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Occupancy statistics arising from weighted particle rearrangements

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Abstract
The box-occupancy distributions arising from weighted rearrangements of a particle system are investigated. In the grand-canonical ensemble, they are characterized by determinantal joint probability generating functions. For doubly non-negative weight matrices, fractional occupancy statistics, generalizing Fermi–Dirac and Bose–Einstein statistics, can be defined. A spatially extended version of these balls-in-boxes problems is investigated.

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1. Introduction and outline

The purpose of this work is to study a class of combinatorial balls-in-boxes models as a random allocation scheme of particles. Although the urn model under study is formally in the spirit of those found, for example, in Charalambides [6], Johnson and Kotz [21], or Kolchin [24], it is however not covered by these manuscripts. Another unrelated balls-in-boxes process of similar flavor was recently revisited in [20], developing some equilibrium aspects of the zeta-urn model first introduced in [4]. In some sense made precise later, the model we shall deal with here is concerned with random box filling of an interacting particle system derived from weighted permutations of its constitutive items.

We first describe our model in some detail. Suppose we are given a total amount of $k \geqslant 1$ labeled particles (items) of n different types (or colors), with $n \geqslant 2$. Let $k_m, m = 1, \ldots, n$, be the number of type-m particles in some initial configuration, with $|\mathbf{k}_n| := k_1 + \cdots + k_n = k$ and $\mathbf{k}_n = (k_m, m = 1, \ldots, n)$. Initially place these k particles in boxes and, more specifically, place the k_m type-m particles in box number $m, m = 1, \ldots, n$, respectively. Suppose the energy required to move a particle from box m to box m' is $-\log W_{m,m'}$, where $W_{m,m'}$ is the $m \times m'$ entry of some non-negative $n \times n$ weight matrix W. We shall address the problem of evaluating the configurational weight of all particle rearrangements which end up with

$\mathbf{k}_n$ particles in different boxes, regardless of their type. Upon suitable normalization, for each Boltzmann weight matrix W, we shall use this to define the Gibbs canonical probability generating function of the random box occupancies $\mathbf{K}_{n,k} = (K_{n,k}(m), m = 1, \ldots, n)$, given a total population of k particles. From this model, the event $\mathbf{K}_{n,k} = \mathbf{k}_n$ will be realized not only because there are k_m type-m particles in box number m, but also because there is rearrangement of this peculiar configuration, the weight of each being needed to evaluate its occurrence probability. After suitably randomizing the particle number k, we shall rather work with the grand-canonical probability generating function of the random occupancies $\mathbf{K}_{n,z}$ where the 'fugacity' parameter z is in one-to-one correspondence with the average number κ of particles in the system. We shall show that it has a determinantal form and that the associated probabilities are rather permanental, that is, can be expressed in terms of the permanence of some enlarged matrix derived from W. Since W has non-negative entries, it turns out that the joint distribution of $\mathbf{K}_{n,z}$ is infinitely divisible (that is in the compound Poisson class). As a result, it makes sense to raise the probability generating function of $\mathbf{K}_{n,z}$ to the power α, for all $\alpha \in (0, \infty)$. This leads to a fractional occupancy statistics of order α, the special case $\alpha = 1$ corresponding to the standard Bose–Einstein occupancy model. Under the additional condition that W is definite non-negative, it makes sense to raise the probability generating function of $\mathbf{K}_{n,z}$ to the power α, for all $\alpha \in \{\ldots, -2, -1\}$: for such distributions, the maximal number of particles within each box cannot exceed $-\alpha$. The special case $\alpha = -1$ corresponds to the usual Fermi–Dirac occupancy model involving an exclusion principle: no more than one particle within each box. Therefore, for doubly non-negative weight matrices (that is, both non-negative and definite non-negative), fractional occupancies of all order $\alpha \in \{\ldots, -2, -1\} \cup (0, \infty)$ can be defined. In the limit $|\alpha| \nearrow \infty$, a Maxwell–Boltzmann occupancy model is found: grand-canonical box occupancies turn out to be independent and Poisson distributed. All these allegations can easily be derived from the version of the MacMahon master theorem which is relevant to our balls-in-boxes context, respecting transition weights.

We now briefly describe the content of this paper in more details.

Section 2 is devoted to generalities on thermalized urn models and occupancies which are of common use in the physics literature. Its purpose is to put this work in the physical context of standard urn models. The remaining part concerns our specific balls-in-boxes problem just described.

In section 3, we start illustrating our ideas in the case where W is a weight matrix with $\{0, 1\}-$entries, starting with the flat matrix. Here, the configurational weight of particle rearrangements simply counts the number of admissible rearrangements when a transition from box m to box m' is either forbidden or allowed, depending on whether $W_{m,m'}$ is 0 or 1. We discuss some examples in subsections 3.1 and 3.2; some are solvable, some are more involved. Subsection 3.3 considers the full case of a real-valued weight matrix that is doubly non-negative. Here we compute, for instance, the factorial moments of $\mathbf{K}_{n,z}$, the 2-boxes joint law of the occupancies $(K_{n,z}(m_1); K_{n,z}(m_2))$ and the marginal law of $K_{n,z}(m)$. We prove that the limiting distribution of $\mathbf{K}_{n,z}$ when $\alpha \nearrow \infty$ is the Maxwell–Boltzmann distribution. We characterize the limit law of $\mathbf{K}_{n,z}/\kappa$ when the expected number κ of particles goes to infinity, in terms of a specific multivariate gamma distribution.

Section 4 is devoted to what is needed of MacMahon master theorem which is relevant to our balls-in-boxes context.

Finally, we shall address the following problem. Assume that particles can only be placed in boxes in the positions $-\infty < x_1 \leqslant x_2 \leqslant \cdots \leqslant x_n < \infty$ on the real line. The box number of a particle now is the index of its position on $\mathbb{R}$ and the model is spatially extended; a particle is attached to the box number m if it stands at the mth position x_m. The purpose of section 5 is to construct natural doubly non-negative weight matrices W which are indexed by $\mathbf{x} := (x_1, \ldots, x_n) \in \mathbb{R}^n$, representing particle positions on the line. They are adapted to the spatially extended version of the occupancy problem. In such models, the $m \times m'$ entry $W_{m,m'}$ of W is of the form $W(x_m, x_{m'})$; using this, occupancy statistics can be considered when $-\log W(x_m, x_{m'})$ is now the energy required to move a particle from position x_m to position $x_{m'}$. The construction of such matrices parallels that of non-negative correlation functions whose spectral measure is positive. We shall also discuss the relevance of the recent notion of an infinitely divisible weight matrix, in the context of our investigations. Several examples are supplied.

2. Generalities on thermalized urn models and occupancies

To fix the background and notations, we start with generalities on standard classes of thermalized urn models before concentrating on the class of rearrangement urn models which is the main purpose of this paper. Urn problems consist in simplified models at the cornerstone between statistical mechanics and probability theory. The purpose of this introductory section is to put this work in the physical context of 'standard' urn models.

Consider an urn model with n distinguishable boxes within which k particles are to be allocated 'at random'. Suppose first the energy required to put k_m particles within the box number $m, m = 1, \ldots, n$, is $e_{k_m,m} > 0$. We shall let $\mathbf{k}_n := (k_1, \ldots, k_n)$ and $|\mathbf{k}_n| := \sum_{m=1}^{n} k_m = k$. Two cases then arise as follows.

(1) Either $e_{k_m,m}$ depends explicitly on the box label m. A familiar example is $e_{k_m,m} = k_m\epsilon_m$ where ϵ_m is the energy required to put a *single* particle within the box number $m, m = 1, \ldots, n$. Typically, $\epsilon_m = m^{\gamma}$, for some $\gamma > 1$. Note that $e_{k_m,m}$ is an increasing sequence in both arguments (k_m, m). In this case, energy is box dependent (say BDE for short).

(2) Or $e_{k_m,m}$ does not depend on m; hence, $e_{k_m,m} = e_{k_m}$ where e_{k_m} is simply assumed to increase with k_m. In this case, energy is box independent (say BIE).

Define the total energy of a configuration or state $\mathbf{k}_n$, satisfying $|\mathbf{k}_n| = k$, to be $\sum_{m=1}^{n} e_{k_m,m}$. Suppose the occupancy numbers within boxes are now random; call each of them $K_{k,n}(m)$; $m = 1, \ldots, n$. With $\mathbb{N} := \{0, 1, 2, \ldots\}$, we use the notational convenience

$$\mathbf{K}_{k,n} := (K_{k,n}(1), \ldots, K_{k,n}(n)) \in \mathbb{N}^n.$$

Therefore, $\mathbf{K}_{k,n}$ is the integral-valued random vector of occupancies counting the number of particles within the n different boxes in a k-particle system.

Equilibrium occupancy distributions which can be dealt with are Gibbs distributions for the probability law $\mathbb{P}(\mathbf{K}_{k,n} = \mathbf{k}_n)$ of $\mathbf{K}_{k,n}$. These laws can be obtained while maximizing occupancies' distribution entropy under the constraint that the average total energy $\mathfrak{h} := \mathbb{E}(\mathcal{H}_{k,n})$ of the k-particle system configurations within n boxes is fixed; naturally, $\mathbb{E}(\mathcal{H}_{k,n})$ denotes the mathematical expectation of $\mathcal{H}_{k,n} := \sum_{m=1}^{n} e_{K_{k,n}(m),m}$. In this Lagrangian setup, as usual, a parameter β (the reciprocal temperature) pops in; it is the Legendre conjugate of the average energy $\mathfrak{h}$.

Depending now on whether particles to be allocated are distinguishable (labeled) or not (unlabeled), two additional cases arise; finally, we are left with four possible cases which we shall briefly outline.

- First, assume that particles to be allocated within labeled boxes are *distinguishable* or labeled (as in the Maxwell–Boltzmann statistics, say MB for short).

(a) If energy is box dependent, $\mathbf{K}_{k,n}$ follows the BDE-MB (box-dependent energy, distinguishable particles) distribution if

$$\mathbb{P}(\mathbf{K}_{k,n} = \mathbf{k}_n) = \frac{1}{Z_{k,n}(\beta)} \prod_{m=1}^{n} \frac{\sigma_{k_m,m}^{-\beta}}{k_m!},$$

where the partition function

$$Z_{k,n}(\beta) = [z^k] \prod_{m=1}^{n} Q_{\beta,m}(z) \qquad \text{and} \qquad Q_{\beta,m}(z) = \sum_{k_m \in \mathbb{N}} \frac{z^{k_m}}{k_m!} \mathrm{e}^{-\beta e_{k_m,m}}$$

is a product of 'exponential' generating functions[1]. Here, $\sigma_{k_m,m}^{-\beta} := \mathrm{e}^{-\beta e_{k_m,m}}$ are the usual Boltzmann weights. In addition, β and $\mathfrak{h} := \mathbb{E}(\mathcal{H}_{k,n})$ are Legendre conjugates, related as usual through $-\partial_\beta \log Z_{k,n}(\beta) = \mathfrak{h}$ for each (k, n) fixed.

(b) When energy is box independent, $\mathbf{K}_{k,n}$ follows the BIE-MB (box-independent energy, distinguishable particles) distribution if

$$\mathbb{P}(\mathbf{K}_{k,n} = \mathbf{k}_n) = \frac{1}{Z_{k,n}(\beta)} \prod_{m=1}^{n} \frac{\sigma_{k_m}^{-\beta}}{k_m!},$$

where, with $\sigma_k := \exp e_k$,

$$Z_{k,n}(\beta) = [z^k] Q_\beta(z)^n \qquad \text{and} \qquad Q_\beta(z) = \sum_{k \in \mathbb{N}} \frac{z^k}{k!} \mathrm{e}^{-\beta e_k}.$$

In this case, the random variables $\mathbf{K}_{k,n}$ are exchangeable in the sense that, for all permutation σ of $\{1, \ldots, n\}$,

$$\mathbb{P}(K_{k,n}(m) = k_m;\, m = 1, \ldots, n) = \mathbb{P}(K_{k,n}(m) = k_{\sigma_m};\, m = 1, \ldots, n),$$

and the joint law of $\mathbf{K}_{k,n}$ is a symmetric function of $\mathbf{k}_n = (k_1, \ldots, k_n)$.

