Point Processes with Specified Low Order Correlations

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Abstract

Given functions $\rho_k(\mathbf{r}_1, ..., \mathbf{r}_k)$, defined on $(\mathbb{R}^d)^k$ or $(\mathbb{Z}^d)^k$ for $k = 1, ..., n$, we wish to determine whether they are the first n correlation functions of some point process in $\mathbb{R}^d$ or $\mathbb{Z}^d$, respectively, and if so what we can say about the process. We give partial answers to these questions and discuss some examples.

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Running head: Realizability of Point Processes.

1 Introduction

Let $\eta(\mathbf{r})$, $\mathbf{r} \in \Omega$, be a random empirical field describing a point process in a domain $\Omega \subset \mathbb{R}^d$; for concreteness we will always take Ω to be either $\mathbb{R}^d$ or $\mathbb{Z}^d$. Then

$$\eta(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{x}_i), \tag{1.1}$$

where the $\mathbf{x}_i$ are the positions of the points of the process, with $\mathbf{x}_i \neq \mathbf{x}_j$ for $i \neq j$, distributed according to some measure μ defined on the family of all locally finite collections of points in Ω. Here δ is either the Dirac or the Kronecker delta function, depending on whether we are in the continuum or on the lattice; in the latter case $\eta(\mathbf{r})$ has value 0 or 1. Depending on context the $\mathbf{x}_i$ can represent the positions of particles in a fluid or of the stars in the sky, the occurrence times of members of a train of neural spikes, or more generally the space-time locations of the events of some specified physical process.

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The correlation functions $\rho_k(\mathbf{r}_1, ..., \mathbf{r}_k)$ are defined via averages, with respect to μ, of products of $\eta(\mathbf{r})$'s involving distinct particles:

$$\rho_1(\mathbf{r}_1) \quad = \quad \langle \eta(\mathbf{r}_1) \rangle, \tag{1.2}$$

$$\rho_2(\mathbf{r}_1, \mathbf{r}_2) \quad = \quad \left\langle \sum_{i \neq j} \delta(\mathbf{r}_1 - \mathbf{x}_i) \delta(\mathbf{r}_2 - \mathbf{x}_j) \right\rangle, \tag{1.3}$$

and in general

$$\rho_k(\mathbf{r}_1, \ldots, \mathbf{r}_k) = \left\langle \sum_{i_1 \neq i_2 \neq \cdots \neq i_k} \prod_{j=1}^{k} \delta(\mathbf{r}_j - \mathbf{x}_{i_j}) \right\rangle. \tag{1.4}$$

Note that the correlation function ρ_2 is not simply the two-point correlation of η, rather,

$$\rho_2(\mathbf{r}_1, \mathbf{r}_2) = \langle \eta(\mathbf{r}_1) \eta(\mathbf{r}_2) \rangle - \rho_1(\mathbf{r}_1) \delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{1.5}$$

with similar expressions for the higher order correlations. Note also that on the lattice $\rho_k(\mathbf{r}_1, ..., \mathbf{r}_k)$ vanishes when $\mathbf{r}_i = \mathbf{r}_j$.

For translation invariant processes, the only ones we shall consider here, we shall write $\rho_1(\mathbf{r}_1) = \rho$, $\rho_2(\mathbf{r}_1, \mathbf{r}_2) = \rho^2 g(\mathbf{r}_2 - \mathbf{r}_1)$, $\rho_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \rho^3 g_3(\mathbf{r}_2 - \mathbf{r}_1, \mathbf{r}_3 - \mathbf{r}_1)$, etc. The function $g(\mathbf{r})$ is known in the fluids literature [1], where it is additionally assumed that g is a function only of $|\mathbf{r}|$, as the *radial distribution function*. We shall also assume generally that $\rho_k(\mathbf{r}_1, \ldots, \mathbf{r}_k) \to \rho^k$ when $|\mathbf{r}_i - \mathbf{r}_j| \to \infty$ for all i, j with $1 \leq i < j \leq k$.

We study the following problem. Suppose we are given functions which might determine the first few correlations, say ρ and $g(\mathbf{r})$; does there then exist an underlying process with these correlations and, if so, what can we say about it?[5] The given putative correlations may come from averaging and smoothing of observations, as in the study of neural spike trains [2, 3], or from some approximate theory, such as the Percus-Yevick equation for the radial distribution function of a classical fluid [1]. They may also just express target correlations for a material or process with certain desired properties [4].

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[5]We mention here a technical point: in the continuum, (1.4) in fact defines the ρ_k as measures, and the correlation functions, also denoted ρ_k, are in fact their densities (which we will always assume to exist) with respect to Lebesgue measure. These densities are measurable functions which are *a priori* defined only almost everywhere. Thus unless the given functions are continuous we can only require that the correlation functions of the realizing point process agree with them almost everywhere.

