the large deviation rate function $\mathcal{I}_\beta : \mathcal{M}_{+1}([0,1]^2)$ for the empirical measure of $((x_1,y_1),\ldots,(x_n,y_n))$ on $[0,1]^2$

$$m^{(n)}_{((x_1,y_1),\ldots,(x_n,y_n))}(\bullet) = \frac{1}{n} \sum_{k=1}^n 1_\bullet((x_k,y_k)).$$

We start with his formula for the rate function, and we show that there is a unique optimizer. There is a straightforward connection between $\mu_{n,\beta}$ and $P_{n,q}$. Therefore, this gives a direct probabilistic method to find the weak limit law for $\mu_{n,\beta}$.

### 1.1 Discussion of proof technique and relation to known results

Following the approach suggested by the height functions, we consider the 4-square problem. Given $\theta \in (0,1)$ define $L_1(\theta) = [0,\theta]$ and $L_2(\theta) = (\theta,1]$. Given $\theta_1,\theta_2 \in (0,1)$ define $\Lambda_{ij}(\theta_1,\theta_2) = L_1(\theta_1) \times L_2(\theta_2)$ in $[0,1]^2$. Then, finally, given $t_{11},t_{12},t_{21},t_{22} \geq 0$ such that $t_{11} + t_{12} + t_{21} + t_{22} = 1$, define

$$W_{\theta_1,\theta_2}(t_{11},t_{12},t_{21},t_{22}) = \{ \nu \in \mathcal{M}_{+1}([0,1]^2) : \forall i,j \in \{1,2\}, \nu(\Lambda_{ij}(\theta_1,\theta_2)) = t_{ij} \}.$$ 

We give an explicit formula for $\mathcal{I}_\beta(W_{\theta_1,\theta_2}(t_{11},t_{12},t_{21},t_{22}))$. Intuitively, this is the simplest possible problem one can consider, starting from Mukherjee’s formula for $\mathcal{I}_\beta$. Moreover, for each $(\theta_1,\theta_2) \in (0,1)^2$, there is a unique choice of $t_{11}^*(\theta_1,\theta_2)$ maximizing this formula. Moreover,

$$R_\beta(\theta_1,\theta_2) = t_{11}^*(\theta_2,\theta_2),$$

defined for each $\theta_1,\theta_2 \in [0,1]$ (and extended continuously at the boundary) corresponds to the joint cumulative distribution function of a measure $\rho_\beta \in \mathcal{M}_{+1}([0,1]^2)$: $\rho_\beta([0,\theta_1] \times [0,\theta_2]) = R_\beta(\theta_1,\theta_2)$.

As a corollary, elementary results imply that $m^{(n)}_{((x_1,y_1),\ldots,(x_n,y_n))}$ converge in distribution to the non-random measure $\rho_\beta$, when for each $n$ we have $((x_1,y_1),\ldots,(x_n,y_n))$ distributed according to $\rho_\beta$. Then, due to the connection to the Mallows measure, the same result holds when applied to $m^{(n)}_{((x_1,y_1),\ldots,(x_n,y_n))}$ if, for each $n$ we define $x_k = k/n$ and $y_k = \pi_k/n$ for $k = 1,\ldots,n$, where we select a random permutation $\pi \in S_n$, distributed according to $P_{n,q_n}$, as long as $(q_1,q_2,\ldots)$ is a sequence such that $\lim_{n \to \infty} n(1-q_n) = \beta$. Note that $\beta \in \mathbb{R}$ is fixed. (For $\beta < 0$ this means that $q_n$ is slightly greater than 1 instead of less than 1, as it would be for $\beta > 0$.) So this result also gives a simpler, more direct proof of an old result from [27], which had previously been proved by an obscure method.

### 1.1.1 The Mallows model is a frustration free, mean-field model

The Hamiltonian in [11] is a mean-field Hamiltonian. Mean-field Hamiltonians have the property that considering a subsystem, the inverse-temperature $\beta$ needs to be rescaled because of the explicit dependence of $H_n$ on $n$. The consideration of a sub-system is sometimes known as the cavity method to find the weak limit law for $H_n$. Temperature renormalization means that if there is an explicit formula for the optimizing Hamiltonian on $[0,1]^2$ in the thermodynamic limit, then restricting attention to the sub-squares $\Lambda_{ij}(\theta_1,\theta_2)$, the restriction of the measure to these sets may be an optimizer for different choices of $\beta$, due to dilution on the sub-squares. (We will refer to the $\Lambda_{ij}(\theta_1,\theta_2)$’s as “sub-squares” even though they are rectangles.)

Of course, since the model is a mean-field model, there is an interaction between all particles in $[0,1]^2$, including between different sub-squares. But then there is a special symmetry of the model. In two dimensions, it is common to see conformally invariant models, which is the symmetry one finds from local rotational symmetry as well as dilution covariance. For the Mallows model, instead of $SO(2)$ symmetry the group which leaves the model invariant is the group of hyperbolic rotations $SO^+(1,1)$,
because one may rescale the two dimensions as long as the area remains fixed, in what is sometimes known as a “squeeze transformation.”

Moreover, one can factorize the degrees of freedom of a measure on a square by first considering its \( x \) and \( y \) marginals, and then considering the measure in the square with those marginals, which we call the “coupling measure.” In the Mallows model, the different sub-squares only interact through their marginals. We think of the \( x \) and \( y \) marginals as data living on the boundary of each square, and the coupling measure as data interior. Then the choice of the coupling measure in the interior of each subsquare is not affected by the choice of the boundary marginal measures. So for each sub-square, the coupling measure is an un-restricted optimizer of the rate function \( I_{\beta_{ij}} \), but at a diluted value of the inverse-temperature \( \beta_{ij} \). In this sense, the problem is “frustration free.” Moreover, this shifts the problem to determining the optimal choices of \( \beta_{11}, \beta_{12}, \beta_{21}, \beta_{22} \), which are in turn explicit functions of \( t_{11}, t_{12}, t_{21}, t_{22} \) due to the explicit formula for the pressure \( p(\beta) = \lim_{n \to \infty} n^{-1} \ln(Z_n(\beta)). \) So, in this sense the data \( R_\beta(\theta_1, \theta_2) \) may be deduced just from the general formula for the pressure \( p : \mathbb{R} \to \mathbb{R}. \)

### 1.1.2 Discrete symmetry and integrability

The main point of this paper is to give a simple proof of the uniqueness of the optimizer of \( I_\beta \), exploiting the symmetry just described in the continuum limit. But there is a related symmetry of the Mallows measure even for finite \( \beta \). For example, it is related to the Fisher-Yates-Knuth algorithm for perfectly simulating permutations. This is also related to the powerful bounds and approximations of Bhatnagar and Peled [7]. The symmetry may also be deduced from the “height-function” approach of Wilson [32], which was exploited by [5], relating the biased card-shuffling algorithm of Diaconis and Ram [9] to the Markov chain projection, which is the asymmetric exclusion process (ASEP). (Of course, in the present paper, we only consider invariant measures, not the actual stochastic dynamics, which is at least one level higher.)

The ASEP is also unitarily equivalent to the anisotropic Heisenberg model, known as the XXZ model, with the anisotropy parameter \( \Delta = (q + q^{-1})/2 \) with “kink soliton” boundary conditions. For more information on the XXZ model, see [24, 14]. This relation has a long history. See, for example, [8]. Also, for the relation between the Mallows model and the ASEP, an important reference point is to consider \( q = 1 \) where one sees the relation between the uniform measure on permutations and the SEP, where Liggett’s stirring process gives a graphical representation, which one may see in Chapter VIII of [16]. (This also leads to duality, and in this regard, one may also refer for the \( q \neq 1 \) case to [11].)

The most important points for us are 2: first the XXZ model is also frustration free [13]. This is important, because that implies certain properties such as a spectral gap [22] and certain correlation structure in the ground state [23]. Secondly, there are certain equations related to the thermodynamic limits of the XXZ model such as the Liouville PDE [25]. The Liouville PDE is known to have the boundary symmetry we mentioned in the last subsection, related to the frustration free property [15]. (Also, see Section 1.1 of the published version of Tao’s blog, year 3, [29], for an elementary derivation of the symmetries and solution of the Liouville equation.) In this paper we avoid the partial differential equations. But that is an alternative route which has been explored before [27].

We do not try to relate the frustration free property of the XXZ model to the frustration free property of the LDP optimization problem. But we will state, in an appendix, the discrete version of the frustration free property of the LDP.

### 1.1.3 Outline for the rest of the paper

A brief summary of our paper is this. It is known that the “pressure” for the Mallows model is explicitly calculable. More precisely, this is related to the \( q \)-Stirling’s formula, which is also related to the dilogarithm (although we will not discuss that). Because of the symmetry we can reduce the 4-square problem to the calculation of the pressure at diluted inverse-temperatures. This dilution, or “temperature renormalization,” arises in all mean-field problems (where the statistical mechanics setup
is deficient because the Hamiltonian itself explicitly depends on the system size). The important point
is that, due to the frustration free property, we may reduce the four-square problem of calculating
\( I_\beta(W_{n,\beta}(s)) \) to a 1-dimension optimization problem related to the density of points in each
subsquare, not the sub-permutations. Even though the weak LDP is not strictly convex, this particular
problem is. That explains why there is a unique minimizer in this problem, despite the lack of convexity.

Although the problem is related to interesting topics in quantum statistical mechanics, the main
results and tools, henceforth, will be purely probabilistic. We do not make any further reference to
quantum spin systems (such as the XXZ model) or partial differential equations (such as the Liouville
PDE). The approach may be viewed as purely probabilistic by probabilists.

2 Set-up

Let \( \lambda \) be the standard Lebesgue measure on \([0, 1] \). Let \( \lambda^{\otimes 2} \) denote the standard Lebesgue measure on
\([0, 1]^2 \), which is a Borel probability measure on \( \mathbb{R}^2 \).

For any \( n \in \{2, 3, \ldots \} \) and \( \beta \in \mathbb{R} \), let us define the measure \( \mu_{n,\beta} \in M_{+,1}([0, 1]^n) \) to be the
absolutely continuous measure with respect to \( (\lambda^{\otimes 2})^{\otimes n} \) such that

\[
\frac{d\mu_{n,\beta}}{d(\lambda^{\otimes 2})^{\otimes n}}((x_1, y_1), \ldots, (x_n, y_n)) = \frac{1}{Z_n(\beta)} \exp \left[ -\beta H_n((x_1, y_1), \ldots, (x_n, y_n)) \right],
\]

where

\[
H_n((x_1, y_1), \ldots, (x_n, y_n)) = \frac{1}{n-1} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} h((x_i, y_i), (x_j, y_j)),
\]

for

\[
h((x_i, y_i), (x_j, y_j)) = 1_{(-\infty, 0)}((x_i - x_j)(y_i - y_j)), \tag{2}
\]

and where \( Z_n(\beta) \) is a normalization constant

\[
Z_n(\beta) = \int_{([0, 1]^2)^n} \exp \left[ -\beta H_n((x_1, y_1), \ldots, (x_n, y_n)) \right] \prod_{i=1}^{n} d\lambda^{\otimes 2}(x_i, y_i).
\]

The main result of this paper relates to the weak large deviation principle for this sequence of measures.