Examples. If we set $e_k = -\delta(k, 0)$ with δ the Kronecker symbol, then we get the Backgammon model whose glassy behavior has been extensively studied [16, 17, 27].

When $\beta \searrow 0$ (the infinite temperature limit), regardless of the energy sequence e_k, the limiting occupancy distribution is multinomial as it reads

$$\mathbb{P}(\mathbf{K}_{k,n} = \mathbf{k}_n) = \frac{1}{n^k} \frac{k!}{\prod_{m=1}^{n} k_m!}.$$

It corresponds to the equilibrium occupancies of the celebrated Ehrenfest model with $n \geqslant 2$ boxes [10]. Solving the corresponding transient Fokker–Planck equation of the Ehrenfest model requires some computational skill. For this, see [22, 23] and also the recent combinatorial 'tour de force' of [13].

- Assume now that particles are *undistinguishable* or unlabeled (as in the Bose–Einstein statistics, say BE).

(a) If energy is box dependent, $\mathbf{K}_{k,n}$ follows the BDE-BE distribution if

$$\mathbb{P}(\mathbf{K}_{k,n} = \mathbf{k}_n) = \frac{1}{Z_{k,n}(\beta)} \prod_{m=1}^{n} \sigma_{k_m,m}^{-\beta},$$

where the partition function

$$Z_{k,n}(\beta) = [z^k] \prod_{m=1}^{n} P_{\beta,m}(z) \qquad \text{with} \qquad P_{\beta,m}(z) = \sum_{k_m \in \mathbb{N}} z^{k_m} \mathrm{e}^{-\beta e_{k_m,m}}$$

is now the product of 'ordinary' generating functions.

[1] In the latter formula and in the forthcoming article, $[z^k] f(z)$ will stand for the z^k-coefficient in the series expansion of the function $f(z)$.

(b) If energy is box independent, $\mathbf{K}_{k,n}$ follows the BIE-BE distribution if

$$\mathbb{P}(\mathbf{K}_{k,n} = \mathbf{k}_n) = \frac{1}{Z_{k,n}(\beta)} \prod_{m=1}^{n} \sigma_{k_m}^{-\beta},$$

where

$$Z_{k,n}(\beta) = [z^k] P_\beta(z)^n \quad \text{and} \quad P_\beta(z) = \sum_{k \in \mathbb{N}} z^k \, \mathrm{e}^{-\beta e_k}.$$

Example. Assume that one further specifies in that

$$\frac{e_k}{k} \underset{k \nearrow \infty}{\to} 0,$$

meaning that energy is sub-linear. The first example one could think of is $e_k = k^\gamma$ where $\gamma \in (0, 1)$; as a second suitable example, $e_k = \log(1 + k)$ would do. Interest in such specific allocation models is because they are likely to present a phase transition (condensation) phenomenon at all temperatures in the first example and when temperature is small enough in the second example.

The BIE-BE model, with $e_k = \log(1+k)$ or equivalently $\sigma_k = 1+k$, corresponds precisely to the zeta urn model (see [4, 15]).

We now proceed with the rearrangement urn models under concern.

3. Multi-type weighted particle rearrangements

From now on, the remaining part of the paper concerns our specific balls-in-boxes problem as one arising from weighted particle rearrangements, as was briefly described in the introduction. The model we shall deal with is concerned with random box filling of an interacting particle system derived from weighted permutations of its constitutive items. As also indicated in the introduction, we first start with the simplest rearrangement case before extending the construction to more general weight matrices.

3.1. The simple rearrangement case

Suppose we are given a total amount of $k \geqslant 1$ labeled particles (items) of n different types (or colors), with $n \geqslant 2$. Let $k_m, m = 1, \ldots, n$, be the number of type-m particles in some initial configuration, with $|\mathbf{k}_n| := k_1 + \cdots + k_n = k$. Place k_m particles in the box number $m, m = 1, \ldots, n$, respectively. When considering the problem of enumerating the number of ways to permute these $\mathbf{k}_n$ particles ending up with $\mathbf{k}_n$ particles in the different boxes (or urns), the following generating function proves necessary:

$$\frac{1}{1 - z(u_1 + \cdots + u_n)} = \sum_{\mathbf{k}_n \in \mathbb{N}^n} z^{|\mathbf{k}_n|} \frac{|\mathbf{k}_n|!}{\prod_{m=1}^n k_m!} \prod_{m=1}^{n} u_m^{k_m}.$$

Here $\mathbf{u} := (u_1, \ldots, u_n) \in [0, 1]^n$ 'marks' the different types of particles and $z \in [0, z_\mathrm{c} := 1/n)$ is a 'marker' of the total number of particles. From this, interpreting the above generating function as an 'exponential' generating function, extracting the Taylor coefficients in the variables $\prod_{m=1}^n u_m^{k_m}$ of its series expansion, as conventional wisdom suggests, there are $|\mathbf{k}_n|! = k!$ ways to permute the $\mathbf{k}_n$ labeled (distinguishable) particles. In other words, if $\mathcal{S}(\mathbf{k}_n)$ is the set of all such permutations, then $|\mathcal{S}(\mathbf{k}_n)| = |\mathbf{k}_n|!$. This is poorly informative, so far.

Would the particles be unlabeled within each type class, there would clearly be $\frac{|\mathbf{k}_n|!}{\prod_{m=1}^n k_m!}$ ways to permute the $\mathbf{k}_n$ unlabeled particles, looking the above generating function as an 'ordinary' generating function and simply extracting the coefficients in the variables $\prod_{m=1}^{n} u_m^{k_m}$ of its series expansion. In this case, a permutation is called a rearrangement of the word $1^{k_1}, \ldots, n^{k_n}$. Clearly, when assigning $u_1 = \cdots = u_n = 1$, the $[z^k]$-coefficient of $(1 - zn)^{-1}$, which is n^k, will count the number of ways to permute (rearrange) k unlabeled particles of n different types, regardless of the number of particles within each class.

Assuming for example $n = 2, k_1 = 2, k_2 = 1, k = 3$, identifying the two particles of the first type, there are three different possible rearranged words out of $1^2 2^1$, namely 11 2, 12 1 and 21 1, whereas there are $2^3 = 8$ ways to permute three unlabeled particles of two different types: Ø 222, (1 22, 2 12, 2 21), (11 2, 12 1, 21 1) and 111 Ø corresponding respectively to the partitions $(k_1, k_2) = (0, 3), (1, 2), (2, 1)$ and $(3, 0)$ of $k = 3$. Here Ø is the empty box 'word'. For more details on rearrangements, see [5].

Let $W = J$ where J is the $n \times n$ flat 'weight' matrix whose entries are all equal to 1, for which $\text{Spect}(W) = \{0, \ldots (n-1) \text{ times} \ldots, 0; n\}$. With $|W| := \det(W)$ and $U := \text{diag}(\mathbf{u})$, it turns out that

$$\frac{1}{1 - z(u_1 + \cdots + u_n)} = |I - zUW|^{-1}.$$

Next, we note that

$$\left[z^{|\mathbf{k}_n|} \prod_{m=1}^{n} \frac{u_m^{k_m}}{k_m!}\right] \log|I - zUW|^{-1} = (|\mathbf{k}_n| - 1)!$$

counts the number of ways to permute cyclically the $\mathbf{k}_n$ labeled particles, when restricting $\mathcal{S}(\mathbf{k}_n)$ to $\mathcal{S}_c(\mathbf{k}_n)$, the set of all connected (one cycle) permutations, clearly with $|\mathcal{S}_c(\mathbf{k}_n)| = (|\mathbf{k}_n| - 1)!$.

With $\alpha > 0$ now 'marking' the number of cycles, this suggests us to also consider the generating function

$$|I - zUW|^{-\alpha} = \mathrm{e}^{-\alpha \log|I - zUW|}.$$

With $p \in \mathbb{N}$, the generating function $[\alpha^p]|I - zUW|^{-\alpha}$ is the one counting the permutations of n types of particles, when restricting them to be a collection of p disconnected cycles. In particular, $[\alpha]|I - zUW|^{-\alpha} = -\log|I - zUW|$ counts the permutations of n types of particles, when restricting them to be simple cycles. We shall return to this point later.

3.1.1. Canonical and grand-canonical randomization. Let $\mathbf{K}_{n,k} := (K_{n,k}(m), m = 1, \ldots, n)$ denote an integral-valued random vector which will stand for occupancies of the boxes $m = 1, \ldots, n$ given a total population of k particles.

Given $|\mathbf{k}_n| = k$, define naturally the (conditional) probability that $K_{n,k}(m) = k_m, m = 1, \ldots, n$, by the ratio of their configuration numbers

$$\mathbb{P}(\mathbf{K}_{n,k} = \mathbf{k}_n) = \frac{\binom{k}{k_1, \ldots, k_n}}{[z^k](1 - zn)^{-1}} \mathbf{1}(|\mathbf{k}_n| = k).$$

The event $\mathbf{K}_{n,k} = \mathbf{k}_n$ will be realized not only because there are k_m type-m particles in the box number m, but also because there is rearrangement of this peculiar configuration. In other words,

$$\mathbb{E}\left(\prod_{m=1}^{n} u_m^{K_{n,k}(m)}\right) = \frac{[z^k](1 - z(u_1 + \cdots + u_n))^{-1}}{[z^k](1 - zn)^{-1}}$$

is its canonical (conditional) probability generating function.

To avoid considering the simplex $|\mathbf{k}_n| = k$, suppose one randomizes the total number k of particles as follows: let there be a random number $K_{n,z}$ of particles, where

$$\mathbb{P}(K_{n,z} = k) = \frac{z^k [z^k](1 - zn)^{-1}}{(1 - zn)^{-1}}.$$

In other words, with $u \in [0, 1]$,

$$\mathbb{E}(u^{K_{n,z}}) = \frac{|I - zW|}{|I - zuW|} = \frac{1 - zn}{1 - zun}$$

is the (geometric) generating function of $K_{n,z}$. Then, parameters z and $0 < \kappa := \mathbb{E}(K_{n,z})$ are related through

$$\kappa := \kappa(z) = \frac{zn}{1 - zn},$$

and, since 'fugacity' $z \in [0, z_c = 1/n)$, these are in one-to-one correspondence. Given $\kappa := \mathbb{E}(K_{n,z}) = \frac{zn}{1-zn}$, define next the probability that $K_{n,z}(m) = k_m$, $m = 1, \ldots, n$, simply by

$$\mathbb{P}(\mathbf{K}_{n,z} = \mathbf{k}_n) = \frac{z^{|\mathbf{k}_n|}\binom{|\mathbf{k}_n|}{k_1,\ldots,k_n}}{(1 - zn)^{-1}}, \qquad \mathbf{k}_n \in \mathbb{N}^n.$$

In other words, with $W = J$,

$$\mathbb{E}\left(\prod_{m=1}^{n} u_m^{K_{n,z}(m)}\right) = \frac{(1 - z(u_1 + \cdots + u_n))^{-1}}{(1 - zn)^{-1}} = \frac{|I - zW|}{|I - zUW|}$$

stands for its (grand canonical) probability generating function, now conditioned on the expected number $\kappa(z)$ of particles in the system.