The first question above, whether or not there exists a point process or equivalently a measure μ with the given low order correlations, is the *(truncated) realizability problem*. (The full problem, when all the ρ_k, $k = 1, 2, ...$, are given, was studied by A. Lenard [5]). An affirmative answer to this question might come from an explicit construction, an abstract theorem giving a sufficient condition for existence, or simply the fact that the correlations in question arise from observation of an actual physical process; a negative answer from a general necessary condition for existence or from a detailed argument in some special cases. In Section 2 we will review some general results leading to both affirmative and negative answers, and in Section 3 we will describe partial existence results for two related one-parameter families of correlations, one in the lattice and one in the continuum.

Once existence is established, we may next ask about the number and nature of the realizing measures μ which give a specified ρ, $g(r)$, g_3, ..., g_n. This number can be uncountable, as we will see in section 4. We may then wish to ask whether this group includes measures which satisfy some additional criteria, such as being Gibbsian [6, 7] or even Gibbsian with specified type of interactions, e.g., only two body ones. The latter is particularly relevant when considering correlations of an equilibrium fluid. We may also ask about the measure μ in the class of realizing measures which maximizes the Gibbs-Shannon entropy $s(\mu|\mu_0)$ relative to some natural reference measure μ_0. We will define this relative entropy, and discuss these questions further, in Section 4.

2   General conditions for realizability

We begin by considering necessary conditions for existence. There are some obvious conditions which ρ and the g_k must satisfy [4, 8]; certainly

$$\rho > 0, \quad g_k \geq 0 \tag{2.1}$$

and the Fourier transform of $\langle \eta(\mathbf{r}_1)\eta(\mathbf{r}_2) \rangle - \langle \eta(\mathbf{r}_1) \rangle \langle \eta(\mathbf{r}_1) \rangle$ must be positive semi-definite, which for the translation invariant case in $\mathbb{R}^d$ yields

$$\hat{S}(\mathbf{k}) \equiv \rho + \rho^2 \int_{\mathbb{R}^d} e^{i\mathbf{k}\cdot\mathbf{r}} \left[g(\mathbf{r}) - 1 \right] d\mathbf{r} \geq 0. \tag{2.2}$$

If we did not require $\eta(\mathbf{r})$ to correspond to a point process then (2.1) and (2.2) with strict inequality would be sufficient for realizability of $\eta(\mathbf{r})$ as a random field, in particular as a Gaussian process. The requirement that ρ and g come from a point process imposes many additional conditions. There

is in particular a simple condition on the variance V_Λ of the number N_Λ of particles in a region Λ, which follows from the fact that the number of particles in any region must be an integer:

$$V_\Lambda \equiv \rho|\Lambda| + \rho^2 \iint_\Lambda [g(\mathbf{r}_1 - \mathbf{r}_2) - 1]\, d\mathbf{r}_1 d\mathbf{r}_2 \geq \theta(1-\theta). \qquad (2.3)$$

Here $|\Lambda|$ is the volume of Λ and θ is the fractional part of the mean $\rho|\Lambda|$ of N_Λ, i.e., $\rho|\Lambda| = k + \theta$ with $k = 0, 1, \ldots$ and $0 \leq \theta < 1$ [9]. For lattice systems the integrals in (2.2) and (2.3) are replaced by sums.

We now turn to sufficient conditions for existence. We first observe that if there is a point process X with measure μ which realizes the correlations γ, $\gamma^2 g$, ..., $\gamma^n g_n$, then for any density $\rho < \gamma$ there exists a process X_ρ with measure $\mu^{(\rho)}$ which realizes the correlations ρ, $\rho^2 g$, ..., $\rho^n g_n$: we construct X_ρ by "thinning" X [10]; specifically, we independently keep or delete each point $\mathbf{x}_i$ in X with probabilities ρ/γ and $1 - \rho/\gamma$, respectively. In particular, this implies that for given g, ..., g_n there is a critical density ρ_c such that ρ, $\rho^2 g$, ..., $\rho^n g_n$ may be realized for $\rho < \rho_c$ and cannot be realized for $\rho > \rho_c$. On the lattice, a simple compactness argument shows that in fact the correlations may be realized for ρ in the closed interval $[0, \rho_c]$.

We next give a general theorem about realizability in $\mathbb{R}^d$ of a given $g(\mathbf{r})$, $\mathbf{r} \in \mathbb{R}^d$, for sufficiently small ρ.