Let us define the finite-volume approximation to the pressure

\[
p_n(\beta) = \frac{1}{n} \ln (Z_n(\beta)).
\]

2.1 Relation to the Mallows measure on permutations

Given a parameter \( q \in (0, \infty) \), the Mallows measure on permutations is a probability measure on the
symmetric group. More precisely, the probability mass function is \( P_{n,q}: S_n \to \mathbb{R} \), where, for a given
permutation \( \pi = (\pi_1, \ldots, \pi_n) \in S_n \), we define the inversion number and \( P_{n,q} \) as

\[
\text{inv}(\pi) = \# \{(i, j) : i < j \text{ and } \pi_i > \pi_j\} \quad \text{and} \quad P_{n,q}(\pi) = \frac{q^{\text{inv}(\pi)}}{Z_{n,q}}, \text{ where } Z_{n,q} = \sum_{\pi \in S_n} q^{\text{inv}(\pi)}. \tag{3}
\]

Diaconis and Ram showed that the measure \( \mu_{n,q} \) is related to the Iwahori-Hecke algebra \([3]\). One
related fact is the special formula for the normalization:

\[
Z_{n,q} = \prod_{k=1}^{n} \frac{1 - q^k}{1 - q}. \tag{4}
\]
The $q$-integers are defined as $[k]_q = \frac{1 - q^k}{1 - q}$ for each $k \in \mathbb{N} = \{1, 2, \ldots\}$. The $q$-factorial function is

$$[n]_q! = \prod_{k=1}^{n} [k]_q.$$  

Hence $Z_{n,q} = [n]_q!$.

The relation between the measure $\mu_{n,\beta}$ in $\mathcal{M}_{+1}(([0, 1]^2)^n)$ and the probability mass function $P_{n,q} : S_n \to [0, 1]$ is elucidated in the following lemma.

**Lemma 2.1** For each $n \in \mathbb{N}$ and each $\beta \in \mathbb{R}$,

$$p_n(\beta) = \frac{1}{n} \ln \left( \frac{[n]_q!}{n!} \right)_{q = \exp(-\beta/(n-1))}.$$

**Proof:** Since the Lebesgue measure is permutation invariant, we may symmetrize to calculate

$$e^{n p_n(\beta)} = \int_{([0,1]^2)^n} \frac{1}{n!} \sum_{\pi \in S_n} \exp \left[ -\beta H_n((x_{\pi_1}, y_1), \ldots, (x_{\pi_n}, y_n)) \right] \prod_{i=1}^{n} d\lambda(x_i) \prod_{j=1}^{n} d\lambda(y_j).$$

For Lebesgue-a.e. choice of $(x_1, y_1), \ldots, (x_n, y_n)$, we have

$$\sum_{\pi \in S_n} e^{-\beta H_n((x_{\pi_1}, y_1), \ldots, (x_{\pi_n}, y_n))} = \sum_{\pi \in S_n} \left( e^{-\beta/(n-1)} \right)^{\#(i,j) : i < j} \text{ and } (x_{\pi_i} - x_{\pi_j})(y_i - y_j) < 0.$$  

But this quantity is precisely $Z_{n,q}$ for $q = \exp(-\beta/(n-1))$. So the result follows from (4). $\square$

This proof demonstrates the relation between $\mu_{n,\beta}$ and $P_{n,q}$:

$$\frac{d\mu_{n,\beta}}{d(\lambda^\otimes 2)^\otimes n}((x_1, y_1), \ldots, (x_n, y_n)) = P_{n,q}(\pi), \text{ a.s.},$$

where $q = \exp(-\beta/(n-1))$ and $\pi = \pi((x_1, y_1), \ldots, (x_n, y_n))$ is the $(\lambda^\otimes 2)^\otimes n$-almost surely unique permutation such that

$$y_{\pi_i} \leq y_{\pi_j} \iff x_i \leq x_j.$$  

**Corollary 2.2** For each $\beta \in \mathbb{R}$

$$p(\beta) = \int_{0}^{1} \ln \left( \frac{1 - e^{-\beta x}}{\beta x} \right) \, dx.$$  

**Proof:** A more general and precise result is true, which we will mention immediately after this proof. This easy result follows from

$$\frac{1}{n} \ln \left( \frac{[n]_q!}{n!} \right)_{q = \exp(-\beta/n)} = \ln \left( \frac{1 - e^{-\beta/n}}{\beta n} \right) - \frac{1}{\beta} \sum_{k=1}^{n} \ln \left( \frac{1 - e^{-\beta x_{n,k}}}{\beta x_{n,k}} \right) \Delta x_n,$$

where

$$x_{n,k} = \frac{k}{n} \text{ and } \Delta x_n = \frac{1}{n}.$$  

The first term is easily seen to converge to 0. The second term converges to the Riemann-Stieltjes integral. Note that we rescaled $\beta$ by $(n-1)/n$ in this formula, but the limiting formula (involving the integral) is continuous in $\beta$. So this rescaling does not matter in the limit. $\square$

A more general and precise result than this one is true. It is called the $q$-Stirling formula. It was first proved by Moak [19]. We will discuss this further in the Outlook, Section § since it is related to the quantitative version of our main result, which may also be useful for the studying fluctuations, especially in the singular scaling of Bhatnagar and Peled from their paper [7].
3 Statement of main results

For two measures \( \mu, \nu \) on a Borel probability space on a compact metric space \( \mathcal{X} \), let us define the relative entropy in the usual way

\[
S(\mu | \nu) = \begin{cases} 
\infty & \text{if } \mu \not\ll \nu, \\
- \int_{\mathcal{X}} \ln \left( \frac{d\mu}{d\nu}(x) \right) d\mu(x) & \text{if } \mu \ll \nu.
\end{cases}
\]

Then the following is an important consequence of general principles.

**Proposition 3.1** Suppose \( \beta \in \mathbb{R} \) is any fixed number. For any Borel subset \( A \subseteq M_{+1}([0,1]^2) \),

\[
\limsup_{n \to \infty} \frac{1}{n} \ln \left[ \mu_{n,\beta} \left( \left\{ ((x_1, y_1), \ldots, (x_n, y_n)) \in ([0,1]^2)^n : \frac{1}{n} \sum_{k=1}^{n} \delta_{(x_k, y_k)} \in A \right\} \right) \right] \leq \sup_{\nu \in A} \left( S(\nu | \lambda^{\otimes 2}) - \beta \mathcal{E}(\nu) - p(\beta) \right),
\]

and

\[
\liminf_{n \to \infty} \frac{1}{n} \ln \left[ \mu_{n,\beta} \left( \left\{ ((x_1, y_1), \ldots, (x_n, y_n)) \in ([0,1]^2)^n : \frac{1}{n} \sum_{k=1}^{n} \delta_{(x_k, y_k)} \in A \right\} \right) \right] \geq \sup_{\nu \in A^\circ} \left( S(\nu | \lambda^{\otimes 2}) - \beta \mathcal{E}(\nu) - p(\beta) \right),
\]

where \( \mathcal{E}(\nu) \) is the expectation of the energy in a product state \( \nu \otimes \nu \):

\[
\mathcal{E}(\nu) = \frac{1}{2} \int_{[0,1]^2} \int_{[0,1]^2} h((x_1, y_1), (x_2, y_2)) \, d\nu(x_1, y_1) \, d\nu(x_2, y_2),
\]

where \( h \) is as defined before in (5).

**Proof:** This is a special case of a more general theorem proved by Mukherjee in [21]. We will discuss this more, momentarily. Mukherjee also noted that the result had previously been proved by Trashorras [30]. The key for both of them was to rephrase permutations in terms of empirical measures. For us, we are merely focusing on the measures: i.e., the particles in \([0,1]^2\). We did mention the relation to the Mallows measure on \( S_n \) in the last section. We will also return to this issue in the Section 8, outlook. But for now, we merely focus on the measures, not the permutations.

But in this context, one may also refer to a beautiful monograph [10]. Ellis considered large deviation principles for mean-field statistical mechanical models. Then this proposition follows exactly from Theorems II.7.1 and II.7.2 on pages 51-52 of Ellis’s monograph. This is the reference that we are most familiar with.

The large deviation rate function is

\[
\mathcal{I}_\beta(\nu) = - \left( S(\nu | \lambda^{\otimes 2}) - \beta \mathcal{E}(\nu) - p(\beta) \right).
\]

(6)

Part of Mukherjee’s, and Trashorras’s and Ellis’s proof of this proposition entails the fact that \( \mathcal{I}_\beta(\nu) \) has infimum equal to 0, as is needed on basic probabilistic grounds. The large deviation rate function \( \mathcal{I}_\beta \) is lower-semi continuous. Therefore, any infimizing sequence possesses a limit point which is a minimizer. In particular, there is at least one minimizer. Sometimes we will denote this existential minimizer as \( \tilde{\nu}_\beta^* \in M([0,1]^2) \).

Our main result is uniqueness of the minimizer. We state this in a sequence of steps. The main step involves the “four-square problem,” which we describe, shortly. First we would like to comment, briefly, on the papers of Mukherjee and Trashorras, which are critical for our own short article.
3.1 Short discussion

Let us quickly comment on one important aspect of Mukherjee’s paper [21], first. He not only calculated the large deviation principle for the Mallows model, but also for many other non-uniform measures on \( S_n \), of which the Mallows measure is just one. Mallows, himself, considered various measures on \( S_n \), and what we are calling the “Mallows measure,” here, is actually just the Mallows measure relative to a particular distance function, which is the minimum number of nearest neighbor transpositions (i.e., transpositions of the form \((i, i+1)\) for some \(i \in \{1, \ldots, n-1\}\), sometimes called Coxeter generators) needed to transform a given permutation into the identity permutation. Mukherjee has explained all of this. Trashorras has also considered many generalizations of the uniform measure on permutations, too. In this sense, they are the same. But Mukherjee also considered properties of the large deviation problems.

We would also like to mention that Trashorras was motivated by models of permutations arising from Adams, Bru, Dorlas and König relating to Bose condensation [1, 2, 3]. Another important reference is by Betz and Ueltschi [6]. Following a methodology of Ueltschi, they are also related to quantum spin systems [12]. But we have not found a direct connection to the Mallows model, yet, since the cycle type is more important than the inversion number for all of those applications. Nevertheless, there is a direct relation between the Mallows measure and the XXZ model that we mentioned in the introduction. We will return to this in the appendix.