3.1.2. Asymptotics for $\kappa \nearrow \infty$. One suspects that, for fixed n, the following convergence in distribution will hold:

$$\frac{\mathbf{K}_{n,z}}{\kappa} \xrightarrow{d}_{\kappa \nearrow \infty} \mathbf{X}_n,$$

where $\mathbf{X}_n := (X(1), \ldots, X(n))$ is an n-dimensional random vector supported by $\mathbb{R}_+^n$. Let us prove this and characterize the joint law of $\mathbf{X}_n$. Recalling $\kappa := \kappa(z) = \frac{zn}{1-zn}$, let us assume $z = (1 - \epsilon)/n$ where, ϵ being close to 0^+, κ, which is of order ϵ^{-1}, tends to ∞. Then, with $\mathbf{s} := (s_1, \ldots, s_n)$ and $S := \mathrm{diag}(\mathbf{s})$,

$$\begin{aligned}
\mathbb{E}\left(\prod_{m=1}^{n} \mathrm{e}^{-s_m K_{n,z}(m)/\kappa}\right) &\sim \mathbb{E}\left(\prod_{m=1}^{n} \mathrm{e}^{-\epsilon s_m K_{n,n^{-1}(1-\epsilon)}(m)}\right) \\
&= \frac{\epsilon}{1 - (1 - \epsilon)\left(\sum_1^n \mathrm{e}^{-\epsilon s_m}\right)/n} \sim \frac{\epsilon}{1 - (1 - \epsilon)\left(n - \epsilon \sum_1^n s_m\right)/n} \\
&\sim \frac{1}{1 + \left(\sum_1^n s_m\right)/n} = \frac{1}{|I + z_c S W|} = \mathbb{E}\left(\prod_{m=1}^{n} \mathrm{e}^{-s_m X(m)}\right).
\end{aligned}$$

This is the Laplace Stieltjes transform of a symmetric exponentially distributed random vector $\mathbf{X}_n$, with one-dimensional marginals $\mathbb{E}(\mathrm{e}^{-s_m X(m)}) = \frac{1}{1+s_m/n}$, $m = 1, \ldots, n$, those of exponentially distributed random variables on $\mathbb{R}_+$ with mean n^{-1}.

3.1.3. Fractional statistics. Let $z_\alpha := z/\alpha$. We shall also be interested in random variables with distributions $\mathbb{P}_\alpha$ defined by

$$\mathbb{E}_\alpha\left(\prod_{m=1}^{n} u_m^{K_{n,z}(m)}\right) = \frac{\left(1 - \frac{z}{\alpha}(u_1 + \cdots + u_n)\right)^{-\alpha}}{\left(1 - \frac{z}{\alpha} n\right)^{-\alpha}} = \left(\frac{|I - z_\alpha W|}{|I - z_\alpha U W|}\right)^{\alpha},$$

where $\alpha \in \{\ldots, -2, -1\} \cup (0, \infty)$ and $z < \alpha/n$ if $\alpha > 0$ or $z \geqslant 0$ if $\alpha \in \{\ldots, -2, -1\}$. Since $W = J$, with $(\alpha)_k := \alpha(\alpha+1)\ldots(\alpha+k-1)$, this is

$$\mathbb{P}_\alpha(\mathbf{K}_{n,z} = \mathbf{k}_n) = (1 - z_\alpha n)^\alpha \cdot z_\alpha^{|\mathbf{k}_n|} \frac{(\alpha)_{|\mathbf{k}_n|}}{\prod_{m=1}^n k_m!}, \qquad \mathbf{k}_n \in \mathbb{N}^n.$$

When $\alpha = -i < 0$, the range of $\mathbf{K}_{n,z}$ is $\mathbf{k}_n \in \{0, \ldots, i\}^n$. For instance, for $\mathbf{k}_n \in \{0, 1\}^n$, $\mathbb{P}_{-1}(\mathbf{K}_{n,z} = \mathbf{k}_n)$ is the (Fermi-) joint probability to find one (respectively, no) particle in the box number m_q if $k_{m_q} = 1$ (respectively, if $k_{m_q} = 0$). Thus, when $W = J$, $\mathbf{K}_{n,z}$ is well defined under $\mathbb{P}_\alpha$ for all $\alpha \in \{\ldots, -2, -1\} \cup (0, \infty)$. In particular,

$$\mathbb{E}_\alpha(u^{K_{n,z}}) = \left(\frac{1 - z_\alpha n}{1 - z_\alpha un}\right)^\alpha,$$

showing that $K_{n,z}$ has negative binomial $(\alpha, z_\alpha n)$ distribution (when $\alpha > 0$) or multinomial $(-\alpha, (-z_\alpha n)/(1-nz_\alpha))$ distribution ($\alpha \in \{\ldots, -2, -1\}$), with mean $\kappa := \mathbb{E}_\alpha(K_{n,z}) = \frac{zn}{1-nz_\alpha}$. Such α-distributions may be thought of as fractional occupancy statistics of order α. When $\alpha = -1, \alpha = +1, |\alpha| \nearrow \infty$ we get a usual Fermi–Dirac, Bose–Einstein or Maxwell–Boltzmann distribution for $\mathbf{K}_{n,z}$, respectively. When $\alpha = k/2$ where k is any integer, we get a para-Boson statistics (see [1, 19]). One of the questions next raised is: for which W is $\mathbf{K}_{n,z}$ well defined for all α in the positivity spectrum $\{\ldots, -2, -1\} \cup (0, \infty)$?

3.2. Weighted restricted rearrangements: $\{0, 1\}$*-weight matrix*

These elementary considerations first suggest to introduce more generally the quantities $|I - zUW|^{-1}$, where W is now a $n \times n$ weight matrix whose entries all belong to $\{0, 1\}$. By doing so, we address the problem of enumerating the number of ways to permute the $|\mathbf{k}_n| = k$ particles when the transition from type m to type m' is allowed at the only condition that entry $W_{m,m'} = 1$. Define formally the energy (cost) of transition $m \to m'$ as $H_{m,m'} := -\log W_{m,m'}$. Then, would $W_{m,m'} = 0$, the transition from type m to type m' is forbidden as the energy required to realize this transition is infinite. Would $W_{m,m'} = 1$, the transition $m \to m'$ requires no particular energy. Proceeding in this way, the random occupancies $\mathbf{K}_{n,z}$ are now dictated by the weighted restricted rearrangements encoded by W. For related problems, see [9].

The quantity $|I - zUW|^{-1}$ is defined for $\mathbf{u} := (u_1, \ldots, u_n) \in [0, 1]^n$ and $z \in [0, z_c := 1/\rho(W))$ where, with λ_m; $m = 1, \ldots, n$, the spectrum of W, $\rho(W) = \|W\| = \max(|\lambda_m|, m = 1, \ldots, n)$ is the spectral radius of W. The critical fugacity z_c is the reciprocal of the spectral radius of W and $|I - zUW|^{-1}$ first becomes singular at z_c. Since all such W are non-negative, by the Perron–Foebenius theorem, the eigenvalue with the largest modulus is real. Since W only has $\{0, 1\}$−entries, $\rho(W) \in [1, n]$ and so $z_c \in [1/n, 1]$. The weighted random occupancies $K_{n,z}(m)$, $m = 1, \ldots, n$, can be defined accordingly. As we shall indeed see later in the following section, such random variables are well defined; in fact they are always well defined as soon as W has non-negative entries. This is because the Taylor coefficients in the variables $\prod_{m=1}^n u_m^{k_m}$ of the series expansion of $\frac{|I-zW|}{|I-zUW|}$ are the permanents $\mathrm{Per}(W(\mathbf{k}_n))$. Here, $W(\mathbf{k}_n)$ are the $|\mathbf{k}_n| \times |\mathbf{k}_n|$ matrix obtained by repeating (removing and deleting) each $W_{m,m'}$ into a size $k_m \times k_{m'}$ block if k_m and $k_{m'}$ are both positive (otherwise). Permanents of a matrix with non-negative entries are non-negative. Note that the basic quantity appearing in the law of $K_{n,z}$ reads $|I - zW|^{-1} = \prod_{m=1}^n (1 - z\lambda_m)^{-1}$.

Similarly, random variables $\mathbf{K}_{n,z}$ with law $\mathbb{P}_\alpha$ parameterized by $\alpha > 0$ are well defined for all $\alpha > 0$ when W has in particular non-negative entries. This is because the Taylor coefficients in the variables $\prod_{m=1}^n u_m^{k_m}$ of the series expansion of $\left(\frac{|I-z_\alpha W|}{|I-z_\alpha UW|}\right)^\alpha$ are now proportional to the α-permanents $\mathrm{Per}_\alpha(W(\mathbf{k}_n))$. α-permanents of a matrix with non-negative entries are non-negative (see the following section). In all such cases, random variables $\mathbf{K}_{n,z}$ with law

$\mathbb{P}_\alpha$ (where $\alpha > 0$) are infinitely divisible that is in the compound Poisson class. When $\alpha \in \{\ldots, -2, -1\}$, a necessary and sufficient condition for $\mathbf{K}_{n,z}$ with law $\mathbb{P}_\alpha$ to be well defined is that W has all its 2^n principal minors non-negative (see [29], Prop. 6.1 for the necessity condition). If $\mathbf{K}_{n,z}$ with law $\mathbb{P}_\alpha$ is to be defined for all $\alpha \in \{\ldots, -2, -1\} \cup (0, \infty)$, a sufficient condition is that W has all its principal minors non-negative and is non-negative. If W is in addition symmetric, then a doubly non-negative W would do (doubly non-negative matrices are those which are both definite non-negative and with non-negative entries).

Examples.

- Assume $W = I$. Then, with $z < z_c = 1$,

$$|I - zUW|^{-1} = \prod_{m=1}^{n} (1 - zu_m)^{-1} = \frac{1}{1 - \oplus_{m=1}^{n} (zu_m)},$$

where $x_1 \oplus x_2 = x_1 + x_2 - x_1 x_2$ is the commutative and associative probabilistic sum. Here,

$$\left[z^{|\mathbf{k}_n|} \prod_{m=1}^{n} \frac{u_m^{k_m}}{k_m!} \right] |I - zUW|^{-1} = \prod_{m=1}^{n} k_m!$$

counts the number of ways to permute the $\mathbf{k}_n$ labeled particles when the image particle is forced to return back to its own type. Therefore,

$$\mathbb{E}(u^{K_{n,z}}) = \frac{|I - zW|}{|I - zuW|} = \left(\frac{1 - z}{1 - zu} \right)^n$$

is the generating function of $K_{n,z}$, with mean $\kappa = (nz)/(1 - z)$. The z^k-coefficient of $(1 - z)^{-n}$ is $\binom{n+k-1}{k}$.

Clearly, in this interaction-free case,

$$\frac{\mathbf{K}_{n,z}}{\kappa} \xrightarrow{d}_{\kappa \nearrow \infty} \mathbf{X}_n,$$

where the components of the random vector $\mathbf{X}_n$ are independent and identically distributed (iid), mean 1, exponentially distributed random variables on $\mathbb{R}_+$.