Theorem: *Let*

$$g(\mathbf{r}) = \begin{cases} 0, & |\mathbf{r}| \leq D, \\ \exp(-\varphi(\mathbf{r})), & |\mathbf{r}| > D, \end{cases} \qquad (2.4)$$

with $\varphi(\mathbf{r})$ satisfying the condition that for any $n \geq 1$,

$$\sum_{i=1}^n \varphi(\mathbf{r}_i) \geq -2B \quad \text{whenever} \quad |\mathbf{r}_i - \mathbf{r}_j| \geq D, \quad 1 \leq i < j \leq n, \qquad (2.5)$$

for some $B \geq 0$, and all $n \geq 1$. Then ρ and $g(\mathbf{r})$ are realizable whenever

$$\rho \leq \left(e^{1+2B} \int_{\mathbb{R}^d} |g(\mathbf{r}) - 1|\, d\mathbf{r} \right)^{-1}. \qquad (2.6)$$

Note that (2.5) is satisfied for any $D \geq 0$ (with $B = 0$) if $\varphi(\mathbf{r}) \geq 0$ for all $\mathbf{r}$, and for $D > 0$ (i.e., with a hard core) if $\varphi(\mathbf{r})$ decays faster than $|\mathbf{r}|^{-(d+\epsilon)}$ for $|\mathbf{r}| \to \infty$ [6]. There is a similar theorem for realizability on the lattice $\mathbb{Z}^d$, in which the integral in (2.6) is replaced by a sum; note that in this case, by the remark above that $\rho_2(\mathbf{r}, \mathbf{r}) = 0$ for any $\mathbf{r}$, g will automatically satisfy the hard core condition (2.4) for any $D < 1$.

The above theorem is a generalization of a result of R. V. Ambartzumian and H. S. Sukiasian [10], who considered only the case $\varphi \geq 0$, i.e., $g \leq 1$. The construction by Ambartzumian and Sukiasian of the point process corresponding to ρ and $g(\mathbf{r})$ (which we follow) is based on first guessing a full system of correlation function ρ_k from the given $g(\mathbf{r})$ and density ρ; specifically, we define ρ_k via the formula

$$\rho_k(\mathbf{r}_1, ..., \mathbf{r}_k) = \rho^k \prod_{1 \leq i < j \leq k} g(\mathbf{r}_i - \mathbf{r}_j), \quad k = 2, 3, ... \tag{2.7}$$

One then shows that, when (2.6) is satisfied, these ρ_k determine a measure μ.

We show in [11] how to extend this construction to the case when also g_3 is given and satisfies certain conditions (one expects similar results when additional g_k are specified). The maximum density ρ for which the construction is guaranteed to succeed naturally decreases as additional g_k are specified. However, if ρ and g are given, with ρ sufficiently small, then the construction succeeds for an uncountable number of choices of g_3, so that there are an uncountable number of realizations of (ρ, g).

Finally, we remark that general necessary and sufficient conditions for partial realizability can be given in the form of an uncountable number of positivity conditions in a manner similar to that given by Lenard [5] for the full realizability problem. These will be described in [11].

3   Existence: a specific example

Suppose that for $r \in \mathbb{Z}$ we specify [15]

$$g(r) = \begin{cases} 0, & \text{for } r = 0, \pm 1, \\ 1, & \text{for } |r| \geq 2. \end{cases} \tag{3.1}$$

This g describes a model with on-site and nearest neighbor exclusion and with no correlation, on the pair level, for sites separated by two or more lattice spacings. It is then easy to check that (2.1)–(2.3) are satisfied if and only if $\rho \leq 1/3$, so that the critical density for this g must satisfy $\rho_c \leq 1/3$. A computation which we will describe below, however, shows that in fact

$$\rho_c \leq \frac{326 - \sqrt{3115}}{822} \simeq 0.3287. \tag{3.2}$$

On the other hand, it is easy to construct explicitly a realization of (2.5) for $\rho \leq 1/4$, so that certainly $\rho_c \geq 1/4$. To do so we start with a Bernoulli

measure on $\{0,1\}^{\mathbb{Z}}$ with density λ, and then remove the particle from an occupied site x if and only if site $x + 1$ is also occupied. This yields a translation invariant process with density $\rho = \lambda(1 - \lambda) \leq 1/4$ and with $g(r)$ given by (3.1); the maximal ρ which can be obtained in this way is thus $1/4$. A more complicated construction based on a *Markov renewal process*, described below, shows that $\rho_c \geq 0.264$. The actual value of ρ_c in the interval $[0.264, 0.3287]$ is unknown to us at present.

It is clear that in the process just constructed the interparticle distances, which we will call *jumps*, are independent and identically distributed, i.e., the point process is a *renewal* process. We now show that in fact no renewal process with $g(r)$ given by (3.1) can exist for $\rho > 1/4$ (see also [12, 13]). For suppose that, in such a renewal process, a jump of length k occurs with probability $p(k)$, $k = 2, 3, \ldots$. Then the probability $\rho g(k)$ of finding a particle on site $i + k$, given that there is a particle on site i, satisfies

$$\rho g(k) = \sum_{n \geq 1} \sum_{\{k_1, \ldots, k_n | \sum_i k_i = k\}} p(k_1) \cdots p(k_n). \tag{3.3}$$