There is a particular type of statistic, which one may call “linear statistics” for which Mukherjee proved uniqueness of optimizers of the LDP, in those cases. He considered measures \( Q_{n, \theta}(\pi) = \exp[\theta \sum_{i=1}^{n} f(i/n, \pi_i/n) - \ln(Z_n(\theta))] \) for a given continuous function \( f: [0,1]^2 \to \mathbb{R} \). In this case, the large deviation rate function is equal to the Kullback-Leibler divergence (which is the negative of the relative entropy, relative to the uniform measure) plus a linear functional of the measure. But the Kullback-Leibler divergence is strictly convex, and addition of a bounded linear functional does not affect this. One might expect that if there is uniqueness of the optimizer of the LDP for the Mallows measure that this follows from convexity. But, the rate functional \( I \) is not strictly convex on \( \mathcal{M}([0,1]^2) \). (Note that if we describe everything other than the Kullback-Leibler divergence as an effective Hamiltonian, then this is quadratic in the measure, somewhat like the logarithmic potential although less singular, not linear. Hence it need not preserve convexity.) We will give an example calculation to show this in the appendix. Nevertheless, there is a class of events that does lead to convexity for a 1-parameter family of sub-problems. That is how we proceed. This is the 4-square problem, which we now describe.

3.2 Four square problem

For any \( \theta \in (0,1) \), define subsets of \([0,1]\) as

\[
L_1(\theta) = [0, \theta], \quad L_2(\theta) = (\theta, 1].
\]

For each point \((\theta_1, \theta_2) \in (0,1)^2\), we define four rectangular subsets of \([0,1]^2\):

\[
\Lambda_{ij}(\theta_1, \theta_2) = L_i(\theta_1) \times L_j(\theta_2), \text{ for } i, j \in \{1, 2\}.
\]

Let \( \Sigma_4 = \{(t_{11}, t_{12}, t_{21}, t_{22}) \in [0,1]^4 : t_{11} + t_{12} + t_{21} + t_{22} = 1\} \). Given a point in \( M \), we define a Borel subset of \( \mathcal{M}_{4,1}([0,1]^2) \), as

\[
W_{\theta_1, \theta_2}(t_{11}, t_{12}, t_{21}, t_{22}) = \{ \nu \in \mathcal{M}_{4,1}([0,1]^2) : \forall i, j \in \{1, 2\}, \nu(\Lambda_{ij}(\theta_1, \theta_2) = t_{ij} \}
\]

What we call the “four-square problem” is to calculate the large deviation of this set. Solving this problem for all possible values \( \theta_1, \theta_2 \in (0,1)^2 \) and all \((t_{11}, t_{12}, t_{21}, t_{22}) \in \Sigma_4 \) will lead to all the minimizers of \( I_{\beta} \).
Theorem 3.1 For each \( \beta \in \mathbb{R} \), and each \((\theta_1, \theta_2) \in (0, 1)^2\), and each \((t_{11}, t_{12}, t_{21}, t_{22}) \in \Sigma_2\),
\[
\min \{ I_\beta(\nu) : \nu \in W_{\theta_1, \theta_2}(t_{11}, t_{12}, t_{21}, t_{22}) \} = \Phi_\beta(\theta_1, \theta_2; t_{11}, t_{12}, t_{21}, t_{22}),
\]
where
\[
\Phi_\beta(\theta_1, \theta_2; t_{11}, t_{12}, t_{21}, t_{22}) \overset{\text{def}}{=} p(\beta) + \sum_{i,j=1}^2 t_{ij} \ln \left( \frac{t_{ij}}{|X|_{ij}} \right) + \sum_{i,j=1}^2 t_{ij} p(\beta t_{ij})
- (t_{11} + t_{12}) p(\beta (t_{11} + t_{12})) - (t_{11} + t_{21}) p(\beta (t_{11} + t_{21}))
- (t_{12} + t_{22}) p(\beta (t_{12} + t_{22})) - (t_{21} + t_{22}) p(\beta (t_{21} + t_{22}))
+ \beta t_{12} t_{21}.
\]
Actually a subset of the four-square problems suffices to find the minimizers of \( I_\beta \).

Given a measure \( \nu \in \mathcal{M}_{\nu}([0,1]^2) \), let us define the \( x \) and \( y \) marginals as \( \nu_X, \nu_Y \in \mathcal{M}_{\nu}([0,1]) \) defined as
\[
\nu_X(\cdot) = \nu(\cdot \cap [0,1]) \quad \text{and} \quad \nu_Y(\cdot) = \nu([0,1] \cap \cdot).
\]

Theorem 3.2 For each \( \beta \in \mathbb{R} \), any \( \nu \in \mathcal{M}_{\nu}([0,1]^2) \) satisfying \( I_\beta(\nu) = 0 \), \( \nu_X = \nu_Y = \lambda \).

Because of the lemma, we may restrict to \((t_{11}, t_{12}, t_{21}, t_{22}) \in \Sigma_2\) such that \( t_{11} + t_{12} = \theta_1 \) and \( t_{11} + t_{21} = \theta_2 \) because those are the \( \lambda \) measures of \([0, \theta_1]\) and \([0, \theta_2]\). This reduces the parameter from general \((t_{11}, t_{12}, t_{21}, t_{22}) \in \Sigma_2\) to just \( t_{11} \) in a certain interval. We define
\[
I_{\theta_1, \theta_2} = [\max \{0, \theta_1 + \theta_2 - 1\}, \min \{\theta_1, \theta_2\}].
\]
Then we define \( \Phi_\beta(\theta_1, \theta_2; \cdot) : I_{\theta_1, \theta_2} \to \mathbb{R} \) as
\[
\Phi_\beta(\theta_1, \theta_2; t) = \Phi_\beta(\theta_1, \theta_2; t, \theta_1 - t, \theta_2 - t, 1 - \theta_1 - \theta_2 + t).
\]

Theorem 3.3 For each \( \beta \in \mathbb{R} \), and each \((\theta_1, \theta_2) \in (0, 1)^2\), the function \( \Phi_\beta(\theta_1, \theta_2; \cdot) : I_{\theta_1, \theta_2} \to \mathbb{R} \) is strictly convex, and the unique critical point is given by
\[
t = R_\beta(\theta_1, \theta_2) \overset{\text{def}}{=} - \frac{1}{\beta} \ln \left( 1 - \frac{(1 - e^{-\beta \theta_1})(1 - e^{-\beta \theta_2})}{1 - e^{-\beta}} \right).
\]

This theorem easily leads to the following, which is the main summary of the results.

Theorem 3.4 The unique measure \( \nu \in \mathcal{M}_{\nu}([0,1]^2) \) such that \( I_\beta(\nu) = 0 \) is \( \nu = \nu_\beta^* \), where \( d\nu_\beta^*(x,y) = \rho_\beta^*(x,y) \, dx \, dy \) for \( x, y \in [0,1]^2 \), where
\[
\rho_\beta(x,y) = \frac{\partial^2}{\partial x \, \partial y} R_\beta(x,y).
\]

Proof: Any measure \( \nu \in \mathcal{M}_{\nu}([0,1]^2) \) such that \( I_\beta(\nu) = 0 \) must satisfy \( \nu_X = \nu_Y = \lambda \) by Theorem 3.2. Then, for any \((\theta_1, \theta_2) \in \mathcal{M}_{\nu}([0,1]^2)\) the measure \( \nu \) is in \( W_{\theta_1, \theta_2}(t, \theta_1 - t, \theta_2 - t, 1 - \theta_1 - \theta_2 + t) \) for \( t = \nu(\Lambda_{\theta_1}(\theta_2)) \). So by Theorem 3.3 \( \Phi_\beta(\theta_1, \theta_2; t, \theta_1 - t, \theta_2 - t, 1 - \theta_1 - \theta_2 + t) = 0 \). But then, by Theorem 3.3 we see that this means that \( t = R_\beta(\theta_1, \theta_2) \). In other words, \( \nu([0, \theta_1] \times [0, \theta_2]) = R_\beta(\theta_1, \theta_2) \). These rectangular measures completely characterize \( \nu \): in fact they give the standard formula for the multidimensional distribution function. So uniqueness is proved. We now call it \( \nu_\beta^* \). Note that \( \nu_\beta^* \ll \lambda_{\otimes 2} \) because the relative entropy is not \(-\infty\). Therefore, there is a density, which may be calculated by differentiating the distribution function. \( \square \)
Proposition 4.2 Suppose that from (10) and the chain rule we have \( \nu = \) then we obtain that
\[
\text{In the second integral we integrate over } y \nu \text{ function } g x \text{ for } g x \text{ and } \nu y \nu \text{ function } h y \nu \text{ for } h y \nu .
\]

Proof: The fact about the marginals follows directly from the definition (10) and the definition of the marginals (3) and \( \nu x = \nu y = \lambda \).

Let us write \( \rho x : [0, 1] \rightarrow [0, \infty) \) for the density associated to \( \nu x \). Note that \( \int_0^1 \rho x(x, y) dy = 1 \) for \( x \), \( \lambda \)-a.e., and similarly \( \int_0^1 \rho x(x, y) dx = 1 \) for \( y \), \( \lambda \)-a.e., because \( \nu x = \nu y = \lambda \). Let us write \( g x : [0, 1] \rightarrow [0, \infty) \) and \( g y : [0, 1] \rightarrow [0, \infty) \) for the density functions associated to \( g x \) and \( g y \). Then, from (10) and the chain rule we have
\[
\frac{d\nu}{d\lambda^{\otimes 2}}(x, y) = \rho x(G x(x), G y(y))g x(x)g y(y).
\]
Therefore,
\[
S(\nu | \lambda^{\otimes 2}) = - \int_0^1 \int_0^1 \ln \left( \rho x(G x(x), G y(y)) \right) \rho x(G x(x), G y(y))g x(x)g y(y) dx dy
- \int_{[0, 1]^2} \ln(g x(x)) d\nu(x, y) - \int_{[0, 1]^2} \ln(g y(y)) d\nu(x, y).
\]
In the second integral we integrate over \( y \) first and use the fact that the marginal \( \nu x \) has density function \( g x \) and in the third integral we integrate over \( x \) first and use the fact that \( \nu y \) has density function \( g y \). In the first integral we make the change of variables \( x = G x(u) \) and \( y = G y(v) \), and then we obtain
\[
S(\nu | \lambda^{\otimes 2}) = - \int_0^1 \int_0^1 \ln(\rho x(x, y)) \rho x(x, y) dx dy
- \int_0^1 \ln(f x(x)) f x(x) dx - \int_0^1 \ln(f y(y)) f y(y) dy.
\]

4 Standardizing the measure

This is a solvable model. This is manifest in the symmetry of \( I \nu \). We describe this, now.