- In the last two examples, the weight matrix is definite non-negative. It has all principal minors non-negative. The canonical form of a $\{0, 1\}$-valued definite non-negative weight matrix W is made of p flat Jordan blocks J_q (of type J), $q = 1, \ldots, p$, where the sizes of J_q are $n_q \times n_q$, $q = 1, \ldots, p$, with $\sum_{q=1}^{p} n_q = n$ and $1 \leqslant n_1 \leqslant \cdots \leqslant n_p$. Since W is symmetric, outside the Jordan blocks, W has zero entries and so is block diagonal. The number of such matrices, therefore, is the number of partitions of n. The spectrum of W is $\mathrm{Spect}(W) = \cup_{q=1}^{p} \{0, \ldots (n_q - 1) \text{ times} \ldots, 0; n_q\}$ and with $n_0 := 0$ and $\overline{n}_q := \sum_{r=0}^{q} n_q$, $q = 0, \ldots, p$,

$$|I - zUW|^{-1} = \prod_{q=1}^{p} \left(1 - z\left(u_{\overline{n}_{q-1}+1} + \cdots + u_{\overline{n}_q}\right)\right)^{-1}$$
$$= \left[1 - \oplus_{q=1}^{p} \left(z(u_{\overline{n}_{q-1}+1} + \cdots + u_{\overline{n}_q})\right)\right]^{-1},$$

defined for $z < 1/n_p$. Representing the above partition sequence $1 \leqslant n_1 \leqslant \cdots \leqslant n_p$ by the sequence $0 =: m_0 < 1 \leqslant m_1 < \cdots < m_r$ where each m_q, $q = 1, \ldots, r$, has multiplicity d_q now with $\sum_{q=1}^{r} d_q m_q = n$,

$$\mathbb{E}(u^{K_{n,z}}) = \frac{|I - zW|}{|I - zuW|} = \prod_{q=1}^{r} \left(\frac{1 - zm_q}{1 - zum_q} \right)^{d_q}$$

is the generating function of $K_{n,z}$, with mean

$$\kappa = \sum_{q=1}^{r} (zd_q m_q)/(1 - zm_q).$$

The first introductory example ($W = J$) corresponds to an irreducible case with $r = 1, m_1 = n$ and $d_1 = 1$, whereas the second example ($W = I$) is completely reducible with $r = 1, m_1 = 1$ and $d_1 = n$.

For this class of W, $\mathbf{K}_{n,z}$ is well defined under $\mathbb{P}_\alpha$ for all $\alpha \in \{\ldots, -2, -1\} \cup (0, \infty)$.

- (Derangements) Assume now that $W = J - I$ which is symmetric but not definite positive. One can check that $\mathrm{Spect}(W) = \{-1, \ldots (n-1) \text{ times} \ldots, -1; n-1\}$. Then, with $z < z_c = 1/(n-1)$, it holds that

$$|I - zUW|^{-1} = \frac{1}{1 - \sum_{p=2}^{n} z^p (p-1) \sigma_p(\mathbf{u})},$$

where

$$\sigma_p(\mathbf{u}) = \sum_{1 \leqslant m_1 < \cdots < m_p \leqslant n} \prod_{q=1}^{p} u_{m_q}$$

are the elementary symmetric functions. For this example,

$$\left[z^{|\mathbf{k}_n|} \prod_{m=1}^{n} \frac{u_m^{k_m}}{k_m!} \right] |I - zUW|^{-1}$$

counts the number of ways to permute the $\mathbf{k}_n$ labeled particles, when no permuted particle is allowed to return to its own type. A permutation in this class is called a derangement (see [18]).

In this case, with $0 \leqslant z < 1/\rho(W) = 1/(n-1)$, we get

$$|I - zW|^{-1} = \frac{1}{1 - \sum_{p=2}^{n} z^p (p-1) {n \atop p}} = \frac{1}{(1+z)^{n-1}[1 - (n-1)z]}$$

with $[z^k]|I - zW|^{-1} = \sum_{l=0}^{k} (-1)^l \binom{n+l-2}{l} (n-1)^{k-l} \geqslant 0$. So, for instance,

$$\mathbb{E}(u^{K_{n,z}}) = \frac{|I - zW|}{|I - zuW|} = \left(\frac{1+z}{1+zu} \right)^{n-1} \frac{1 - (n-1)z}{1 - (n-1)zu}$$

is the generating function of $K_{n,z}$, with mean

$$\kappa = (n-1)z \left[\frac{1}{1 - (n-1)z} - \frac{z}{1+z} \right].$$

For this class of W, $\mathbf{K}_{n,z}$ is well defined under $\mathbb{P}_\alpha$ for all $\alpha \in (0, \infty)$ (see [14]) but, since the principal minors can be negative, not for $\alpha \in \{\ldots, -2, -1\}$.

- If W is any of the $(n-1)!$ orthogonal matrices of a cyclic (connected) permutation

$$|I - zUW|^{-1} = \frac{1}{1 - \prod_{m=1}^{n} (zu_m)}, \qquad z < z_c = 1.$$

For this example, there is no way to permute the $\mathbf{k}_n$ labeled particles, unless all $k_m = k_1, m = 1, \ldots, n$, in which case this number is $(k_1!)^n$. Here,

$$\mathbb{E}(u^{K_{n,z}}) = \frac{|I - zW|}{|I - zuW|} = \frac{1 - z^n}{1 - (zu)^n}$$

is the generating function of $K_{n,z}$, with mean $\kappa = (nz^n)/(1 - z^n)$. Note that the spectrum of W consists in the n roots of unity. With $\lambda_m = \mathrm{e}^{2\mathrm{i}\pi(m-1)/n}$, $m = 1, \ldots, n$, note the identity $\sum_{m=1}^{n} \frac{z\lambda_m}{1-z\lambda_m} = \frac{nz^n}{1-z^n} = \kappa$.

Clearly, in this case

$$\frac{\mathbf{K}_{n,z}}{\kappa} \xrightarrow{d}_{\kappa \nearrow \infty} \mathbf{X}_n,$$

where, with $\mathbb{E}\big(\prod_{m=1}^{n} \mathrm{e}^{-s_m X(m)}\big) = \big(1 + \big(\sum_1^n s_m\big)/n\big)^{-1}$, $\mathbf{X}_n$ has symmetric multivariate exponential distribution.

For this class of W, $\mathbf{K}_{n,z}$ is well defined under $\mathbb{P}_\alpha$ for all $\alpha \in (0, \infty)$ but, since the principal minors can be negative, not for $\alpha \in \{\ldots, -2, -1\}$.

The next two examples are more involved and would require some additional knowledge of the weight matrix spectrum.

- *Periodic nearest neighbors interactions*. Assume $W_{1,2} = W_{1,n} = 1$; $W_{m,m+1} = W_{m,m-1} = 1$, $m = 2, \ldots, n-1$, and $W_{n,1} = W_{n,n-1} = 1$, the other entries being all equal to 0. In this case, $\rho(W) = 2$ and $z_c = 1/2$. Matrix W is symmetric with real eigenvalues. In a standard (non-periodic) nearest neighbors interactions model, $W_{1,n} = W_{n,1} = 0$ and W is strictly tridiagonal.
- *Tournaments*. Assume $W_{m,m} = 0$, $m = 1, \ldots, n$. For all $m' > m$, fix $W_{m,m'} \in \{0, 1\}$ and force $W_{m',m} = 1 - W_{m,m'}$ so that $\sum_{m,m'} W_{m,m'} = \binom{n}{2}$. Each W fulfills $W + W' = J - I$. There are $2^{n(n-1)/2}$ tournaments as issues of pair matching games with n players.

Remark. The distribution of $\mathbf{K}_{n,z}$ is exchangeable if and only if $\mathbb{E}\big(\prod_{m=1}^{n} u_m^{K_{n,z}(m)}\big) = \mathbb{E}\big(\prod_{m=1}^{n} u_{\sigma_m}^{K_{n,z}(m)}\big)$ for all permutation σ of $\{1, \ldots, n\}$, in other words, if and only if $|I - zUW|$ is a symmetric function of $\mathbf{u} := (u_1, \ldots, u_n)$. This will be the case under the following special conditions: $W = aI + b(J - I)$, where a and b belong to $\{0, 1\}$. Thus, when $W = I$, $W = J - I$ or $W = J$. This is also the case when W is the weight matrix of a cyclic (connected) permutation. In all these cases, for each order, all principal minors of W coincide, which is a necessary and sufficient condition for the distribution of $\mathbf{K}_{n,z}$ to be exchangeable. This is clear from the development of $|I - zUW|$ in terms of all principal minors of W.

3.3. Rearrangements from doubly non-negative weight matrices

Let W be an arbitrary weight matrix with real non-negative entries and with non-negative principal minors. With $z_\alpha := z/\alpha$, we are interested in random variables $\mathbf{K}_{n,z}$ with probability generating functions

$$\mathbb{E}_\alpha\left(\prod_{m=1}^{n} u_m^{K_{n,z}(m)}\right) = \left(\frac{|I - z_\alpha W|}{|I - z_\alpha UW|}\right)^{\alpha},$$

where $\alpha \in \{\ldots, -2, -1\} \cup (0, \infty)$ and $z < \alpha/n$ if $\alpha > 0$ or $z \geqslant 0$ if $\alpha \in \{\ldots, -2, -1\}$. These random variables are well defined for all α in the prescribed range and infinitely divisible when $\alpha > 0$. They correspond to occupancy α-distributions arising from rearrangements with weight W. If W is in addition symmetric, then W belongs to the class of doubly non-negative matrices.

For general doubly non-negative real-valued matrices, $\mathbf{K}_{n,z}$ is well defined under $\mathbb{P}_\alpha$ where α varies in the announced range.

3.3.1. Factorial moments of $\mathbf{K}_{n,z}$. Let $k_m \geqslant 0$, $m = 1, \ldots, n$, and $\{n\}_k := n(n-1)\ldots(n-k+1)$, $\{n\}_0 := 1$. Define the factorial moments of $\mathbf{K}_{n,z}$ to be

$$\mu_\alpha(\mathbf{k}_n) := \mathbb{E}_\alpha\left(\prod_{m=1}^{n}\{K_{n,z}(m)\}_{k_m}\right).$$

We have

$$\mathbb{E}_\alpha\left(\prod_{m=1}^{n} u_m^{K_{n,z}(m)}\right) = \left(\frac{|I - z_\alpha W|}{|I - z_\alpha U W|}\right)^\alpha = \left(\frac{|I - z_\alpha W|}{|I - z_\alpha W - z_\alpha (U - I) W|}\right)^\alpha$$
$$= (|I - (U - I) z_\alpha W (I - z_\alpha W)^{-1}|)^{-\alpha} =: \left(\left|I - (U - I) W_{z_\alpha}\right|\right)^{-\alpha}.$$

Therefore, the factorial moments $\mu_\alpha(\mathbf{k}_n)$ of $\mathbf{K}_{n,z}$ exist; they are given by the Taylor coefficients in the variables $\prod_{m=1}^{n}(u_m - 1)^{k_m}$ of the series expansion of $\left(\left|I - (U - I) W_{z_\alpha}\right|\right)^{-\alpha}$, namely $\mathrm{Per}_\alpha\left(W_{z_\alpha}(\mathbf{k}_n)\right)$, where $W_{z_\alpha} = z_\alpha W (I - z_\alpha W)^{-1}$ is the resolvent matrix of W. If W has non-negative entries, so does W_{z_α} and therefore the factorial moments of $\mathbf{K}_{n,z}$, namely $\mathrm{Per}_\alpha\left(W_{z_\alpha}(\mathbf{k}_n)\right)$ are non-negative. If W is definite positive with positive eigenvalues λ_m, so does W_{z_α} with eigenvalues $(z_\alpha \lambda_m)/(1 - z_\alpha \lambda_m)$. For doubly non-negative weight matrices, $\mu_\alpha(\mathbf{k}_n)$ are well defined for all α in the full range $\{\ldots, -2, -1\} \cup (0, \infty)$.