Equation (3.3) may be expressed in terms of the generating functions

$$G(z) = \sum_k \rho g(k) z^k, \qquad f(z) = \sum_k p(k) z^k, \tag{3.4}$$

as $G = \sum_{n=1}^{\infty} f^n = f/(1 - f)$. But from (3.1) we have $G(z) = \rho z^2/(1 - z)$, which identifies f:

$$f(z) = \frac{\rho z^2}{1 - z + \rho z^2} = \frac{\rho^2 z^2}{\sqrt{1 - 4\rho}} \left[\frac{z_+}{1 - z/z_-} - \frac{z_-}{1 - z/z_+} \right], \tag{3.5}$$

where $z_\pm = (2\rho)^{-1}(1 \pm \sqrt{1 - 4\rho})$. For $\rho > 1/4$ the roots $z_\pm$ are complex and the coefficients $p(k)$ of the Taylor series of $f(z)$ are not all positive, so the renewal process does not exist. Note that existence of the renewal process for $\rho \leq 1/4$ also follows from (3.5), since the coefficients of the Taylor series are then clearly positive. One needs here and in examples below the construction of a translation invariant point process from a translation invariant jump process (in the continuum the latter corresponds to a Palm measure); see [14].

The analysis of the corresponding realizability problem for a point process on the real line, in which (3.1) is replaced by a unit step function [4]

$$g(r) = \begin{cases} 0, & |r| < 1, \\ 1, & |r| > 1, \end{cases} \tag{3.6}$$

where now $r \in \mathbb{R}$, is quite similar. Conditions (2.1)–(2.3) are now satisfied if and only if $\rho \leq 1/2$, while an explicit construction, starting with a Poisson measure with density λ, then removing all points which have another point lying within a unit distance to their right, yields a measure μ with a density $\rho = \lambda e^{-\lambda} \leq 1/e$ satisfying (2.3); thus $\rho_c \in [1/e, 1/2]$. The measure μ just described corresponds to a renewal process, and one can again prove that $\rho = 1/e$ is the maximal density for a renewal process satisfying (3.6) [12, 13]. In this case numerical investigation of an appropriate Markov renewal process suggests that $\rho_c \geq 0.395$; see below.

3.1   Derivation of the upper bound

We now discuss the derivation of upper bounds for ρ_c. If μ is a translation invariant measure on configurations on $\mathbb{Z}$ which realizes (3.1) at some density ρ, then the restriction μ_N of μ to configurations in a finite box $\Lambda_N \equiv \{1, 2, \ldots, N\}$ realizes the same ρ and g for sites in the box. Thus if one shows that such a restriction μ_N cannot exist at some density ρ_*, then necessarily $\rho_c \leq \rho_*$. Computations in the box are simplified by the observations that (i) μ_N is the restriction of μ_{N+1} to Λ_N, and (ii) by averaging over reflections we may assume that μ is reflection invariant and hence that μ_N is invariant under reflections about the center of the box.

As a first application of this idea we observe that for $\rho = 1/3$ a simple hand computation shows that a restriction μ_N can exist only if $N < 12$; so that $\rho_c < 1/3$. First one sees by inspection that there is a unique possible μ_4: writing $\eta = (\eta_1 \cdots \eta_N)$ with $\eta_i = 0, 1$ for a configuration in Λ_N we have from (3.1) that

$$\mu_4(1010) = \mu_4(1001) = \mu_4(0101) = 1/9; \tag{3.7}$$

for example,

$$\mu_4(1010) = \langle \eta_1(1 - \eta_2)\eta_3(1 - \eta_4) \rangle = \langle \eta_1 \eta_3 \rangle = \rho^2 = 1/9. \tag{3.8}$$

Moreover, once (3.7) is established we have

$$\left.\begin{array}{l} \mu_4(1000) = \mu_4(0001) = 1/9, \\ \mu_4(0100) = \mu_4(0010) = 2/9, \end{array}\right\} \quad \text{from } \langle \eta(r) \rangle = 1/3, \tag{3.9}$$

$$\mu_4(\eta) = 0 \quad \text{otherwise}, \quad \text{from } \sum_\eta \mu_4(\eta) = 1. \tag{3.10}$$

Next one computes successively μ_5 through μ_{11}, using (i) and (ii) above as well as $\mu_N(00 \cdots 01) = 1/3$, $\mu_N(100 \cdots 001) = 1/9$, finding in each case a unique possible answer; the computation remains of manageable size, and in

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fact $\mu_8, \ldots, \mu_{11}$ are each supported on 18 equally likely configurations. An attempt to extend the computation to μ_{12} fails, however; there is no solution satisfying all the constraints.