Definition 4.1 Suppose that \( \nu^0 \in M_{+1}([0, 1]^2) \) satisfies \( \nu^0 \ll \lambda^{\otimes 2} \). Suppose that \( g x, g y : [0, 1] \rightarrow [0, \infty) \) are two absolutely continuous probability distribution functions. Then we may define a new measure \( \nu = \mathcal{R}(\nu^0, g x, g y) \) as
\[
\nu([0, x] \times [0, y]) = \nu^0([0, G x(x)] \times [0, G y(y)]).
\]

Proposition 4.2 Suppose that \( \nu^0 \in M_{+1}([0, 1]^2) \) satisfies \( \nu^0 \ll \lambda^{\otimes 2} \) and \( \nu^0 = \nu^0 = \lambda \). Suppose that \( g x, g y : [0, 1] \rightarrow [0, \infty) \) are two absolutely continuous probability distribution functions. Defining \( \nu = \mathcal{R}(\nu^0, g x, g y) \), we have that \( \nu x([0, a]) = g x(a), \nu y([0, a]) = g y(a) \) for all \( a \in [0, 1] \). Moreover,
\[
S(\nu | \lambda^{\otimes 2}) = S(\nu^0 | \lambda^{\otimes 2}) + S(\nu x | \lambda^{\otimes 1}) + S(\nu y | \lambda^{\otimes 1}),
\]
and
\[
\mathcal{E}(\nu) = \mathcal{E}(\nu^0).
\]
The first integral follows from the chain rule for Stieltjes integrals. See, for example, [26], Chapter III, especially Section 58.

The result for the energy follows from a similar calculation, using the same method.

Now, given any \( \nu \in \mathcal{M}_{\mathbb{R}}([0, 1]^2) \), if \( \nu \ll \lambda_*^2 \), then \( \nu_X \) and \( \nu_Y \), defined in \( \Box \) are both absolutely continuous with respect to \( \lambda \). We define \( F_{\nu,X}, F_{\nu,Y} : [0, 1] \rightarrow [0, 1] \) as

\[
F_{\nu,X}(a) = \nu_X([0, a]) \quad \text{and} \quad F_{\nu,Y}(a) = \nu_Y([0, a]),
\]

for each \( a \in [0, 1] \). These functions are both continuous.

**Definition 4.3** Given a distribution function \( G : [0, 1] \rightarrow [0, 1] \), let us denote the generalized inverse as \( G^I : [0, 1] \rightarrow [0, 1] \), where the condition to be a generalized inverse is

\[
\forall x \in [0, 1], \quad G^I(y) = \inf(U_G(x)), \quad \text{where} \quad U_G(x) = \{ a \in [0, 1] : G(a) \geq x \}.
\]

Generally speaking, by right-continuity of \( G \), we have \( G(G^I(x)) = \inf\{G(a) : a \in U_G(x)\} \geq x \). Also, if \( y < G^I(x) \) then \( y \notin U_G(x) \) so \( G(y) < x \). Hence,

\[
G(G^I(x)) \geq x, \quad \text{and} \quad (y < G^I(x) \Rightarrow G(y) < x) . \tag{14}
\]

That is true for any distribution function. More is true if \( G \) is continuous.

**Lemma 4.4** Suppose that \( G : [0, 1] \rightarrow [0, 1] \) is a continuous distribution function. Then \( G^I \) is a right inverse for \( G \): for all \( x \in [0, 1] \), \( G(G^I(x)) = x \).

**Proof:** Suppose that we had \( G(G^I(x)) > x \). Since \( G \) is continuous, there would exist some \( y < G^I(x) \) such that \( G(y) > x \), as well. But this contradicts (14). \( \Box \)

**Definition 4.5** If \( \nu \in \mathcal{M}_{\mathbb{R}}([0, 1]^2) \) satisfies \( \nu \ll \lambda_*^2 \), then define \( \tilde{\nu} \in \mathcal{M}_{\mathbb{R}}([0, 1]^2) \) to be the measure such that

\[
\tilde{\nu}([0,x] \times [0,y]) = \nu([0,F^I_{\nu,X}(x)] \times [0,F^I_{\nu,Y}(y)]), \quad \tag{15}
\]

with the notation as above.

The important relation between \( \nu \) and \( \tilde{\nu} \) is the following.

**Lemma 4.6** If \( \nu \in \mathcal{M}_{\mathbb{R}}([0, 1]^2) \) satisfies \( \nu \ll \lambda_*^2 \), then \( \tilde{\nu}|_X = \nu|_X = \lambda \) and

\[
\nu([0,x] \times [0,y]) = \tilde{\nu}([0,F^I_{\nu,X}(x)] \times [0,F^I_{\nu,Y}(y)]), \quad \tag{16}
\]

for all \( x, y \in [0, 1] \). In other words, \( \nu = \mathcal{N}(\tilde{\nu}, F_{\nu,X}, F_{\nu,Y}) \).

**Proof:** To simplify notation, let us just write \( F_X, F_Y, F^I_X, F^I_Y \) in place of \( F_{\nu,X}, F_{\nu,Y}, F^I_{\nu,X}, F^I_{\nu,Y} \).

By definition

\[
(\tilde{\nu}|_X)([0,x]) = \tilde{\nu}([0,x] \times [0,1]) = \nu([0,F^I_X(x)] \times [0,F^I_Y(1)]).
\]

Now we note that this means

\[
(\tilde{\nu}|_X)([0,x]) \leq \nu([0,F^I_X(x)] \times [0,1]) = \nu_X([0,F^I_X(x)]) = F_X(F^I_X(x)) = x,
\]

using Lemma 4.4. But in fact,

\[
x - (\tilde{\nu}|_X)([0,x]) = \nu([0,F^I_X(x)] \times (F^I_Y(1), 1]) \leq \nu([0,1] \times (F^I_Y(1), 1]) = \nu_Y((F^I_Y(1), 1],
\]

and this equals \( F_Y(1) - F_Y(F^I_Y(1)) \), i.e., \( 1 - F_Y(F^I_Y(1)) \), which is 0, again by Lemma 4.4. So this proves that \( (\tilde{\nu}|_X) = \lambda \), and the corresponding fact for the \( y \) marginal follows, similarly.
Now, applying (15) with \( x \) replaced by \( F_X(x) \) and \( y \) replaced by \( F_Y(y) \),
\[
\hat{\nu}([0, F_X(x)] \times [0, F_Y(y)]) = \nu([0, F_X^1(F_X(x))] \times [0, F_Y^1(F_Y(y))]) .
\] (17)
We note that (14) implies that if \( a < F_X^1(F_X(x)) \) then \( F_X(a) < F_X(x) \). Since \( F_X \) is non-decreasing this implies that for every \( a \in [0, 1] \), if we have \( a < F_X^1(F_X(x)) \) then \( a < x \). In other words, this all implies that \( F_X^1(F_X(x)) \leq x \). Using this, we may see that (17) implies that
\[
\hat{\nu}([0, F_X(x)] \times [0, F_Y(y)]) \leq \nu([0, x] \times [0, y]) .
\]
But then by the same type of argument as before, using (17), we actually have
\[
\nu([0, x] \times [0, y]) - \hat{\nu}([0, F_X(x)] \times [0, F_Y(y)])
\leq \nu_X([0, x]) - \nu_X([0, F_X^1(F_X(x))]) + \nu_Y([0, y]) - \nu_Y([0, F_Y^1(F_Y(y))]) .
\]
And this equals 0.

Finally, we state the scaling properties of the entropy and energy, under the transformation of \( \nu \) to \( \hat{\nu} \).

**Corollary 4.7** For any \( \nu \in \mathcal{M}_{+1}([0, 1]^2) \) with \( \nu \ll \lambda^{\otimes 2} \),
\[
S(\nu | \lambda^{\otimes 2}) = S(\hat{\nu} | \lambda^{\otimes 2}) + S(\nu_X | \lambda^{\otimes 1}) + S(\nu_Y | \lambda^{\otimes 1}) ,
\]
and
\[
\mathcal{E}(\nu) = \mathcal{E}(\hat{\nu}).
\] (19)

**Proof:** Combine Proposition 4.3 and Lemma 4.6.

We may now prove Theorem 3.2 (We will prove Theorem 3.1 in a later section.)

**Proof of Theorem 3.2** From (18) and (19), it follows that
\[
\mathcal{I}_\beta(\nu) = \mathcal{I}_\beta(\hat{\nu}) - S(\nu_X | \lambda) - S(\nu_Y | \lambda) .
\] (20)
Hence
\[
\mathcal{I}_\beta(\hat{\nu}) = \mathcal{I}_\beta(\nu) + S(\nu_X | \lambda) + S(\nu_Y | \lambda) .
\]
But the relative entropy is nonpositive and equals 0 only at the unique maximizer \( \lambda \). Therefore, since \( \mathcal{I}_\beta \) can never be negative, we see that \( \mathcal{I}_\beta(\nu) \) can equal 0 only if \( \nu_X = \nu_Y = \lambda \).

We can think of this proof as a partial solution of the one-square problem, for \([0, 1]^2\). More specifically, while it does not give the unique measure \( \nu \in \mathcal{M}([0, 1]^2) \) solving \( \mathcal{I}_\beta(\nu) = 0 \), it does give the \( x \) and \( y \) marginals. The next step is to consider the two-square problem. For the two-square problem, we will not determine the exact marginals. But we will prove a scaling which will ultimately let us solve the four-square problem.