3.3.2. Marginal distribution of $K_{n,z}(m)$. With U_m a diagonal matrix whose $m \times m$ entry is u_m, all other diagonal entries being 1, with $z_\alpha := z/\alpha$, we have

$$\mathbb{E}_\alpha\left(u_m^{K_{n,z}(m)}\right) = \left(\frac{|I - z_\alpha W|}{|I - z_\alpha U_m W|}\right)^\alpha = \left(\frac{|I - z_\alpha W|}{|I - z_\alpha W - z_\alpha (U_m - I) W|}\right)^\alpha$$
$$= (|I - (U_m - I) z_\alpha W (I - z_\alpha W)^{-1}|)^{-\alpha} = \left(\left|I - (U_m - I) W_{z_\alpha}\right|\right)^{-\alpha}$$
$$= \left(1 - (u_m - 1)\left(W_{z_\alpha}\right)_{m,m}\right)^{-\alpha} =: \left(\frac{1 - p_m}{1 - p_m u_m}\right)^\alpha.$$

Since $\left(W_{z_\alpha}\right)_{m,m} \geqslant 0$, when $\alpha > 0$, this is the distribution of a negative binomial random variable with parameters $\left(\alpha, p_m := \frac{(W_{z_\alpha})_{m,m}}{1 + (W_{z_\alpha})_{m,m}}\right)$. Here, p_m is the success probability depending on z and α. When $\alpha \in \{\ldots, -2, -1\}$, this generating function is that of a multinomial distribution with parameters $\left(-\alpha, \pi_m := -\left(W_{z_\alpha}\right)_{m,m}\right)$, where π_m now is the probability that the underlying Bernoulli random variable takes the value 1.

Note from this analysis that in any case for α,

$$\kappa := \mathbb{E}_\alpha(K_{n,z}) = \alpha \sum_{m=1}^{n} \left(W_{z_\alpha}\right)_{m,m} = \alpha \cdot \mathrm{tr}\left(W_{z_\alpha}\right).$$

3.3.3. Joint distribution of $(K_{n,z}(m_1), K_{n,z}(m_2))$. Let $1 \leqslant m_1 < m_2 \leqslant n$. With U_{m_1,m_2} a diagonal matrix whose entries $m_1 \times m_1$ and $m_2 \times m_2$ are u_{m_1} and u_{m_2} respectively, all other diagonal entries being 1, we have

$$\mathbb{E}_\alpha\left(u_{m_1}^{K_{n,z}(m_1)} u_{m_2}^{K_{n,z}(m_2)}\right) = \left(\frac{|I - z_\alpha W|}{|I - z_\alpha U_{m_1,m_2} W|}\right)^\alpha = \left(\left|I - \left(U_{m_1,m_2} - I\right) W_{z_\alpha}\right|\right)^{-\alpha}$$
$$= \left(1 - \sum_{i \in \{1,2\}} \left(u_{m_i} - 1\right)\left(W_{z_\alpha}\right)_{m_i,m_i} + \left(u_{m_1} - 1\right)\left(u_{m_2} - 1\right)\left|W_{z_\alpha}(m_1, m_2)\right|\right)^{-\alpha},$$

where $\left|W_{z_\alpha}(m_1, m_2)\right|$ is the corresponding minor of W_{z_α}. From this, we get in particular

$$\begin{aligned}\mathrm{Cov}_\alpha(K_{n,z}(m_1), K_{n,z}(m_2)) &= \alpha\left[\left(W_{z_\alpha}\right)_{m_1,m_1}\left(W_{z_\alpha}\right)_{m_2,m_2} - \left|W_{z_\alpha}(m_1, m_2)\right|\right]\\ &= \alpha\left(W_{z_\alpha}\right)_{m_1,m_2}\left(W_{z_\alpha}\right)_{m_2,m_1},\end{aligned}$$

which is non-negative when W_{z_α} (or W) is non-negative or when W_{z_α} (or W) is symmetric (in particular, definite positive). When $\alpha > 0$, $(K_{n,z}(m_1), K_{n,z}(m_2))$ are positively correlated. Note that the above covariance decreases with α and that $\mathrm{Cov}_\alpha(K_{n,z}(m_1), K_{n,z}(m_2)) \to_{\alpha\nearrow\infty} 0$. In sharp contrast, when $\alpha \in \{\ldots, -2, -1\}$, these random variables are negatively correlated.

3.3.4. Limiting distribution of $\mathbf{K}_{n,z}$ *when* $\alpha \nearrow \infty$. To the first order in α, the exponential-trace expression of the determinant gives

$$\mathbb{E}_\alpha\left(\prod_{m=1}^n u_m^{K_{n,z}(m)}\right) = \left(\frac{|I - z_\alpha W|}{|I - z_\alpha UW|}\right)^\alpha \underset{\alpha\nearrow\infty}{\to} \mathrm{e}^{-\,\mathrm{tr}(zW) + \,\mathrm{tr}(zUW)} = \prod_{m=1}^n \mathrm{e}^{-z(1-u_m)W_{m,m}}.$$

This shows that asymptotically

$$\mathbf{K}_{n,z} \overset{d}{\underset{\alpha\nearrow\infty}{\to}} \mathbf{P}_{n,z},$$

where $\mathbf{P}_{n,z} := (P_{n,z}(1), \ldots, P_{n,z}(n))$ are mutually independent Poisson distributed random variables with respective intensities $zW_{m,m}$, proportional to the diagonal terms of W. This is the limiting Maxwell–Boltzmann distribution for $\mathbf{K}_{n,z}$.

3.3.5. Limit law of $\mathbf{K}_{n,z}/\kappa$ *when* $\kappa \nearrow \infty$. First assume that $\alpha = 1$ and let $z_\mathrm{c} := 1/\rho(W)$. Assume that W differs from the identity. Letting $z := z_\mathrm{c}(1-\epsilon)$, $\kappa = \mathrm{tr}(W_z)$ grows like ϵ^{-1}, to the first order in ϵ. This is because $\kappa = \sum_1^n (z\lambda_m)/(1 - z\lambda_m)$ where $(\lambda_m, m = 1, \ldots, n)$ are the eigenvalues of W with $\rho(W)$ being the largest (real) of these: this model does not show phase transition phenomena because $\kappa := \kappa(z)$ is always divergent at critical fugacity z_c.

Now, with $\mathbf{s} := (s_1, \ldots, s_n)'$ and $S := \mathrm{diag}(\mathbf{s})$,

$$\begin{aligned}\mathbb{E}\left(\prod_{m=1}^n \mathrm{e}^{-\epsilon s_m K_{n,z}(m)}\right) &\underset{\epsilon\searrow 0}{\sim} \frac{|I - z_\mathrm{c}(1-\epsilon)W|}{|I - z_\mathrm{c}(1-\epsilon)(1-\epsilon S)W|}\\ &\underset{\epsilon\searrow 0}{\sim} \frac{|I - z_\mathrm{c}W + \epsilon z_\mathrm{c}W|}{|I - z_\mathrm{c}W + \epsilon z_\mathrm{c}(I+S)W|}.\end{aligned}$$

Observing $|I - z_\mathrm{c}W| = 0$, the exponential-trace expansion of the determinant gives, in this singular case,

$$|I - z_\mathrm{c}W + \epsilon z_\mathrm{c}W| \underset{\epsilon\searrow 0}{\sim} \epsilon \cdot \mathrm{tr}(z_\mathrm{c}W \cdot \mathrm{adj}(I - z_\mathrm{c}W)),$$

where $\mathrm{adj}(A)$ is the adjugate matrix of A. Thus,

$$\mathbb{E}\left(\prod_{m=1}^n \mathrm{e}^{-\epsilon s_m K_{n,z}(m)}\right) \underset{\epsilon\searrow 0}{\to} \frac{\mathrm{tr}(z_\mathrm{c}W \cdot \mathrm{adj}(I - z_\mathrm{c}W))}{\mathrm{tr}((I+S)z_\mathrm{c}W \cdot \mathrm{adj}(I - z_\mathrm{c}W))} =: \mathbb{E}\left(\prod_{m=1}^n \mathrm{e}^{-s_m X_n(m)}\right).$$

This shows that asymptotically

$$\frac{\mathbf{K}_{n,z}}{\kappa} \overset{d}{\underset{\kappa\nearrow\infty}{\to}} \mathbf{X}_n,$$

where the law of $\mathbf{X}_n := (X_n(1), \ldots, X_n(n))$ is characterized by the above joint Laplace–Stieltjes transform. Developing the traces, with $\langle \mathbf{s}, \mathbf{X}_n\rangle$ the scalar product of $\mathbf{s} \geqslant \mathbf{0}$ and $\mathbf{X}_n$, we get more specifically

$$\mathbb{E}(\mathrm{e}^{-\langle \mathbf{s}, \mathbf{X}_n \rangle}) = \left(1 + \sum_{m=1}^{n} s_m \mu_m\right)^{-1} = (1 + \langle \mathbf{s}, \mu_n \rangle)^{-1},$$

where $\mu_n := (\mu_1, \ldots, \mu_n)$, $\mu_m = b_m \big/ \sum_1^n b_k$ and $b_m = (z_c W \cdot \operatorname{adj}(I - z_c W))_{m,m}$, $m = 1, \ldots, n$, are the diagonal terms of the matrix $z_c W \cdot \operatorname{adj}(I - z_c W)$. In any case, it holds that $\sum_1^n \mu_m = 1$ so that $\sum_1^n X_n(m)$ has mean 1 exponential law. The marginals of $\mathbf{X}_n$ are exponentially distributed with mean μ_m. Note that, unless some special conditions hold on W, the distributions of $\mathbf{K}_{n,z}$ and $\mathbf{X}_n$ are not exchangeable. The telling feature of the $\mathbf{X}_n$-law is that any linear non-negative combination of its components remains exponentially distributed.

When $\alpha > 0$, considering the model $\mathbf{K}_{n,z}$ now under $\mathbb{P}_\alpha$, similar arguments would show that, with $\kappa = \operatorname{tr}(W_{z_\alpha})$,

$$\frac{\mathbf{K}_{n,z}}{\kappa} \underset{\kappa \nearrow \infty}{\overset{d}{\to}} \mathbf{X}_n,$$

where the law of $\mathbf{X}_n$ is now a multivariate-gamma distribution given by

$$\mathbb{E}(\mathrm{e}^{-\langle \mathbf{s}, \mathbf{X}_n \rangle}) = \left(1 + \sum_{m=1}^{n} s_m \mu_m\right)^{-\alpha} = (1 + \langle \mathbf{s}, \mu_n \rangle)^{-\alpha},$$

where μ_n is now given in terms of the following b_m:

$$b_m = (z_{c,\alpha} W \cdot \operatorname{adj}(I - z_{c,\alpha} W))_{m,m}, \qquad m = 1, \ldots, n,$$

with $z_{c,\alpha} := z_c/\alpha$. The latter Laplace–Stieltjes transform of $\mathbf{X}_n$ is well defined because for all $\mathbf{s} > \mathbf{0}$, all $\lambda > 0$, $\mathbb{E}(\mathrm{e}^{-\lambda \langle \mathbf{s}, \mathbf{X}_n \rangle})$, which is the Laplace–Stieltjes transform of the positive scalar random variable $\langle \mathbf{s}, \mathbf{X}_n \rangle$, is a Bernstein (completely monotone) function of the gamma type. The general shape of the moment generating function of a multivariate gamma random variable $\mathbf{X}_n$ is determinantal such as $\mathbb{E}(\mathrm{e}^{-\langle \mathbf{s}, \mathbf{X}_n \rangle}) = |I + SM|^{-\alpha}$ for some admissible matrix M. In our case, M takes the particular form: $M = [\mu_1 \mathbf{1}, \ldots, \mu_n \mathbf{1}]$, where $\mathbf{1} := (1, \ldots, 1)'$. The spectrum of such matrices is $\{0, \ldots (n-1) \text{ times} \ldots, 0; \sum_1^n \mu_m = 1\}$ with non-negative real eigenvalues only; by Proposition 4.6 of Vere-Jones [29], it gives a well-defined Laplace–Stieltjes transform.