To obtain the upper bound (3.2) we note that existence of μ_N at density ρ corresponds to the feasibility of a linear programming problem in $(p_\eta)_{\eta \in T}$, where p_η is $\mu_N(\eta)$ and T is the set of configurations η such that for no i is $\eta_i = \eta_{i+1} = 1$:

$$\sum_{\eta \in T} p_\eta \;=\; 1, \tag{3.11}$$

$$\sum_{\{\eta \in T \mid \eta_i = 1\}} p_\eta \;=\; \rho, \quad 1 \le i \le N \tag{3.12}$$

$$\sum_{\{\eta \in T \mid \eta_i = \eta_j = 1\}} p_\eta \;=\; \rho^2, \quad 3 \le i + 2 \le j \le N, \tag{3.13}$$

$$p_\eta \;\ge\; 0, \quad \eta \in T, \tag{3.14}$$

But (3.11)–(3.14) is feasible if and only if the dual problem, which is to minimize the objective function

$$A_{N,\rho}(s) \equiv 1 + \sum_{1 \le i \le N} s_i \rho + \sum_{3 \le i + 2 \le j \le N} s_{ij} \rho^2, \tag{3.15}$$

subject to the constraints

$$1 + \sum_{\{i \mid \eta_i = 1\}} s_i + \sum_{\{i+2 \le j \mid \eta_i = \eta_j = 1\}} s_{ij} \ge 0, \qquad \eta \in T, \tag{3.16}$$

has a nonnegative solution [16] (this condition is closely related to a general sufficient condition for existence presented in [11]). For moderate values of N one may use software available through the NEOS Server web site [17, 18, 19] to produce a set of coefficients $\bar{s}_i, \bar{s}_{ij}$ which satisfy (3.16) and are such that $A_{N,1/3}(\bar{s})$ minimizes $A_{N,1/3}(s)$; in particular we know from the above argument that $A_{N,1/3}(\bar{s}) < 0$ if $N \ge 12$. (It is in practice convenient to use reflection symmetry to reduce the size of the problem, but this does not affect the nature of the argument). It follows that if $A_{N,\rho_*}(\bar{s}) < 0$ then $\rho_c < \rho_*$. For $18 \le N \le 22$, one finds that $A_{N,\rho}(\bar{s})$ is proportional to $1644\rho^2 - 1304\rho + 251$, leading to (3.2).

3.2 Derivation of the lower bound

We observed above that a computation of the generating function $f(z)$ furnishes a construction of the renewal process satisfying (3.1). Here we generalize this construction using a *Markov renewal process*, in which the jth

state σ_j of an underlying Markov chain determines the distribution of the jth jump of the point process.

We will take the underlying Markov chain to have two states, so that $\sigma_j \in \{0, 1\}$, $j \in \mathbb{Z}$. The transition matrix is

$$M = \begin{bmatrix} p_{0 \to 0} & p_{0 \to 1} \\ p_{1 \to 0} & p_{1 \to 1} \end{bmatrix} = \begin{bmatrix} a & 1-a \\ 1-b & b \end{bmatrix}, \tag{3.17}$$

where the parameters a and b, which will be specified later, lie in $[0, 1]$. The invariant measure P for this Markov process is the (left) eigenvector, with eigenvalue 1, of M, normalized to have the sum of the entries equal to 1:

$$P = [p_0, p_1] = \left[\frac{1-b}{2-a-b}, \frac{1-a}{2-a-b} \right]. \tag{3.18}$$

We will always assume that this underlying process is in its stationary state.

If $\sigma = (\sigma_j)_{j \in \mathbb{Z}}$ is known then the jth jump is chosen, independently of all other jumps, from a distribution which depends only on σ_j. Specifically, this jump has value k with probability $p_0(k)$, if $\sigma_j = 0$, and $p_1(k)$, if $\sigma_j = 1$. Then (3.1) implies that $p_0(1) = p_1(1) = 0$. Here we consider only the case in which the distributions p_0 and p_1 have disjoint support:

$$p_0(k)p_1(k) = 0, \qquad \text{for all } k \geq 1. \tag{3.19}$$

In this case the state σ_j is a function of the jump and therefore the sequence of jumps is itself a Markov process.

It remains to determine whether, for a given ρ, one may choose a and b and the distributions p_0 and p_1 to achieve density ρ and two-point function $\rho^2 g$, with g given by (3.1). The computation is quite similar to that for the renewal process. Let us take G to be the generating function of $\rho g(k)$, as in (3.4), and f_σ to be the generating function of the distribution $p_\sigma(k)$:

$$f_\sigma(z) = \sum_{k=2}^{\infty} p_{\sigma,k} z^k, \quad \sigma = 0, 1, \tag{3.20}$$

Suppose that we condition on the occurrence of a particle at site i, and without loss of generality suppose that the jumps are labelled so that the distribution of the jump immediately succeeding this particle is p_{σ_1}, i.e., that the probability of the next particle being at site $i + k$ is $p_{\sigma_1}(k)$. Then given $\sigma_1, \sigma_2, ..., \sigma_n$, the probability that the nth particle after site i lies on site $i + k$ is given by the kth Taylor coefficient of the function $f_{\sigma_1} f_{\sigma_2} ... f_{\sigma_n}$, which leads to

$$G = \sum_{n=1}^{\infty} \sum_{\sigma_1, ..., \sigma_n} \text{Prob}(\sigma_1, ..., \sigma_n) \prod_{j=1}^{n} f_{\sigma_j}, \tag{3.21}$$

where the probability of the sequence $\sigma_1, \ldots, \sigma_n$, is

$$\text{Prob}(\sigma_1, \ldots, \sigma_n) = P_{\sigma_1} p_{\sigma_1 \to \sigma_2} \cdots p_{\sigma_{n-1} \to \sigma_n} \tag{3.22}$$