## 5 The two-square problem

Given any \( \theta \in (0, 1) \) we define \( \Lambda_1(\theta) = [0, 1] \times [0, \theta] \) and \( \Lambda_2(\theta) = [0, 1] \times (\theta, 1] \). Since \( \nu_Y = \lambda \), we have \( \nu(\Lambda_1) = \theta \) and \( \nu(\Lambda_2) = 1 - \theta \). We define two new measures \( \nu^{(1)}, \nu^{(2)} \in \mathcal{M}_{+1}([0, 1]^2) \) by
\[
\nu^{(1)}(\cdot) = \theta^{-1} \nu(\cdot \cap \Lambda_1) \quad \text{and} \quad \nu^{(2)}(\cdot) = (1 - \theta)^{-1} \nu(\cdot \cap \Lambda_2). \]
Since \( \nu_Y = \lambda \), we have for the \( y \)-marginals of \( \nu^{(1)} \) and \( \nu^{(2)} \):
\[
\nu^{(1)}_Y(\cdot) = \theta^{-1} \lambda(\cdot \cap [0, \theta]) \quad \text{and} \quad d\nu^{(2)}_Y(y) = (1 - \theta)^{-1} \lambda(\cdot \cap (\theta, 1]).
\] (21)
The \( x \) marginals \( \nu^{(1)}_X \) and \( \nu^{(2)}_X \) may be more complicated. But we can prove the following result.
Lemma 5.1 Assuming that $\nu \in M_{+1}([0,1]^2)$ has $\nu \ll \lambda^\otimes 2$ and $\nu_\gamma = \lambda$, using the notation above,

$$I_\beta(\nu) = p(\beta) - \theta p(\beta\theta) - (1 - \theta)p(\beta(1 - \theta)) + \theta I_{\beta\theta}(\nu^{(1)}) + (1 - \theta)I_{\beta(1 - \theta)}(\nu^{(2)})$$

$$- \theta S(\nu^{(1)}_X | \lambda) - (1 - \theta)S(\nu^{(2)}_X | \lambda) + \beta(1 - \theta) \int_0^1 \int_0^1 1_{(\infty,0)}(x_2 - x_1) d\nu^X_\gamma(1)(x_1) d\nu^X_\gamma(2)(x_2).$$

Proof: A straightforward computation using the definition of the entropy shows that, defining $s(\theta, 1 - \theta) = -\theta \ln(\theta) - (1 - \theta)\ln(1 - \theta)$,

$$I_\beta(\nu) = p(\beta) - s(\theta, 1 - \theta) - \theta S(\nu^{(1)} | \lambda^\otimes 2) - (1 - \theta)S(\nu^{(2)} | \lambda^\otimes 2) + \beta^2 E(\nu^{(1)}) + (1 - \theta)^2 E(\nu^{(2)})$$

$$+ \beta(1 - \theta) \int_0^1 \int_0^1 h((x_1, y_1), (x_2, y_2)) d\nu^X_\gamma(1)(x_1) d\nu^X_\gamma(2)(x_2).$$

We note that, because $\nu^{(1)}$ has support in $\Lambda^{(1)}$ and $\nu^{(2)}$ has support in $\Lambda^{(2)}$ we may rewrite this as

$$I_\beta(\nu) = p(\beta) - s(\theta, 1 - \theta) - \theta S(\nu^{(1)} | \lambda^\otimes 2) - (1 - \theta)S(\nu^{(2)} | \lambda^\otimes 2) + \beta^2 E(\nu^{(1)}) + (1 - \theta)^2 E(\nu^{(2)})$$

$$+ \beta(1 - \theta) \int_0^1 \int_0^1 1_{(\infty,0)}(x_2 - x_1) d\nu^X_\gamma(1)(x_1) d\nu^X_\gamma(2)(x_2).$$

Now we note that using the definition of $I_\beta$ for all $\beta$’s, this may be rewritten as

$$I_\beta(\nu) = p(\beta) - s(\theta, 1 - \theta) + \theta I_{\beta\theta}(\nu^{(1)}) - \theta p(\beta\theta) + (1 - \theta)I_{\beta(1 - \theta)}(\nu^{(2)}) - (1 - \theta)p(\beta(1 - \theta))$$

$$+ \beta(1 - \theta) \int_0^1 \int_0^1 1_{(\infty,0)}(x_2 - x_1) d\nu^X_\gamma(1)(x_1) d\nu^X_\gamma(2)(x_2),$$

Finally, using [20], we may rewrite this as

$$I_\beta(\nu) = p(\beta) - s(\theta, 1 - \theta) - \theta p(\beta\theta) - (1 - \theta)p(\beta(1 - \theta)) + \theta I_{\beta\theta}(\nu^{(1)}) + (1 - \theta)I_{\beta(1 - \theta)}(\nu^{(2)})$$

$$- \theta S(\nu^{(1)}_X | \lambda) - \theta S(\nu^{(1)}_X | \lambda) - (1 - \theta)S(\nu^{(2)}_X | \lambda) - (1 - \theta)S(\nu^{(2)}_X | \lambda)$$

$$+ \beta(1 - \theta) \int_0^1 \int_0^1 1_{(\infty,0)}(x_2 - x_1) d\nu^X_\gamma(1)(x_1) d\nu^X_\gamma(2)(x_2),$$

Using [21], we may calculate $S(\nu^{(1)}_Y | \lambda)$ and $S(\nu^{(2)}_Y | \lambda)$. This yields the desired result. \(\square\)

Corollary 5.2 For any measures $\mu, \bar{\mu} \in M_{+1}([0,1])$, both of which are absolutely continuous with respect to $\lambda$, we have, for each $\beta \in \mathbb{R}$ and each $\theta \in (0,1)$,

$$- \theta S(\mu | \lambda) - (1 - \theta)S(\bar{\mu} | \lambda) + \beta(1 - \theta) \int_0^1 \int_0^1 1_{(\infty,0)}(x_2 - x_1) d\mu(x_1) d\bar{\mu}(x_2)$$

$$\geq \theta p(\beta\theta) + (1 - \theta)p(\beta(1 - \theta)) - p(\beta).$$

Moreover, there does exist a pair of measures $\mu, \bar{\mu} \in M_{+1}([0,1])$ giving equality.

Proof: Recall that for each $\beta \in \mathbb{R}$, we do know that there exists at least one measure in $M_{+1}([0,1]^2)$ which minimizes $I_\beta$, using soft analysis, especially lower semi-continuity and weak-compactness. For each $\beta \in \mathbb{R}$, we choose such one measure and call it $\nu^{\beta}$.

Let us define $\kappa, \bar{\kappa} \in M_{+1}([0,1])$ by $d\kappa(y) = \theta^{-1}I_{[0,\theta]}(y) d\gamma$ and $d\bar{\kappa}(y) = (1 - \theta)^{-1}I_{[\theta,1]}'(y) d\gamma$. Then we may define two measures $\xi, \bar{\xi} \in M([0,1]^2)$ by $\xi = 9(\nu^{\beta}_{\theta\beta}, F_\mu, F_\kappa)$, where $F_\mu$ and $F_\kappa$ are the distribution functions for $\mu$ and $\kappa$, respectively, and with a similar definition for $\xi$ based on $\nu^{\beta}_{\beta(1 - \theta)}$, $\bar{\mu}$ and $\bar{\kappa}$. Then taking $\nu = \theta \xi + (1 - \theta)\bar{\xi}$, we will have $\nu^{(1)} = \xi$, $\nu^{(2)} = \bar{\xi}$, et cetera. In particular, we
will have $I_{\beta\theta}(\tilde{\nu}^{(1)}) = I_{\beta(1-\theta)}(\tilde{\nu}^{(2)}) = 0$ because $I_{\beta\theta}(\tilde{\nu}_{\beta\theta}) = 0$ and $I_{\beta(1-\theta)}(\tilde{\nu}_{\beta(1-\theta)}) = 0$. So applying Lemma 5.1 and using Proposition 5.1, we obtain the inequality.

To prove that there does exist a case of equality, take $\nu \in \mathcal{M}_{++,1}([0,1]^2)$ to be $\tilde{\nu}_\beta$, which we know exists since we do know that a minimizer for $I_\beta$ does exist. Then taking the $\nu_{X}^{(1)}$ and $\nu_{X}^{(2)}$’s as at the beginning of the section, we obtain equality. \hfill $\square$

6 The four-square problem

Suppose that $\theta_1, \theta_2 \in (0, 1)$. In order to simplify notation, let us denote $\Lambda_{ij}(\theta_1, \theta_2)$ just as $\Lambda_{ij}$, for this section. We assume that we have $(t_{11}, t_{12}, t_{21}, t_{22}) \in \Sigma_4$, defined. Let us assume, for now, that all four numbers are positive. We will say later what changes if some $t_{ij}$ equals 0.

We consider $\nu \in W_{\theta_1, \theta_2}(t_{11}, t_{12}, t_{21}, t_{22})$. We define four measures, $\nu^{(i,j)}$ for $i, j \in \{1, 2\}$ by

$$d\nu^{(i,j)}(x, y) = t_{ij}^{-1} \mathbf{1}_{\Lambda_{ij}}(x, y) d\mu(x, y).$$

Lemma 6.1 Assuming that $\nu \ll \lambda^{22}$ and $\nu_X = \nu_Y = \lambda$, using the notation above,

$$I_\beta(\nu) = p(\beta) + t_{11} \ln(t_{11}) + t_{12} \ln(t_{12}) + t_{21} \ln(t_{21}) + t_{22} \ln(t_{22})$$

$$+ \sum_{i,j=1}^{2} \left( -t_{ij} S(\nu^{(i,j)}_X | \lambda) - t_{ij} S(\nu^{(i,j)}_Y | \lambda) + t_{ij} I_{\beta t_{ij}}(\tilde{\nu}^{(i,j)}) - t_{ij} p(\beta t_{ij}) \right)$$

$$+ \beta t_{11} t_{12} \int_0^1 \int_0^1 1_{(-\infty,0)}(x_2 - x_1) d\nu^{(1,1)}_X(x_1) d\nu^{(1,2)}_X(x_2)$$

$$+ \beta t_{11} t_{21} \int_0^1 \int_0^1 1_{(-\infty,0)}(y_2 - y_1) d\nu^{(1,1)}_Y(y_1) d\nu^{(1,2)}_Y(y_2)$$

$$+ \beta t_{21} t_{22} \int_0^1 \int_0^1 1_{(-\infty,0)}(x_2 - x_1) d\nu^{(2,1)}_X(x_1) d\nu^{(2,2)}_X(x_2)$$

$$+ \beta t_{12} t_{21} \int_0^1 \int_0^1 1_{(-\infty,0)}(x_2 - x_1) d\nu^{(1,2)}_Y(y_1) d\nu^{(2,2)}_Y(y_2)$$

$$+ \beta t_{12} t_{22} \int_0^1 \int_0^1 1_{(-\infty,0)}(x_2 - x_1) d\nu^{(1,2)}_Y(y_1) d\nu^{(2,1)}_X(x_1)$$

(23)

Proof: One goes through the same steps as in the proof of Lemma 5.1. \hfill $\square$

We want to use this to prove Theorem 5.1. The idea of the completion of the proof is to use Corollary 5.2. But first we generalize it slightly.

Corollary 6.2 Suppose $\nu_1^{(1)}, \nu_1^{(2)} \in \mathcal{M}_{++,1}([0,1]^2)$, both have support inside an interval $[a, b]$ with $b-a = \theta \in (0, 1)$. Then, for each $\beta \in \mathbb{R}$ and each $t_1, t_2 \in (0, 1)$,

$$-t_1 S(\nu_1^{(1)} | \lambda) - t_2 S(\nu_1^{(2)} | \lambda) + \beta t_1 t_2 \int_0^1 \int_0^1 1_{(-\infty,0)}(x_2 - x_1) d\nu_1^{(1)}(x_1) d\nu_1^{(2)}(x_2)$$

$$\geq -(t_1 + t_2) \ln(\theta) + t_1 p(\beta t_1) + t_2 p(\beta t_2) - (t_1 + t_2) p(\beta(t_1 + t_2)) \ .$$

(24)

Moreover, there does exist a pair of measures $\nu_1^{(1)}, \nu_1^{(2)} \in \mathcal{M}_{++,1}([0,1]^2)$, both having support inside $[a, b]$, giving equality.