4. Combinatorics related to MacMahon master theorem

In this section, we shall develop some combinatorial aspects of the MacMahon master theorem which are useful to our purposes. We shall let $\mathbb{N} = \{0, 1, 2, \ldots\}$, $\mathbb{N}_* = \{1, 2, \ldots\}$.

We shall assume that W is an $n \times n$ non-negative weight matrix, with $|W| = \det(W)$. We shall let Per W stand for the permanent of W. We recall that $\mathbf{k}_n = (k_1, \ldots, k_n) \in \mathbb{N}^n$, $|\mathbf{k}_n| = k_1 + \cdots + k_n$. $\mathbf{u} = (u_1, \ldots, u_n) \in [0, 1]^n$ and that $U = \operatorname{diag}(\mathbf{u})$, $I =$ Identity. Define $W(\mathbf{k}_n)$ to be the $|\mathbf{k}_n| \times |\mathbf{k}_n|$ matrix obtained by repeating (removing and deleting) each $W_{m,m'}$ into a size $k_m \times k_{m'}$ block if k_m and $k_{m'}$ are both positive (otherwise). Assuming that $z \in [0, 1/\rho(W))$, we have

$$\begin{aligned}
|I - zUW|^{-1} &= \sum_{\mathbf{k}_n \in \mathbb{N}^n} z^{|\mathbf{k}_n|} \prod_{m=1}^{n} u_m^{k_m} \left[\prod_{m=1}^{n} u_m^{k_m}\right] \prod_{m=1}^{n} (W\mathbf{u})_m^{k_m} \\
&= \sum_{\mathbf{k}_n \in \mathbb{N}^n} z^{|\mathbf{k}_n|} \prod_{m=1}^{n} \frac{u_m^{k_m}}{k_m!} \operatorname{Per} W(\mathbf{k}_n) \\
&= \sum_{\mathbf{k}_n \in \mathbb{N}^n} z^{|\mathbf{k}_n|} \prod_{m=1}^{n} \frac{u_m^{k_m}}{k_m!} \sum_{\sigma \in \mathcal{S}(\mathbf{k}_n)} \prod_{m,l_m} W_{m,\sigma_1(m,l_m)}
\end{aligned}$$

where if $\sigma(m, l_m) = (m', l')$, $l_m = 1, \ldots, k_m$, $m = 1, \ldots, n$, $\sigma_1(m, l_m) = m'$ gives the type of the image of particle l_m in the class m. In the formulae displayed above, the first identity is due to MacMahon (see [8], for a short proof). It took some time to realize that the Taylor coefficients in $\mathbf{u}$ of the above expression can in fact be identified to the permanent of $W(\mathbf{k}_n)$ which is the content of the subsequent expressions (see [29, 30] for historical remarks and background).

Remark. If W is diagonal, with positive diagonal entries $(\lambda_m, m = 1, \ldots, n)$, one can check that $\mathrm{Per}\, W(\mathbf{k}_n) = \prod_{m=1}^{n} \left(k_m! \lambda_m^{k_m}\right)$ so that, as required,

$$|I - zUW|^{-1} = \sum_{\mathbf{k}_n \in \mathbb{N}^n} z^{|\mathbf{k}_n|} \prod_{m=1}^{n} u_m^{k_m} \lambda_m^{k_m} = \prod_{m=1}^{n} (1 - z u_m \lambda_m)^{-1}.$$

Let $\alpha > 0$ or $\alpha \in \{-1, -2, \ldots\}$. Let $\mathrm{cyc}(\sigma)$ be the number of cycles in $\sigma \in \mathcal{S}(\mathbf{k}_n)$. Then,

$$\begin{aligned}
|I - zUW|^{-\alpha} &= \sum_{\mathbf{k}_n \in \mathbb{N}^n} z^{|\mathbf{k}_n|} \prod_{m=1}^{n} \frac{u_m^{k_m}}{k_m!} \mathrm{Per}_\alpha W(\mathbf{k}_n) \\
&= \sum_{\mathbf{k}_n \in \mathbb{N}^n} z^{|\mathbf{k}_n|} \prod_{m=1}^{n} \frac{u_m^{k_m}}{k_m!} \sum_{\sigma \in \mathcal{S}(\mathbf{k}_n)} \alpha^{\mathrm{cyc}(\sigma)} \prod_{m, l_m} W_{m, \sigma_1(m, l_m)} \\
&= \sum_{\mathbf{k}_n \in \mathbb{N}^n} (\alpha z)^{|\mathbf{k}_n|} \prod_{m=1}^{n} \frac{u_m^{k_m}}{k_m!} \sum_{\sigma \in \mathcal{S}(\mathbf{k}_n)} \left(\frac{1}{\alpha}\right)^{|\mathbf{k}_n| - \mathrm{cyc}(\sigma)} \prod_{m, l_m} W_{m, \sigma_1(m, l_m)}.
\end{aligned}$$

Thus,

$$\left|I - \frac{z}{\alpha} UW\right|^{-\alpha} = \sum_{\mathbf{k}_n \in \mathbb{N}^n} z^{|\mathbf{k}_n|} \prod_{m=1}^{n} \frac{u_m^{k_m}}{k_m!} \sum_{\sigma \in \mathcal{S}(\mathbf{k}_n)} \left(\frac{1}{\alpha}\right)^{|\mathbf{k}_n| - \mathrm{cyc}(\sigma)} \prod_{m, l_m} W_{m, \sigma_1(m, l_m)}$$

and

$$\left|I - \frac{z}{\alpha} UW\right|^{-\alpha} = \frac{1}{1 - \left(1 - |I - \frac{z}{\alpha} UW|^{\alpha}\right)}$$

with

$$1 - \left|I - \frac{z}{\alpha} UW\right|^{\alpha} = \sum_{\mathbf{k}_n \in \mathbb{N}^n} (-z)^{|\mathbf{k}_n|} \prod_{m=1}^{n} \frac{u_m^{k_m}}{k_m!} \sum_{\sigma \in \mathcal{S}(\mathbf{k}_n)} \left(\frac{-1}{\alpha}\right)^{|\mathbf{k}_n| - \mathrm{cyc}(\sigma)} \prod_{m, l_m} W_{m, \sigma_1(m, l_m)}.$$

Further, with ‘tr’ standing for trace, the weight function

$$\sigma \to w_\alpha(\sigma) = \alpha^{\mathrm{cyc}(\sigma)} \prod_{m, l_m} W_{m, \sigma_1(m, l_m)}$$

being multiplicative (equal to the product of the weights over the connected components of σ),

$$\begin{aligned}
-\alpha \log \left|I - \frac{z}{\alpha} UW\right| &= \sum_{k \geqslant 1} \left(\frac{1}{\alpha}\right)^{k-1} \frac{z^k}{k} \mathrm{tr}(\{UW\}^k) \\
&= \sum_{\mathbf{k}_n \in \mathbb{N}_*^n} z^{|\mathbf{k}_n|} \prod_{m=1}^{n} \frac{u_m^{k_m}}{k_m!} \sum_{\sigma \in \mathcal{S}_c(\mathbf{k}_n)} \left(\frac{1}{\alpha}\right)^{|\mathbf{k}_n| - 1} \prod_{m, l_m} W_{m, \sigma_1(m, l_m)},
\end{aligned}$$

where $\mathcal{S}_c(\mathbf{k}_n)$ is the subset of connected permutations σ from $\mathcal{S}(\mathbf{k}_n)$, satisfying $\mathrm{cyc}(\sigma) = 1$ and $\sigma(n, k_n) = (1, 1)$. Thus,

$$\left[z^{|\mathbf{k}_n|}\prod_{m=1}^{n}\frac{u_m^{k_m}}{k_m!}\right]\left\{-\alpha\log\left|I-\frac{z}{\alpha}UW\right|\right\}=\sum_{\sigma\in\mathcal{S}_c(\mathbf{k}_n)}\left(\frac{1}{\alpha}\right)^{|\mathbf{k}_n|-1}\prod_{m,l_m}W_{m,\sigma_1(m,l_m)}$$

involves cyclic weight products $\prod_{m=1}^{n}\prod_{l_m=1}^{k_m}W_{m,\sigma_1(m,l_m)}$, since $\sigma\in\mathcal{S}_c(\mathbf{k}_n)$ with $\sigma_1(n,k_n)=1$. In particular,

$$\left[z^{|\mathbf{k}_n|}\prod_{m=1}^{n}\frac{u_m^{k_m}}{k_m!}\right]\{-\log|I-zUW|\}=\sum_{\sigma\in\mathcal{S}_c(\mathbf{k}_n)}\prod_{m,l_m}W_{m,\sigma_1(m,l_m)}=w_1(\mathcal{S}_c(\mathbf{k}_n)).$$

If in particular $\alpha=-1$, then

$$|I+zUW|=\sum_{\mathbf{k}_n\in\mathbb{N}^n}z^{|\mathbf{k}_n|}\prod_{m=1}^{n}\frac{u_m^{k_m}}{k_m!}\sum_{\sigma\in\mathcal{S}(\mathbf{k}_n)}(-1)^{|\mathbf{k}_n|-\mathrm{cyc}(\sigma)}\prod_{m,l_m}W_{m,\sigma_1(m,l_m)},$$

where

$$\sum_{\sigma\in\mathcal{S}(\mathbf{k}_n)}(-1)^{|\mathbf{k}_n|-\mathrm{cyc}(\sigma)}\prod_{m,l_m}W_{m,\sigma_1(m,l_m)}=|W(\mathbf{k}_n)|,$$

which is null unless $\mathbf{k}_n\in\{0,1\}^n$. Thus, with $|W(\{m_1,\ldots,m_p\})|$ a principal minor of W

$$|I+zUW|=1+\sum_{p=1}^{n}z^p\sum_{1\leqslant m_1<\cdots<m_p\leqslant n}\prod_{q=1}^{p}u_{m_q}|W(\{m_1,\ldots,m_p\})|.$$

Note that

$$1-|I-zUW|=\sum_{p=1}^{n}(-1)^{p-1}z^p\sum_{1\leqslant m_1<\cdots<m_p\leqslant n}\prod_{q=1}^{p}u_{m_q}|W(\{m_1,\ldots,m_p\})|$$

so that

$$|I-zUW|^{-1}=\frac{1}{1-(1-|I-zUW|)}.$$

From these combinatorial developments, it is clear (from positivity of induced probabilities) that if W is definite non-negative, the occupancies $\mathbf{K}_{n,z}$ are well defined under $\mathbb{P}_\alpha$ for all $\alpha>0$ and infinitely divisible. If in addition W is definite non-negative, all principal minors of W are non-negative and so $\mathbf{K}_{n,z}$ are well defined under $\mathbb{P}_\alpha$ for all $\alpha\in\{\ldots,-2,-1\}$. For more on permanents, determinants, MacMahon master theorem and the like, see [2, 5, 7, 26, 29, 30].

5. Doubly non-negative and infinitely divisible weight matrices. Spatially extended boxes

Recall a weight matrix which is both non-negative and non-negative definite is a doubly non-negative matrix. As underlined before, doubly non-negative weight matrices play a special role in our occupancy problems.

5.1. A probabilistic construction of doubly non-negative weight matrices

Let us first give a systematic construction which generates doubly non-negative matrices. In the process, we shall obtain the spatially extended system on the real line discussed in the introduction.