The function G can be computed. Define

$$M' = \begin{bmatrix} a f_0 & (1-a) f_1 \\ (1-b) f_0 & b f_1 \end{bmatrix} \quad \text{and} \quad Q = \begin{bmatrix} 1 \\ 1 \end{bmatrix}. \tag{3.23}$$

Then (3.21) becomes

$$G(z) = \sum_{n=1}^{\infty} P(M')^n Q = PM'(1 - M')^{-1} Q. \tag{3.24}$$

A straightforward computation leads to

$$G(z) = \frac{(b-1)f_0 + (a-1)f_1 - (a+b-2)(a+b-1)f_0 f_1}{(a+b-2)(1 - a f_0 - b f_1 + (a+b-1)f_0 f_1)}, \tag{3.25}$$

Finally we require that g be given by (3.1), i.e., that $G(z) = \rho z^2/(1-z)$:

$$\rho \frac{z^2}{1-z} = \frac{(b-1)f_0 + (a-1)f_1 - (a+b-2)(a+b-1)f_0 f_1}{(a+b-2)(1 - a f_0 - b f_1 + (a+b-1)f_0 f_1)}. \tag{3.26}$$

Next we must choose p_0 and p_1 (or equivalently f_0 and f_1), a, and b. For simplicity of computation we will choose $p_1(k)$ to be nonzero only if $k = 2$ or $k = 3$. Since then $p_0(2) = p_0(3) = 0$, by (3.19), the condition that $g(2) = g(3) = 1$ implies that $p_1(2) = p_1(3) = 1/2$ and that $P_1 = 2\rho$, so that

$$f_1(z) = \frac{z^2 + z^3}{2}, \qquad b = 2 - a + \frac{a-1}{2\rho}. \tag{3.27}$$

Substituting (3.27) into (3.26) we obtain

$$f_0 = z^4 \frac{N(z)}{D(z)}, \tag{3.28}$$

where

$$\begin{align}
N(z) &= \rho(1 - a + 2a\rho) + \rho(1 - a - 4\rho + 2a\rho)z, \tag{3.29} \\
D(z) &= (4\rho - 8\rho^2)(1 - z) + (1 - a - 2\rho + 4a\rho^2)z^2 \\
&\quad + (-1 + a + 3\rho - a\rho - 2\rho^2)z^4 + (\rho - a\rho - 2\rho^2)z^5. \tag{3.30}
\end{align}$$

Now (3.1) will be realizable at density ρ if for some a the Taylor series of (3.28) has nonnegative coefficients $p_0(4), p_0(5), \ldots$ (equations (3.28)–(3.30)

imply trivially that these coefficients satisfy $p_0(k) = 0$, $k = 1, 2, 3$, and that $f_0(1) = 1$, so that $p_0(k)$ forms a probability distribution). With this construction we can obtain realizations for $\rho > 1/4$—in particular, as an immediate consequence of the next lemma, for $\rho = 0.264$.

Lemma: *Suppose that $\rho = 0.264$ and $a = 0.41$. Then the roots $z_1, \ldots, z_5$ of D may be numbered so that $0 < z_1 < \inf_{2 \le i \le 5} |z_k|$, and then the coefficients in the partial fraction expansion $N(z)/D(z) = \sum_{i=1}^{5} a_i/(1 - z/z_i)$ satisfy*

$$a_1 > \sum_{i=2}^{5} |a_i|, \tag{3.31}$$

so that the coefficients of z^k in the expansion

$$\frac{N(z)}{D(z)} = \sum_{k=0}^{\infty} \left(\sum_{i=1}^{5} \frac{a_i}{z_i^{k+1}} \right) z^k \tag{3.32}$$

are positive.

We sketch the proof very briefly; it was carried out using a computer algebra system (in fact, with Mathematica and Maple independently), but only for computations involving rational numbers. One first, using the root-finding abilities of the computer algebra system for guidance, chooses approximations $\tilde{z}_1, \ldots, \tilde{z}_5$, rational or complex with rational real and imaginary parts, to the roots of D; these then determine an approximate denominator $\tilde{D}(z) = (\rho - a\rho - 2\rho^2) \prod_{k=1}^{5} (z - \tilde{z}_k)$. Since one knows the (rational) coefficients of D and $\tilde{D}$ exactly, one may use a result of Beauzamy [20] to show that $|z_k - \tilde{z}_k| < \delta$, $k = 1, \ldots, 5$, for some small, explicitly known, and rational δ. It is then straightforward to compute

$$a_k = -\frac{N(z_k)}{z_k D'(z_k)} \approx -\frac{N(\tilde{z}_k)}{\tilde{z}_k D'(\tilde{z}_k)}, \tag{3.33}$$

using only rational arithmetic, with enough accuracy to verify (3.31).