Proof: This follows from Corollary 5.2 by making some scaling transformations. We may define $\tilde{\nu}_1^{(1)}$ and $\tilde{\nu}_1^{(2)}$ by

$$\tilde{\nu}_1^{(1)}(A) = \nu_1^{(i)}(\{a + (b-a)x : x \in A\}) .$$
It is easy to see that \( S(\nu_X^{(i)} | \lambda) = \ln(\theta) + S(\nu_X^{(i)} | \lambda) \). With this, the result follows by straightforward calculations.

Now we may prove Theorem 3.1, including the case where some \( t_{ij} \) may equal 0.

**Proof of Theorem 3.1.** At first, assume that all \( t_{ij} \)'s are strictly positive, as we have been assuming in this section, up to this point. Combining Lemma 6.1 with Corollary 6.2, and writing \(|\Lambda_{ij}|\) for \( \lambda^{\otimes 2}(\Lambda_{ij}) \), we obtain

\[
I(\beta) \geq p(\beta) + \sum_{i,j=1}^{2} t_{11} \ln \left( \frac{t_{11}}{|\Lambda_{ij}|} \right) + \sum_{i,j=1}^{2} t_{ij} \beta t_{ij} \beta t_{ij} \cdot p(\beta t_{ij}) - (t_{11} + t_{12}) p(\beta(t_{11} + t_{12})) - (t_{11} + t_{21}) p(\beta(t_{11} + t_{21})) - (t_{12} + t_{22}) p(\beta(t_{12} + t_{22})) - (t_{21} + t_{22}) p(\beta(t_{21} + t_{22})) + \beta t_{12} t_{21}.
\]

Finally, using Proposition 3.1 we obtain

\[
I(\beta) \geq p(\beta) + \sum_{i,j=1}^{2} t_{ij} \ln \left( \frac{t_{ij}}{|\Lambda_{ij}|} \right) + \sum_{i,j=1}^{2} t_{ij} \beta t_{ij} \beta t_{ij} \cdot p(\beta t_{ij}) - (t_{11} + t_{12}) p(\beta(t_{11} + t_{12})) - (t_{11} + t_{21}) p(\beta(t_{11} + t_{21})) - (t_{12} + t_{22}) p(\beta(t_{12} + t_{22})) - (t_{21} + t_{22}) p(\beta(t_{21} + t_{22})) + \beta t_{12} t_{21}.
\]

We use Proposition 3.1 to lower bound \( I_{\beta t_{ij}}(\hat{\nu}^{(i,j)}) \) by 0 everywhere.

The cases of equality follow from the cases of equality in Corollary 6.2 as well as the fact that \( \hat{\nu}^* \) measures do exist to give the minimum in \( I \). There is no obstruction to putting these together using \( \mathcal{G}_t \) somewhat similarly to what we did in the proof of 5.2 but with 4 squares instead of 2. Corollary 6.2 give marginals, and \( \hat{\nu}^* \) gives values for \( \hat{\nu}^* \)'s. Then we may use Definition 4.1 as a prescription for obtaining \( \nu^{(i,j)} \).

Finally, for the case that some \( t_{ij} \) equals 0, all that happens is that the actual value of \( \nu^{(i,j)} \) is irrelevant. In particular note that there is no source of discontinuity of \( S \) arising from this. The Lebesgue measure \(|\Lambda_{ij}|\) is fixed and positive because \((\theta_1, \theta_2) \in (0, 1)^2\). All that happens is that the density becomes zero. But \( \phi(x) = -x \ln(x) \) is continuous at 0, since it is defined to be \( \phi(0) = 0 \).

**7 Calculus facts**

We have now proved Theorem 3.1 and Theorem 3.2. (We proved them in opposite order.) The proof of Theorem 3.3 now occupies us. It follows from calculus exercises. We will sometimes write \( t_{ij} \) for \( T_{ij}(\theta_1, \theta_2; t) \), where

\[
T_{11}(\theta_1, \theta_2; t) = t, \quad T_{12}(\theta_1, \theta_2; t) = \theta_1 - t, \quad T_{21}(\theta_1, \theta_2; t) = \theta_2 - t, \quad T_{22}(\theta_1, \theta_2; t) = 1 - \theta_1 - \theta_2 + t.
\]

Let us summarize the main results.

**Lemma 7.1.** (a) For \( t \in \mathcal{T}_{\theta_1, \theta_2} = (\max\{0, \theta_1 + \theta_2 - 1\}, \min\{\theta_1, \theta_2\}) \), we have

\[
\frac{\partial^2}{\partial t^2} \Phi(\theta_1, \theta_2; t) = \sum_{i,j=1}^{2} \frac{\beta}{2 \tanh(\beta t_{ij}/2)}.
\]
(b) The critical point equation \( \frac{\partial}{\partial \beta} \Phi_\beta(\theta_1, \theta_2; t) = 0 \) is equivalent to

\[
\frac{(1 - e^{-\beta_11})(1 - e^{-\beta_22})}{(e^{\beta_{t12} - 1})(e^{\beta_{t21} - 1})} = 1.
\]  

(28)

**Proof:** (a) Using (7) and the definition of \( T_{ij}(\theta_1, \theta_2; t) \), for \( i, j \in \{1, 2\} \), we have

\[
\Phi_\beta(\theta_1, \theta_2; t) = \Phi_\beta(\theta_1, \theta_2; T_{11}(\theta_1, \theta_2; t), T_{12}(\theta_1, \theta_2; t), T_{21}(\theta_1, \theta_2; t), T_{22}(\theta_1, \theta_2; t))
\]

\[
= p(\beta) - \theta_1 p(\beta \theta_1) - \theta_2 p(\beta \theta_2) - (1 - \theta_1) p(\beta(1 - \theta_1)) - (1 - \theta_2) p(\beta(1 - \theta_2))
\]

\[
+ \sum_{i,j=1}^{2} t_{ij} \ln \left( \frac{t_{ij}}{|\Lambda_{ij}|} \right) + \sum_{i,j=1}^{2} t_{ij} p(\beta t_{ij}) + \beta t_{12} t_{21}.
\]

(29)

Moreover, from (5), we see that

\[
\frac{\partial}{\partial \theta} [\theta p(\beta \theta)] = \ln \left( \frac{1 - e^{-\beta \theta}}{\beta \theta} \right).
\]

Using this with (29), we see that

\[
\frac{\partial}{\partial t} \Phi_\beta(\theta_1, \theta_2; t) = \sum_{i,j=1}^{2} \left[ 1 + \ln \left( \frac{t_{ij}}{|\Lambda_{ij}|} \right) \right] \frac{\partial t_{ij}}{\partial t} + \sum_{i,j=1}^{2} \ln \left( \frac{1 - e^{-\beta t_{ij}}}{\beta t_{ij}} \right) \frac{\partial t_{ij}}{\partial t} + \beta t_{12} \frac{\partial t_{21}}{\partial t} + \beta t_{21} \frac{\partial t_{12}}{\partial t}.
\]

Using this with (29), we see that

\[
\frac{\partial}{\partial t} \Phi_\beta(\theta_1, \theta_2; t) = \sum_{i,j=1}^{2} (-1)^{i+j} \ln \left( \frac{t_{ij}}{|\Lambda_{ij}|} \right) + \sum_{i,j=1}^{2} (-1)^{i+j} \ln \left( \frac{1 - e^{-\beta t_{ij}}}{\beta t_{ij}} \right) - \beta (t_{12} + t_{21}).
\]

(30)

This may be rewritten as

\[
\frac{\partial}{\partial t} \Phi_\beta(\theta_1, \theta_2; t) = \sum_{i,j=1}^{2} (-1)^{i+j} \ln \left( \frac{1 - e^{-\beta t_{ij}}}{\beta |\Lambda_{ij}|} \right) - \beta (t_{12} + t_{21}).
\]

(31)

So, taking the second derivative we obtain

\[
\frac{\partial^2}{\partial t^2} \Phi_\beta(\theta_1, \theta_2; t) = \sum_{i,j=1}^{2} (-1)^{i+j} \frac{\beta e^{-\beta t_{ij}}}{1 - e^{-\beta t_{ij}}} \frac{\partial t_{ij}}{\partial t} - \beta \left( \frac{\partial t_{12}}{\partial t} + \frac{\partial t_{21}}{\partial t} \right)
\]

\[
= \sum_{i,j=1}^{2} \frac{\beta e^{-\beta t_{ij}}}{1 - e^{-\beta t_{ij}}} + 2 \beta.
\]

Simplifying, this does give equation (27). Note that for \( \beta = 0 \) we interpret this as the \( \beta \to 0 \) limit which is \( \sum_{i,j=1}^{2} 1/t_{ij} \).

(b) Equation (30) may be rewritten as

\[
\frac{\partial}{\partial t} \Phi_\beta(\theta_1, \theta_2; t) = \ln \left( \frac{(1 - e^{-\beta t_{11}})(1 - e^{-\beta t_{22}})}{(e^{\beta t_{12} - 1})(e^{\beta t_{21} - 1})} \right) - \ln \left( e^{\beta t_{12}} e^{\beta t_{21}} \right)
\]

\[
= \ln \left( \frac{(1 - e^{-\beta t_{11}})(1 - e^{-\beta t_{22}})}{(e^{\beta t_{12} - 1})(e^{\beta t_{21} - 1})} \right).
\]

Therefore, the critical point equation is (28).
Now let us prove Theorem 3.3.