Let (X_1,X_2) be a pair of iid random variables on $\mathbb{R}$ with a density, say $\phi(x)$. Consider the random variable $X=X_1-X_2$. Its density, say $f(x)$, exists and is given by $f(x)=\phi*\overset{\vee}{\phi}(x)$,

$x \in \mathbb{R}$, where $\overset{\vee}{\phi}(x) := \phi(-x)$ and $*$ stands for convolution. Clearly, $f(x) = f(-x)$ and f is symmetric. Let $\Phi(\mathrm{i}\lambda) = \mathbb{E}(\mathrm{e}^{\mathrm{i}\lambda X_1})$ be the common characteristic function of both X_1 and X_2. Then $|\Phi(\mathrm{i}\lambda)|^2$ is the (real) Fourier transform of $f(x)$ or the characteristic function of X. Clearly $g(\lambda) := \frac{1}{2\pi}|\Phi(\mathrm{i}\lambda)|^2 \geqslant 0$ for almost allλ and since f is continuous and integrable, by Bochner theorem, f is definite non-negative in that, for all integer n, all real numbers $\mathbf{x} := (x_m, m = 1, \ldots, n)$ and all $\mathbf{z} \in \mathbb{C}^n : \mathbf{z}'[f(x_m - x_{m'})]\mathbf{z} \geqslant 0$. In this interpretation, the function $g(\lambda)$ should be regarded as the integrable spectral density associated with the correlation function$f$. Here, $[f(x_m - x_{m'})]$ is the $n \times n$ square matrix whose (m, m') entry is $f(x_m - x_{m'})$. Assuming $W = [W_{m,m'}]$ and $W_{m,m'} = f(x_m - x_{m'})$, then the weight matrix is doubly non-negative. It should be emphasized that strictly speaking, $W = W(\mathbf{x})$, which is now a function of $\mathbf{x}$. Also note also that this construction yields a correlation function which is also a probability density function so that the total mass of f is 1, which is purely arbitrary.

Let $\psi(x) \geqslant 0$ be any non-negative function on $\mathbb{R}$. Then, with $W_{m,m'} = \psi(x_m) f(x_m - x_{m'})\psi(x_{m'})$, $W := [W_{m,m'}]$ is diagonally congruent to the latter and so is also doubly non-negative. Clearly, its entries are indeed non-negative and definite positiveness is preserved under congruence. If $\psi(x) = C > 0$, this constant can be used to readjust the mass of f if needed.

Remarks.

(i) Let P be the permutation matrix which maps the indices of $(x_m, m = 1, \ldots, n)$ into the those of $-\infty < x_1 \leqslant \cdots \leqslant x_n < \infty$, where now x_m are ordered on the real line. By considering instead the novel congruent weight matrix $P'WP$, we can assume, without loss of generality, that $W_{m,m'} = \psi(x_m) f(x_m - x_{m'})\psi(x_{m'})$, where x_m are ordered. Note that in this construction, a particle is attached to the box number m if and only if it stands at the mth position x_m on the real line. In this context, $H_{m,m'} := -\log W_{m,m'}$ is now the energy required to move a particle from site x_m to site $x_{m'}$.

(ii) Let w_x be a (stationary) white noise (δ-correlated) process, indexed by $x \in \mathbb{R}$. Let $z_x := (\phi * w)_x$, where ϕ is as above. Then $z_x, x \in \mathbb{R}$, is a stationary process whose correlation function is $\mathrm{Cov}[z_{x'} z_{x'+x}] = f(x) = \phi * \overset{\vee}{\phi}(x)$.

(iii) Assume that both (X_1, X_2) have a common law supported by $(0, \infty)$ in the above construction. Then, it can be checked that $f(x) = h(|x|)$, where $h(z) = \int_0^\infty \phi(y + z)\phi(y)\,\mathrm{d}y, z > 0$.

(iv) Assume that both (X_1, X_2) have a symmetric common law supported by $\mathbb{R}$. Then $f(x) = \phi^{*2}$ and $\mathbb{E}(\mathrm{e}^{\mathrm{i}\lambda X_1})$ is real. A given f belongs to this class if it is 2-divisible on $\mathbb{R}$. Note that $f(x) = h(|x|)$, where $h(z) = \int_{\mathbb{R}} \phi(z - y)\phi(y)\,\mathrm{d}y, z > 0$.

(v) Exploiting this Fourier isomorphism on integrable positive functions, reversing the role played by 'space' x and wave number λ, we conclude that $f(x) = \frac{1}{2\pi}|\Phi(\mathrm{i}x)|^2$ is a correlation function whose associated spectral measure is $g(\lambda) = \phi * \overset{\vee}{\phi}(\lambda), \lambda \in \mathbb{R}$.

Examples.

(i) Let $\phi(x) = \mathrm{e}^{-x}\mathbf{1}(x > 0)$. Then, $f(x) = \mathrm{e}^{-|x|}/2, x \in \mathbb{R}$, is a continuous integrable correlation function with spectral density $g(\lambda) = 1/[\pi(1 + \lambda^2)]$. For all n and $-\infty < x_1 \leqslant \cdots \leqslant x_n < \infty$, the matrix $W = [\mathrm{e}^{-|x_m - x_{m'}|}]$ has the required properties. Let $\psi(x) = \mathrm{e}^x$. Then, with $W_{m,m'} = \mathrm{e}^{x_m}\,\mathrm{e}^{-|x_m - x_{m'}|}\,\mathrm{e}^{x_{m'}} = \min(\mathrm{e}^{2x_m}, \mathrm{e}^{2x_{m'}})$, $W := [W_{m,m'}]$ also has the required properties. Specifying x_m to $x_m = (\log m)/2$, the matrix with entries $\min(m, m')$ has the required properties. Putting $t_m = \mathrm{e}^{x_m}$, $W := [\min(t_m, t_{m'})]$ has the required property where we recognize the correlation kernel of the standard Brownian motion on $\mathbb{R}_+$.

(ii) Let $\phi(x) = \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{-x^2/2}$, $x \in \mathbb{R}$.
Then $g(\lambda) = \frac{1}{2\pi}\,\mathrm{e}^{-\lambda^2}$, showing that $f(x) = \phi^{*2}(x) = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}\lambda x} g(\lambda)\,\mathrm{d}\lambda = \frac{1}{2\sqrt{\pi}}\,\mathrm{e}^{-x^2/4}$, $x \in \mathbb{R}$.

(iii) Assume $\phi(x) = \exp[-(x+\mathrm{e}^{-x})]$ so that X_1 has Gumbel density on $\mathbb{R}$. One can check that $f(x) = 1/[2(1+\cosh(x))]$. We have $\Phi(\mathrm{i}\lambda) = \Gamma(1-\mathrm{i}\lambda)$ and $g(\lambda) := |\Gamma(1-\mathrm{i}\lambda)|^2/(2\pi) = \lambda/2\sinh(\lambda\pi)$.

More generally, let $\beta > 0$ and assume now $\phi(x) = \exp[-(\beta x + \mathrm{e}^{-x})]$ on $\mathbb{R}$. Then, with $B(.,.)$ the Euler beta function, $f(x) = [1/2(\cosh(x/2))]^{2\beta}/B(\beta,\beta)$. We have $\Phi(\mathrm{i}\lambda) = \Gamma(\beta-\mathrm{i}\lambda)/\Gamma(\beta)$ and $g(\lambda) := |\Gamma(\beta-\mathrm{i}\lambda)|^2/(2\pi)$.

Specifying $\beta = 1/2$, we obtain

$$f(x) = 1/(2\pi\cosh(x/2)) \quad \text{and} \quad g(\lambda) = 1/[2\pi\cosh(\pi\lambda)].$$

This shows that the pair $f(x) = 1/\cosh(x)$ and $g(\lambda) = 1/\cosh(\pi\lambda/2)$ is admissible. Thus $W_{m,m'} = 1/\cosh(x_m - x_{m'})$, but also

$$W_{m,m'} = \mathrm{e}^{x_m}\,\mathrm{e}^{x_{m'}}/[2\cosh(x_m - x_{m'})] = 1/(\mathrm{e}^{-2x_m} + \mathrm{e}^{-2x_{m'}})$$

is doubly non-negative. Assuming a lattice case $x_m = (-\log m)/2$, the Cauchy matrix with entries $1/(m+m')$ has the required properties.

(iv) Assume $f(x) = \frac{1}{2\Gamma(1+1/\gamma)}\,\mathrm{e}^{-|x|^\gamma}$, $x \in \mathbb{R}, \gamma \in (0,1]$. The above construction could apply if, in particular, one could prove that there is a ϕ supported by $(0,\infty)$ such that $\frac{1}{\Gamma(1+1/\gamma)}\,\mathrm{e}^{-z^\gamma} = \int_0^\infty \phi(y+z)\phi(y)\,\mathrm{d}y$, $z > 0$. But, unless $\gamma = 1$, this is not the case. In fact, in this case, there is a symmetric ϕ such that $f(x) \propto \mathrm{e}^{-|x|^\gamma} = \phi^{*2}$. ϕ is characterized by $2\int_0^\infty \cos(\lambda x)\phi(x)\,\mathrm{d}x = [2\pi g(\lambda)]^{1/2}$, where $g(\lambda)$ is a symmetric stable(γ) density (see [11], page 583, for an expression). Indeed, $f(x)$ is a symmetric distribution whose density is restricted to $(0,\infty)$, namely, $f_+(x) = \frac{1}{\Gamma(1+1/\gamma)}\,\mathrm{e}^{-x^\gamma}$, $x \in \mathbb{R}_+, \gamma \in (0,1)$, is completely monotone. By theorem 10.1, page 202 of [28], $f(x)$ is infinitely divisible so that, for k integer, there is a probability density ϕ_k on $\mathbb{R}$ such that $f = \phi_k^{*k}$. The above claim follows from this with $k = 2$.

However, it is not necessary to prove this to conclude that $f(x)$ (even when $\gamma \in (0,2]$) is indeed a correlation function because $g(\lambda) := \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}\lambda x} f(x)\,\mathrm{d}x$ is a stable (strictly positive) density with shape parameter γ and so is $\geqslant 0$ for almost all λ.

(v) Assume $\phi(x) = \mathbf{1}(x \in [0,1])$. Then, $f(x) = (1-|x|)\,\mathbf{1}(x \in [-1,1])$ and $g(\lambda) = \frac{1}{2\pi}\left(\frac{\sin\lambda/2}{\lambda/2}\right)^2$ is an admissible pair. Note that $\mathbf{1}\,(x \in [0,1])$ is not itself a correlation function as its Fourier transform, which is $\frac{1}{\pi}\frac{\sin\lambda}{\lambda}$, is not $\geqslant 0$.

The set of doubly non-negative correlation functions forms a closed cone as this property is preserved under convex linear combinations and point-wise products and if a sequence $(f_k; k \geqslant 1)$ of such correlation functions converges, then the limit remains doubly non-negative.

If f_1 and f_2 are two doubly non-negative correlation functions with associated weight matrices $W_i = [f_i(x_m - x_{m'})]$, $i = 1, 2$, then the weight matrix W associated with $f = f_1 \times f_2$ is $W = W_1 \circ W_2$, where $\circ$ stands for the Hadamard (or Schur) entry-wise product. The Hadamard product of doubly non-negative matrices indeed is a doubly non-negative matrix.