A similar construction of a point process with jumps given by a Markov renewal process can be carried out in the continuum case. We will use again the Markov process $(\sigma_j)_{j \in \mathbb{Z}}$ defined by (3.17), and extract the i-th jump y_i (the distance between particle i and $i + 1$) from a distribution $p_0(y)dy$ if $\sigma_i = 0$ and from $p_1(y)dy$ if $\sigma_i = 1$, where p_0 and p_1 are nonnegative continuum distribution supported on $[1, \infty)$. The generating functions used above are now replaced by Laplace transforms:

$$F_0(s) = \int dy \, e^{-sy} p_0(y), \tag{3.34}$$

$$F_1(s) \;=\; \int dy\, e^{-sy} p_1(y), \tag{3.35}$$

$$G(s) \;=\; \int dy\, e^{-sy} \rho g(y) = \rho \int_1^\infty dy\, e^{-sy} = \rho \frac{e^{-s}}{s}, \tag{3.36}$$

and (3.25) becomes

$$G(s) = \frac{(b-1)F_0 + (a-1)F_1 - (a+b-2)(a+b-1)F_0 F_1}{(a+b-2)(1-aF_0 - bF_1 + (a+b-1)F_0 F_1)}, \tag{3.37}$$

We choose

$$p_1(y) = \begin{cases} 1 & \text{if } 1 \le y \le 2, \\ 0 & \text{otherwise,} \end{cases} \tag{3.38}$$

so that $F_1(s) = (e^{-s} - e^{-2s})/s$. As in the discrete case we choose p_0 and p_1 to have disjoint support, which requires that $P_1 = 1$; for simplicity we also choose $b = 0$ (see the comments below), so that $a = (1 - 2\rho)/(1 - \rho)$. Then

$$F_0(s) = \frac{N(s)}{D(s)}, \tag{3.39}$$

where

$$N(s) = \rho(1 - \rho)s e^s, \tag{3.40}$$

and

$$D(s) = -\rho^2 + \rho(\rho - s)e^s + 2\rho(1 - \rho)s e^{2s} + (1 - \rho)^2 s^2 e^{3s}. \tag{3.41}$$

Now we must check that the distribution $p_0(y)$ obtained from (3.39) is nonnegative. To do so we use the general result that a function $f(y)$ is positive if and only if its Laplace transform $F(s)$ satisfies $F(0) > 0$ and has derivatives $F^{(n)}(0)$ which alternate in sign (see [12, 13] and references therein). In this case we have not proved that p_0 is nonnegative, but numerical computations with Mathematica indicate that that the first 2000 derivatives of F_0 are alternating in sign at density $\rho = 0.395$.

Finally a comment on the choice of b. We do not know what is the optimal b, and indeed the computations with Mathematica suggest that $\rho = 0.395$ can be reached for any $b \in [0, 0.05]$. Numerical investigations at values of ρ slightly larger than 0.395 suggest that the choice $b = 0$ may be optimal.

4 Properties of realizing measures

We suppose in this section that realizing measures for some specified correlations exist, and ask about their properties, focussing on entropy maximization, Gibbsianness, and nonuniqueness.

The Gibbs-Shannon entropy of the measure μ relative to the measure μ_0 is defined by

$$s(\mu|\mu_0) \equiv -\lim_{\Lambda \to \Omega} \frac{1}{|\Lambda|} \int \left[\frac{\mu_\Lambda(\eta)}{\mu_\Lambda^0(\eta)}\right] \log \left[\frac{\mu_\Lambda(\eta)}{\mu_\Lambda^0(\eta)}\right] d\mu_\Lambda^0(\eta), \qquad (4.1)$$

where μ_Λ is the projection of μ on Λ, i.e., the marginal measure on configurations in a finite domain $\Lambda \subset \mathbb{R}^d$ (or $\mathbb{Z}^d$). As reference measure μ_0 we take the measure describing the Poisson point process with density 1, when $\Omega = \mathbb{R}^d$, and the product measure $\nu_{1/2}$ with density $1/2$, when $\Omega = \mathbb{Z}^d$, where the product measure of density ρ, $0 \le \rho \le 1$, is characterized by the projections

$$(\nu_\rho)_\Lambda(\eta) = \prod_{x \in \Lambda}[\rho\eta(x) + (1-\rho)(1-\eta(x))] = \prod_{x \in \Lambda}[e^{\lambda\eta(x)}/(1+e^\lambda)], \qquad (4.2)$$