**Proof of Theorem 3.3.** Firstly, we note that \( \frac{\partial}{\partial \theta_2} \Phi_\beta(\theta_1, \theta_2; t) \) is manifestly positive on \( \mathcal{I}_{\theta_1, \theta_2} \). Therefore, \( \Phi_\beta(\theta_1, \theta_2; \cdot) : \mathcal{I}_{\theta_1, \theta_2} \to \mathbb{R} \) is strictly convex. Next we attempt to solve (28). We recall that \( t_{ij} = T_{ij}(\theta_1, \theta_2; t) \). In particular,

\[
t_{11} = t, \quad t_{12} = \theta_1 - t, \quad t_{21} = \theta_2 - t, \quad t_{22} = 1 - \theta_1 - \theta_2 + t.
\]

So, if we define

\[
u = 1 - e^{-\beta t_{11}} = 1 - e^{-\beta t}.
\]

Then we get

\[
1 - e^{-\beta t_{12}} = 1 - e^{-\beta(\theta_1 + \theta_2 - 1)} e^{-\beta t} = 1 - e^{\beta(1 - \theta_1 - \theta_2)} e^{-\beta t} u,
\]

\[
e^{\beta t_{12}} - 1 = e^{\beta(1 - \theta_1 - \theta_2)} e^{-\beta t} - 1 = e^{\beta(1 - \theta_1 - \theta_2)} (1 - e^{-\beta t} - u),
\]

\[
e^{\beta t_{21}} - 1 = e^{\beta(1 - \theta_1 - \theta_2)} e^{-\beta t} - 1 = e^{\beta(1 - \theta_1 - \theta_2)} (1 - e^{-\beta t} - u).
\]

So (28) is equivalent to

\[
\frac{u (1 - e^{\beta(1 + \theta_2 - 1)} e^{-\beta t} u + e^{\beta(1 + \theta_2 - 1)} e^{-\beta t})}{e^{\beta(1 + \theta_2)} (1 - e^{-\beta t} - u)(1 - e^{-\beta t} - u)} = 1.
\]

The equation is equivalent to

\[
u (1 - e^{-\beta(1 + \theta_2)} - e^{-\beta} + e^{-\beta} u) = (1 - e^{-\beta(1 + \theta_2)} - e^{-\beta} - u).
\]

Doing one more step of simplification, we obtain the equivalent formulation

\[
(1 - e^{-\beta})u^2 - [(1 - e^{-\beta(1 + \theta_2)}) + (1 - e^{-\beta(1 + \theta_2)}) + e^{-\beta(1 + \theta_2)} - e^{-\beta} + (1 - e^{-\beta(1 - \theta_1 - \theta_2)}) = 0.
\]

We may simplify this as

\[
(1 - e^{-\beta})u^2 - [(1 - e^{-\beta(1 + \theta_2)}) + (1 - e^{-\beta(1 + \theta_2)}) + (1 - e^{-\beta(1 + \theta_2)}) + (1 - e^{-\beta(1 - \theta_1 - \theta_2)}) = 0.
\]

Or, splitting the polynomial,

\[
[(1 - e^{-\beta})u - (1 - e^{-\beta(1 + \theta_2)}) (u - 1) = 0.
\]

There are two solutions in the complex plane: \( u = 1 \) which will not correspond to \( u = 1 - e^{-\beta t} \) for any \( t \in \mathcal{I}_{\theta_1, \theta_2} \), and

\[
u = \frac{(1 - e^{-\beta(1 + \theta_2)})(1 - e^{-\beta(1 + \theta_2)})}{1 - e^{-\beta(1 + \theta_2)}}.
\]

This leads to the formula (30).

We should check that \( t = R_\beta(\theta_1, \theta_2) \) is in \( \mathcal{I}_{\theta_1, \theta_2} \). First, we may calculate

\[
\frac{\partial}{\partial \theta_2} R_\beta(\theta_1, \theta_2) = r^{\text{cdf, pdf}}_\beta(\theta_1, \theta_2) = \frac{e^{-\beta(1 - e^{-\beta(1 + \theta_2)})}}{(1 - e^{-\beta}) - (1 - e^{-\beta(1 - \theta_1 - \theta_2)})(1 - e^{-\beta(1 + \theta_2)})}.
\]

(33)

It is easy to see that \( R_\beta(\theta_1, 0) = 0 \) for all \( \theta_1 \in (0, 1) \). Therefore, we do have

\[
R_\beta(\theta_1, \theta_2) = \int_0^{\theta_2} r^{\text{cdf, pdf}}_\beta(\theta_1, y) dy.
\]

(34)
The second derivative calculation is slightly more involved, involving fractions:

\[
\frac{\partial}{\partial \theta_1} r_{\beta}^{\text{cdf,pdf}}(\theta_1, \theta_2) = \frac{\partial}{\partial \theta_1} \frac{e^{-\beta \theta_2}(1 - e^{-\beta \theta_1})}{(1 - e^{-\beta}) - (1 - e^{-\beta \theta_1})(1 - e^{-\beta \theta_2})} \\
= \frac{e^{-\beta \theta_2}}{(1 - e^{-\beta}) - (1 - e^{-\beta \theta_1})(1 - e^{-\beta \theta_2})} \left(1 - \frac{1}{1 - e^{-\beta \theta_1} - (1 - e^{-\beta \theta_2})} \right) \\
= \beta e^{-\beta \theta_2} e^{-\beta \theta_1} \left(1 - \frac{1}{1 - e^{-\beta \theta_1} - (1 - e^{-\beta \theta_2})} \right) + \frac{(1 - e^{-\beta \theta_1})(1 - e^{-\beta \theta_2})}{[(1 - e^{-\beta}) - (1 - e^{-\beta \theta_1})(1 - e^{-\beta \theta_2})]^2} \\
\]

This is manifestly positive for all \(\beta \in \mathbb{R}\). (At \(\beta = 0\) this equals 1 by taking limits.) Moreover, from (33) \(r_{\beta}^{\text{cdf,pdf}}(0, \theta_2) = 0\). So

\[
r_{\beta}^{\text{cdf,pdf}}(\theta_1, \theta_2) = \int_{0}^{\theta_1} \frac{\beta(1 - e^{-\beta})e^{-\beta x}e^{-\beta \theta_2}}{[(1 - e^{-\beta}) - (1 - e^{-\beta \theta_1})(1 - e^{-\beta \theta_2})]^2} dx.
\]

Putting this together with (34), we see that

\[
R_\beta(\theta_1, \theta_2) = \int_{[0, \theta_1] \times [0, \theta_2]} \frac{\beta(1 - e^{-\beta})e^{-\beta x}e^{-\beta y}}{[(1 - e^{-\beta}) - (1 - e^{-\beta \theta_1})(1 - e^{-\beta \theta_2})]^2} dx dy.
\]

Direct calculation of \(R_\beta(\theta_1, 1)\) and \(R_\beta(1, \theta_2)\) shows that it does have the correct marginals. So, it does follow that \(t = R_\beta(\theta_1, \theta_2)\) is in \(I_{\theta_1, \theta_2}^\beta\).

\[\square\]

8 Outlook and extensions

The result that we have presented here is stronger than a weak law of large numbers that was previously proved by one of the authors [27]. Moreover, the present argument is simpler, since the old argument used uniqueness theory for a certain type of partial differential equation. The old proof was not direct. However, the old result, weak as it is, was useful in a subsequent work by Mueller and one of the authors [20]. That was a weak law for the length of the longest increasing subsequence in a Mallows distributed random permutation, when \(q = q_n\) scales such that \(1 - q_n \sim \beta/n\) as \(n \to \infty\), for some \(\beta \in \mathbb{R}\). Bhatnagar and Peled considered the more general case that \(q_n\) may scale with \(n\) in a more singular way. It is therefore interesting to look for a more exact type of result than what has been presented in this article.

The following result is true, and we will prove it in some detail in the appendix.

**Lemma 8.1** Let us define \(\{n\}! := [n]_q! / n!\). Let us define

\[\Sigma_4(n) = \{(n_{11}, n_{12}, n_{21}, n_{22}) \in [0,1,\ldots]^4 : n_{11} + n_{12} + n_{21} + n_{22} = n\} .\]

Then for each such 4-tuple, defining \(P_{n,\beta}(n_{11}, n_{12}, n_{21}, n_{22}; \theta_1, \theta_2)\) to be

\[\mu_{n, \beta} \left(\{(x_1, y_1), \ldots, (x_n, y_n)\} \in [0,1]^n : \frac{1}{n} \sum_{k=1}^{n} \delta_{(x_k, y_k)} \in W_{\theta_1, \theta_2} \left(\frac{n_{11}}{n}, \frac{n_{12}}{n}, \frac{n_{21}}{n}, \frac{n_{22}}{n}\right)\right) ,\]

we have the dependence on \(\beta\), versus the usual multinomial formula for \(\beta = 0\):

\[P_{n, \beta}(n_{11}, n_{12}, n_{21}, n_{22}; \theta_1, \theta_2) = P_{n,0}(n_{11}, n_{12}, n_{21}, n_{22}; \theta_1, \theta_2) \times q^{n_{12}n_{21}} \frac{\{n_{11} + n_{12}\}!\{n_{11} + n_{21}\}!\{n_{12} + n_{21}\}!\{n_{21} + n_{22}\}!\{n_{11} + n_{12} + n_{21} + n_{22}\}!}{\{n_{11}\}!\{n_{12}\}!\{n_{21}\}!\{n_{22}\}!\{n_{11} + n_{12} + n_{21} + n_{22}\}!} q^{\exp(-\beta/(n-1))} .\]
This may be proved using similar symmetries to those already on display here, except at the discrete level.

This leads to a quantitative version of the results on display here, sufficient to establish a local central limit theorem.

But moreover, it may be possible that this applies for $q = q_n$ scaling with $n$ in a more singular way than $1 - q_n \sim c/n$. More precisely, Moak has obtained a full asymptotic expansion for the $q$-factorial numbers such as $\{n\}_q$ in [10]. When $q = \exp(-\beta/(n - 1))$ the leading order part does lead to the large deviation function formulas we have derived here. But there are also correction terms, and more generally the lower order terms may be relevant when $q$ is not scaling as $1 - \beta n^{-1}$ for some finite $\beta \in \mathbb{R}$. That might be useful for trying to further analyze models considered by Bhatnagar and Peled in [7].

In a result related to [20], we are considering a 9-square problem, where the middle square is small, having linear size on the order of $1/n^{1/4}$. That analysis is currently underway, and we hope to report on it soon, in another article.

### A Proof of Lemma 8.1

Let us begin with a lemma.

**Lemma A.1** For each $n \in \mathbb{N}$, the polynomial $P_n(q) = \sum_{\pi \in S_n} q^{\text{inv}(\pi)}$ has the formula

$$P_n(q) = \prod_{k=1}^{n} \left( \frac{1 - q^k}{1 - q} \right)^{\text{def} := [n]_q!},$$

and for any $n \in \mathbb{N}$ and $k \in \{1, \ldots, n\}$

$$\sum_{\pi \in S_{n,k}} q^{\text{inv}(\pi)} = \frac{[n]_q!}{[k]_q! [n-k]_q!} \text{ def} := \left[ \frac{n}{k} \right]_q,$$

where $S_{n,k}$ is the set of all permutations $\pi \in S_n$ such that $\pi_1 < \cdots < \pi_k$ and $\pi_{k+1} < \cdots < \pi_n$.