Fix $1 \leqslant m_1 < \cdots < m_p \leqslant n$ a subsequence of length p from $\{1,\ldots,n\}$. Considering the principal sub-matrices $W(\{m_1,\ldots,m_p\})$ of W, we get a sub-matrix of the same type as the original one. This is useful in the computation of $|W(\{m_1,\ldots,m_p\})|$ since this can be read from that of $|W|$. For instance, if $W = [(\mathrm{e}^{x_m} + \mathrm{e}^{x_{m'}})^{-1}]$, it has been known since Cauchy that

$$|W| = \frac{\prod_{1\leqslant m<m'\leqslant n} (\mathrm{e}^{x_{m'}} - \mathrm{e}^{x_m})^2}{\prod_{1\leqslant m<m'\leqslant n} (\mathrm{e}^{x_{m'}} + \mathrm{e}^{x_m})}.$$

From this, we immediately get

$$|W(\{m_1,\ldots,m_p\})| = \frac{\prod_{1\leqslant q<q'\leqslant p}(\mathrm{e}^{x_{m_{q'}}} - \mathrm{e}^{x_{m_q}})^2}{\prod_{1\leqslant q<q'\leqslant p}(\mathrm{e}^{x_{m_{q'}}} + \mathrm{e}^{x_{m_q}})}.$$

5.2. Infinitely divisible weight matrices

We shall briefly discuss here conditions under which raising W to the power β (in some sense) gives birth to a family of doubly non-negative matrices for all $\beta > 0$.

- Let H be a $n\times n$ symmetric matrix. With $\beta > 0$, consider the weight matrix $W_\beta := \mathrm{e}^{-\beta H}$. For all $\beta > 0$, this weight matrix is definite non-negative (eigenvalues are real and non-negative) but, unless some extraordinary circumstances, its off-diagonal entries have no reason to be non-negative, even if $W = \mathrm{e}^{-H}$ were chosen so as to have itself non-negative entries. A question could be: which are the doubly non-negative weight matrices W whose β-powers remain doubly non-negative for all $\beta > 0$? Preserving positive definiteness and entry-wise positivity of (standard) β-powers together is a very rare combination and very much basis dependent. We now turn to a related question which is more meaningful in our context.
- Let W be a doubly non-negative weight matrix. With $\beta > 0$, let $W^{\circ\beta}$ be the Hadamard β-power of W, with entries $(W^{\circ\beta})_{m,m'} := W^{\beta}_{m,m'}$. This new matrix has non-negative entries and, in any case, when $\beta \geqslant \beta_c := n-2$ it remains definite non-negative (see [12]). However (when $n \geqslant 3$), only under some peculiar circumstances it is still a non-negative definite matrix for all $\beta > 0$ (although by the Schur theorem, it always is when β is an integer). Doubly non-negative matrices whose Hadamard β-powers remain doubly non-negative for all $\beta > 0$ are called infinitely divisible (ID) matrices (see[3]). The Schur product of infinitely divisible matrices yields a novel infinitely divisible matrix. Examples of infinitely divisible matrices are

$$W_{m,m'} = (\mathrm{e}^{x_m} + \mathrm{e}^{x_{m'}})^{-1}, \qquad \Gamma(\mathrm{e}^{x_m} + \mathrm{e}^{x_{m'}} + 1)/[\Gamma(\mathrm{e}^{x_m} + 1)\Gamma(\mathrm{e}^{x_{m'}} + 1)],$$
$$\max(\mathrm{e}^{x_m}, \mathrm{e}^{x_{m'}})^{-1} = \min(\mathrm{e}^{-x_m}, \mathrm{e}^{-x_{m'}}), \qquad \cosh\left(\tfrac{1}{2}(x_m - x_{m'})\right)^{-1},$$
$$\exp[-|x_m - x_{m'}|], \quad \text{and more generally} \quad \exp[-|x_m - x_{m'}|^{\gamma}] \text{ for } \gamma \in (0,2],$$

where $-\infty < x_1 \leqslant x_2 \leqslant \cdots \leqslant x_n < \infty$.

In some (stationary) cases, the correlation kernel $W_{m,m'} = W(x_m, x_{m'})$ only depends on the difference of $(x_m, x_{m'})$.

Remark. In the above language to construct doubly non-negative weight matrices W from positive correlation functions f, it can be checked directly that W is infinitely divisible if and only if $f(x)^\beta$ remains a correlation function for all $\beta > 0$ which clearly is the case for the examples displayed above. If the correlation function f fulfills this property, then, considering its spectral density $g(\lambda)$, for each integer k, there is a spectral measure $g_k(\lambda)$ such that $g = g_k^{*k}$. In this context, infinite divisibility is the eventual property of the spectral density.

For such infinitely divisible doubly non-negative matrices (with strictly positive entries), the Hadamard logarithm of W, defined by

$$H := [H_{m,m'}] \qquad \text{and} \qquad H_{m,m'} = -\log W_{m,m'},$$

satisfies $\mathbf{z}'H\mathbf{z} \leqslant 0$ for all $\mathbf{z} \in \mathbb{C}^n$ such that $\sum_{m=1}^{n} z_m = 0$; the 'energy' matrix H is said to be conditionally definite non-positive. The converse is also true: conditional definite non-positivity of H implies infinite divisibility of $W = \mathrm{e}^{-\circ H}$ (see [25]).

Further, H is conditionally definite non-positive if and only if the $(n-1)\times(n-1)$ matrix Δ with entries

$$\Delta_{m,m'} = H_{m,m'} + H_{m+1,m'+1} - H_{m,m'+1} - H_{m+1,m'}\ ,\ m, m' \in \{1,\ldots,n-1\}$$

is definite non-positive ($\mathbf{z}'H\mathbf{z} \leqslant 0$ for all $\mathbf{z} \in \mathbb{C}^n$).

Example. The matrix $W_{m,m'} = \exp[|x_m|^\gamma + |x_{m'}|^\gamma - |x_m - x_{m'}|^\gamma]$ is ID because it is congruent to an ID matrix when $\gamma \in (0,2]$. Therefore, $-H_{m,m'} := \log W_{m,m'} = |x_m|^\gamma + |x_{m'}|^\gamma - |x_m - x_{m'}|^\gamma$ is conditionally definite non-negative. In the latter expression, we can recognize the correlation kernel of fractional Brownian motion with the Hurst exponent $\gamma/2$.

A block-diagonal matrix whose Jordan blocks are individually infinitely divisible is globally infinitely divisible. So is a matrix which can be brought into this form after a simultaneous permutation of its rows and columns.

Assume that particles can only be placed in boxes in the positions $-\infty < x_1 \leqslant x_2 \leqslant \cdots \leqslant x_n < \infty$ on the real line. In this setting, the box number of a particle is the index of its position on $\mathbb{R}$ and the model is spatially extended. Let $W^{\circ\beta}$ with $W = \mathrm{e}^{-\circ H}$ be infinitely divisible where $H_{m,m'} = H(x_m, x_{m'})$ are, say, as in the previous examples. For such matrices W, for all $\alpha \in (0,\infty]$, $\beta > 0$,

$$\mathbb{E}_\alpha\left(\prod_{m=1}^n u_m^{K_{n,z}(m)}\right) = \left(\frac{|I - z_\alpha W^{\circ\beta}|}{|I - z_\alpha U W^{\circ\beta}|}\right)^\alpha$$

is the probability generating function of a well-defined infinitely divisible random vector corresponding to box occupancies associated with $W^{\circ\beta}$. When $\alpha = 1$ (Bose–Einstein statistics), it addresses the problem of computing the grand-canonical weight of the configurations obtained by rearranging an average number $\kappa = \kappa(z)$ of multi-type particles when the weight associated with the transition m to m' at 'temperature' $1/\beta > 0$ is $\mathrm{e}^{-\beta H_{m,m'}}$. The probability of these configurations follows next upon normalizing. Since for all $\beta > 0$, $W^{\circ\beta}$ has all its minors non-negative, it is also the probability generating function of a well-defined generalized multinomial random variable when $\alpha \in \{\ldots,-2,-1\}$. We note that, since $W^{\circ\beta}$ is definite non-negative,

$$|I - z_\alpha U W^{\circ\beta}|^{-\alpha} = |I - z_\alpha U^{1/2} W^{\circ\beta} U^{1/2}|^{-\alpha} = \prod_{m=1}^n (1 - z_\alpha \lambda_{m,\beta}(\mathbf{u}))^{-\alpha},$$

where $\lambda_{m,\beta}(\mathbf{u})$, $m = 1,\ldots,n$, are the real non-negative eigenvalues of $U^{1/2}W^{\circ\beta}U^{1/2}$ which is congruent to $W^{\circ\beta}$ and definite non-negative for all $\mathbf{u} \in [0,1]^n$. Therefore, with $\lambda_{m,\beta} := \lambda_{m,\beta}(\mathbf{1})$ the eigenvalues of $W^{\circ\beta}$

$$\mathbb{E}_\alpha\left(\prod_{m=1}^n u_m^{K_{n,z}(m)}\right) = \left(\frac{|I - z_\alpha W^{\circ\beta}|}{|I - z_\alpha U W^{\circ\beta}|}\right)^\alpha = \prod_{m=1}^n \left(\frac{1 - z_\alpha\lambda_{m,\beta}}{1 - z_\alpha\lambda_{m,\beta}(\mathbf{u})}\right)^{-\alpha}.$$

This shows that the probability generating function of $\mathbf{K}_{n,z}$ under $\mathbb{P}_\alpha$ can be factorized. As a very particular (interaction-free) example, if $0 < x_1 \leqslant x_2 \leqslant \cdots \leqslant x_n < 1$ and if $W = \mathrm{diag}(x_1,\ldots,x_n)$, then $H = \mathrm{diag}(\epsilon_1,\ldots,\epsilon_n)$ with $\epsilon_m = -\log x_m$, $0 < \epsilon_n \leqslant \cdots \leqslant \epsilon_1$ and

$$\mathbb{E}_\alpha\left(\prod_{m=1}^n u_m^{K_{n,z}(m)}\right) = \left(\frac{|I - z_\alpha W^{\circ\beta}|}{|I - z_\alpha U W^{\circ\beta}|}\right)^\alpha = \prod_{m=1}^n \left(\frac{1 - z_\alpha e^{-\beta\epsilon_m}}{1 - z_\alpha u_m e^{-\beta\epsilon_m}}\right)^\alpha$$

with independent negative binomial factors. In particular, if $\alpha > 0$,

$$\mathbb{P}_\alpha(\mathbf{K}_{n,z} = \mathbf{k}_n) = \prod_{m=1}^n (1 - z_\alpha\,\mathrm{e}^{-\beta\epsilon_m})^\alpha \cdot z_\alpha^{|\mathbf{k}_n|} \prod_{m=1}^n \frac{(\alpha)_{k_m}}{k_m!}\,\mathrm{e}^{-\beta k_m\epsilon_m}\ , \qquad \mathbf{k}_n \in \mathbb{N}^n,$$

which favors states with lower energy. This model is familiar in occupancy problems of discretized energy levels.

Also note that the canonical occupancy probabilities on the simplex $|\mathbf{k}_n| = k$ are

$$\mathbb{P}_\alpha(\mathbf{K}_{k,n} = \mathbf{k}_n) = \frac{1}{Z_{k,n,\alpha}(\beta)} \prod_{m=1}^{n} \frac{(\alpha)_{k_m}}{k_m!} \, \mathrm{e}^{-\beta k_m \epsilon_m}.$$

corresponding when $\alpha = 1$ (respectively $\alpha \nearrow \infty$) to a BDE-BE (respectively BDE-MB) occupancy model in the terminology used in section 2. Here, energy $e_{k_m,m}$ required to put k_m particles within the box number m is box dependent: it reads $e_{k_m,m} = k_m \epsilon_m$, where ϵ_m interprets as the energy required to put a *single* particle within the box number m, $m = 1, \ldots, n$.

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