**Proof:** The first formula is well-known. One may consult [9], for instance, and references, therein.

The second formula is also well-known. But let us review the proof, since we will use the same ideas, subsequently. Given $\pi \in S_n$, and given $k \in \{1, \ldots, n\}$, denote by $\pi^{(k)}$ the permutation such that

$$\{\pi_1^{(k)}, \ldots, \pi_k^{(k)}\} = \{\pi_1, \ldots, \pi_k\} \quad \text{and} \quad \{\pi_{k+1}^{(k)}, \ldots, \pi_n^{(k)}\} = \{\pi_{k+1}, \ldots, \pi_n\},$$

and such that $\pi^{(k)}$ is an element of $S_{n,k}$. Also, let $\pi^{(k,-)}$ denote the permutation in $S_n$ such that $\pi^{(k,-)}_j = j$ for $j > k$ and $\pi^{(k)}_j = \pi^{(k)}_j$ for $j \in \{1, \ldots, k\}$. Similarly, define $\pi^{(k,+)}$ such that $\pi^{(k,+)}_j = j$ for $j \leq k$ and $\pi^{(k,+)}_j = \pi^{(k)}_{\pi_j^{(k,-)}}$ for $j \in \{k+1, \ldots, n\}$. Then it is an easy fact to see that

$$\text{inv}(\pi) = \text{inv}(\pi^{(k)}) + \text{inv}(\pi^{(k,-)}) + \text{inv}(\pi^{(k,+)}).$$

Moreover, defining $S^{-}_{n,k}$ to be the set of all permutations $\pi \in S_n$ such that $\pi_j = j$ for all $j > k$ (which is isomorphic to $S_k$) and $S^{+}_{n,k}$ to be the set of all permutations $\pi \in S_n$ such that $\pi_j = j$ for all $j \leq k$ (which is isomorphic to $S_{n-k}$), we have $S_n \cong S_{n,k} \times S^{-}_{n,k} \times S^{+}_{n,k}$, where the bijection is the mapping $\pi \mapsto (\pi^{(k)}, \pi^{(k,-)}, \pi^{(k,+)})$. Using this, one may easily prove the second formula. \qed

With this, we may give the desired proof.

**Proof of Lemma 8.1.** We are going to start with a particular construction of a set of points $((x_1, y_1), \ldots, (x_n, y_n))$ such that $n^{-1} \sum_{k=1}^{n} \delta_{(x_k, y_k)}$ is in $W_{\theta_1, \theta_2}(\langle n \rangle)^2_{i,j=1}$. 

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First of all we note that the particular ordering of \(((x_1, y_1), \ldots, (x_n, y_n))\) does not affect the density 
\(\mu_{n,\beta}((x_1, y_1), \ldots, (x_n, y_n))\). Therefore, we will only describe the construction modulo a permutation in \(S_n\). We return to this point at the end.

Let us denote
\[
\begin{align*}
n_1^{(1:1)} &= n_1^{(2:1)} = n_{11}, & n_1^{(1:2)} &= n_1^{(2:2)} = n_{12}, & n_1^{(1:1)} &= n_2^{(2:1)} = n_{21}, & n_1^{(1:2)} &= n_2^{(2:2)} = n_{22}.
\end{align*}
\]

Then for each \(i, j \in \{1, 2\}\) let us define \(n^{(i:j)} = n_1^{(i:j)} + n_2^{(i:j)}\).

Let us choose points
\[
0 < \tilde{t}_1^{(1:1)} < \cdots < \tilde{t}_k^{(1:1)} < \theta_1, \quad \theta_1 < \tilde{t}_1^{(1:2)} < \cdots < \tilde{t}_k^{(1:2)} < 1,
\]
and
\[
0 < \tilde{t}_1^{(2:1)} < \cdots < \tilde{t}_k^{(2:1)} < \theta_2, \quad \theta_2 < \tilde{t}_1^{(2:2)} < \cdots < \tilde{t}_k^{(2:2)} < 1.
\]

Next, for each \(i, j \in \{1, 2\}\), let us choose a shuffle permutations \(\pi^{(i:j)} \in \text{Sh}_{n_1^{(i:j)}, n_2^{(i:j)}}\). Then we define
\[
\tilde{t}_k^{(i:j:1)} = \tilde{t}_k^{(i:j)} \pi_k^{(i:j)} \text{ for } k \in \{1, \ldots, n_1^{(i:j)}\}, \text{ and } \tilde{t}_k^{(i:j:2)} = \tilde{t}_k^{(i:j)} \pi_{n_1^{(i:j)}+k}^{(i:j)} \text{ for } k \in \{1, \ldots, n_2^{(i:j)}\}.
\]

Finally, let us choose permutations \(\pi^{(i:j)} \in S_{n_{ij}}\) for each \(i, j \in \{1, 2\}\). Then we define \(Z_{ij} \subset \Lambda_{i,j}(\theta_1, \theta_2)\) with \(|Z_{ij}| = n_{ij}\) for each \(i, j \in \{1, 2\}\), as
\[
\begin{align*}
Z_{11} &= \{(\tilde{t}_k^{(1:1)}, \tilde{t}_k^{(1:1)}) : k = 1, \ldots, n_{11}\}, \\
Z_{12} &= \{(\tilde{t}_k^{(1:2)}, \tilde{t}_k^{(2:1)}) : k = 1, \ldots, n_{12}\}, \\
Z_{21} &= \{(\tilde{t}_k^{(1:1)}, \tilde{t}_k^{(2:2)}) : k = 1, \ldots, n_{21}\}, \\
Z_{22} &= \{(\tilde{t}_k^{(2:2)}, \tilde{t}_k^{(2:2)}) : k = 1, \ldots, n_{22}\}.
\end{align*}
\]

We let \((x_1, y_1), \ldots, (x_n, y_n)\) be an arbitrary choice of points (meaning an arbitrary ordering) comprising \(\bigcup_{i,j=1}^n Z_{ij}\).

For each \(i, j, I, J \in \{1, 2\}\), let us define
\[
\mathcal{N}_{(i,j),(I,J)}((x_1, y_1), \ldots, (x_n, y_n)) = \# \{(k, \ell) : (x_k, y_k) \in \Lambda_{i,j}, (x_\ell, y_\ell) \in \Lambda_{I,J} (x_k - x_\ell)(y_k - y_\ell) < 0\}.
\]

Then it is easy to see that
\[
H_n = \sum_{i,j=1}^2 \mathcal{N}_{(i,j),(i,j)} + \mathcal{N}_{(1,1),(1,2)} + \mathcal{N}_{(1,1),(2,1)} + \mathcal{N}_{(1,2),(2,2)} + \mathcal{N}_{(2,1),(2,2)} + \mathcal{N}_{(1,2),(2,2)}.
\]

We do not need to include \(\mathcal{N}_{(1,1),(2,2)}\) because if \((x_k, y_k) \in \Lambda_{11}\) and \((x_\ell, y_\ell) \in \Lambda_{22}\) then we must have \((x_k - x_\ell)(y_k - y_\ell) > 0\). For similar reasons, we have \(\mathcal{N}_{(1,2),(2,1)}((x_1, y_1), \ldots, (x_n, y_n)) = n_{12}n_{21}\). Finally, we claim that careful inspection shows that
\[
\begin{align*}
\mathcal{N}_{(i,j),(i,j)} &= \text{inv}(\pi^{(i:j)}), \text{ for each } i, j \in \{1, 2\} \\
\mathcal{N}_{(1,1),(1,2)} &= \text{inv}(\pi^{(1:1)}), & \mathcal{N}_{(1,1),(2,1)} &= \text{inv}(\pi^{(2:1)}), \\
\mathcal{N}_{(1,2),(2,2)} &= \text{inv}(\pi^{(2:2)}), & \mathcal{N}_{(2,1),(2,2)} &= \text{inv}(\pi^{(1:2)}).
\end{align*}
\]
Then, using the fact that \( Z_n(\beta) = [n]q!/n!\) for \( q = \exp(-\beta/(n-1))\), we have

\[
\mu_{n,\beta}((x_1, y_1), \ldots, (x_n, y_n)) = \frac{n!}{[n]q!} q^{n_1 n_2} \left[ \prod_{i,j=1}^{2} q^{\inv(\pi(i,j))} \right].
\]

Then summing over each of the independent permutations \( \pi(i,j) \in S_{n_{ij}} \) for \( i, j \in \{1, 2\} \) and \( \pi(i,j) \in \Sh_{n_{i},n_{j}}^{1} \) for \( i, j \in \{1, 2\} \), and using Lemma A.1 we may deduce the result.

**B Another derivation of the main results**

We announce here another approach to derive our main results, without providing all the details. Firstly, there does exist a \( q \)-Stirling’s formula just like the usual Stirling’s formula \([19]\), wherein one may see that the exponential term is as in (5). In fact, the \( q \)-Stirling’s formula may be considered to be superior because the dilogarithm arises in the leading-order exponential term rather than just in the constant term. (In the usual Stirling’s formula the constant \( \sqrt{2\pi} \) must be derived by one of a number of methods. One method is to realize that \( \ln(n!) - (n + \frac{1}{2}) \ln(n) - n + \frac{1}{2} \ln(2\pi) = R_n \) where \( R_n = \int_0^{1/2} \ln(\pi x / \sin(\pi x)) \, dx \). Modulo elementary functions, this is equal to the dilogarithm function at \(-1\), which may be evaluated as easily as it is to calculate \( \zeta(2) \). On the other hand, since (5) is also another expression for the dilogarithm of an exponential, we see that the dilogarithm arises in the leading-order exponential part of the \( q \)-Stirling formula.)

An explicit formulation is as follows: for each \( \beta \in \mathbb{R} \)

\[
\ln \left( \frac{[n]q!}{n!} \right)_{q = \exp(-\beta/(n-1))} = n \int_0^1 \ln \left( \frac{1 - e^{-\beta x}}{\beta x} \right) \, dx + \frac{\beta}{2} + \frac{1}{2} \ln \left( \frac{1 - e^{-\beta}}{\beta} \right) + R_n(\beta), \tag{35}
\]

where \( R_n(\beta) \to 0 \) as \( n \to \infty \). This follows from Moak’s formula. But also, a simple proof is given (by specializing to \( q \)'s of the form \( q_n = 1 - n^{-1}(\beta + o(1)) \) where \( o(1) \to 0 \) as \( n \to \infty \)) in [81]; see Theorem 5.1.1.

Using this formula, keeping only the leading-order exponential term, and using Lemma 8.1 we may prove that

\[
\lim_{n \to \infty} \mu_{n,\beta} \left( \left\{ ((x_1, y_1), \ldots, (x_n, y_n)) : \frac{1}{n} \sum_{k=1}^{n} \delta_{(x_k, y_k)} = W_{\theta_1, \theta_2}((\nu_{1j})_{i,j=1}^{2}) \right\} \right) = \Phi_\beta(\theta_1, \theta_2; \nu_{11}, \nu_{12}, \nu_{21}, \nu_{22}),
\]

the formula from Theorem 5.1. But this is a harder approach. It is proved in complete detail in [81] in Lemma 5.6.2. The advantage of this second approach is that by keeping track of the lower order terms in \([33]\), one may prove local limit theorems. We intend to do this in a later paper for the 9-square problem, where the middle square has both side lengths on the order of \( n^{-1/4} \) as a subset of \([0,1]^2\), so that there are order \( n^{1/2} \) points in the middle square. That is because this is what is needed to obtain the simplest bounds on the fluctuations for the length of the longest increasing subsequence in a Mallows random permutation when \( q_n = 1 - n^{-1}(\beta + o(1)) \). The weak limit of this problem was previously considered in [20]. But we will obtain essentially \( O(n^{(1/4) + \epsilon}) \) bounds in a paper currently in preparation.

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