with

$$\lambda = \log \frac{\rho}{1-\rho}. \qquad (4.3)$$

We now ask: assuming that a specified set of correlations ρ_j, $j \le n$, has at least one realization, will there always be a realization μ_G which is a Gibbs measure with k-body interactions, $k \le n$? That this should formally be so, because the method of Lagrange multipliers implies that the realizing measure which maximizes the entropy (4.1) should be of this form, was pointed out to us by R. Varadhan [21]. On the lattice, in finite volume, one may verify this result [11] by showing that for $\rho < \rho_c$ the maximizing measure occurs in the interior of the set of realizing measures, so that the Lagrange multiplier method applies. However, it has not been shown that the resulting potentials have an infinite volume limit. The only rigorous result in this direction is by L. Koralov [22], who has established the existence of such an infinite-volume Gibbs measure in the lattice case for $n = 2$, ρ small, and g sufficiently close to 1 that $\sum_{r \ne 0}|g(r) - 1| \le 1$.

From now on we consider only the lattice case, and let $\mathcal{M}$ be the (assumed nonempty) set of translation invariant measures realizing some given family ρ_k, $k = 1, \dots, n$ of correlations. It is well known that translation invariant Gibbs measures for a given set of k-body interaction potentials $\phi = (\phi_k)_{k=1}^m$, assumed to be sufficiently rapidly decaying, can be characterized as the maximizers of $A(\mu) \equiv s(\mu|\mu_0) - \mu(\phi)$, where $\mu(\phi)$ is the expected value of the energy per site in the measure μ (see [6] for full details). What is critical here is that, if the ϕ_k involve at most n-body interactions (i.e., if $m \le n$), then $\mu(\phi)$ can be calculated from ϕ and the given ρ_k alone, so that $\mu(\phi)$ is constant on $\mathcal{M}$. Thus if there is in $\mathcal{M}$ a Gibbs measure $\mu^{(\phi)}$ for some potential $(\phi_k)_{k=1}^m$, and $m \le n$, then $\mu^{(\phi)}$ will maximize the entropy over all of $\mathcal{M}$. Since

then any entropy maximizing measure $\mu' \in \mathcal{M}$ must satisfy $A(\mu') = A(\mu^{(\phi)})$, μ' must also be a Gibbs measure for ϕ. In particular, if μ' is known to be a Gibbs measure for the potentials $(\psi_k)_{k=1}^{m'}$ with $m' \leq n$, then a result of Griffiths and Ruelle [23] implies, again under a mild decay condition on the potentials, that the potentials ϕ and ψ must be the same. Thus, for the lattice, the realizability problem can have a Gibbsian solution for at most one set of potentials $(\phi_k)_{k \leq n}$. These potentials will uniquely determine all higher correlation functions and thus the measure, unless the equilibrium system is at a first order phase transition; in the latter case the first n correlations are the same in all phases (since we assume that our ρ_k, $k = 2, \ldots, n$, have at least some mild clustering properties [6]). It also follows from the above considerations that no Gibbs measure in $\mathcal{M}$ with potentials $\phi = (\phi_k)_{k=1}^m$, $m > n$, can maximize the entropy.

We close this section by giving a simple example of a realizability problem for which there are an uncountable number of solutions. Consider, on the lattice $\mathbb{Z}^d$, the correlations

$$\langle \eta(\mathbf{r}) \rangle = 1/2, \tag{4.4}$$

$$g(\mathbf{r}) = \begin{cases} 0, & \text{if } \mathbf{r} = 0 \\ 1, & \text{if } \mathbf{r} \neq 0. \end{cases} \tag{4.5}$$

Clearly (4.4) and (4.5) are realized by the product measure $\nu_{1/2}$, which is the Gibbs measure for the zero potential.

But $\nu_{1/2}$ is not the only realizing measure. To see this, choose some finite set $A \subset \mathbb{Z}^d$ containing at least two sites, and define $A_\mathbf{r}$ as $\mathbf{r} + A$; for example, if $A = (e_1, 2e_1)$, the first two sites to the right of the origin in the direction of the first coordinate axis, then $A_\mathbf{r}$ is the set containing the two sites to the right of $\mathbf{r}$. Consider a random configuration τ with $\tau(\mathbf{r}) \in \{0, 1\}$, distributed according to the product measure $\nu_{1/2}$, and introduce the spin variables $\sigma(\mathbf{r}) = 2\eta(\mathbf{r}) - 1$, $s(\mathbf{r}) = 2\tau(\mathbf{r}) - 1$. Take now a parameter p with $0 \leq p \leq 1$ and let $\eta(\mathbf{r})$ be given by an independent choice at each site, according to

$$\sigma(\mathbf{r}) = \begin{cases} s(\mathbf{r}), & \text{with probability } p, \\ \prod_{\mathbf{r}' \in A_\mathbf{r}} s(\mathbf{r}'), & \text{with probability } 1 - p. \end{cases} \tag{4.6}$$

It is easy to see that this will induce a measure $\mu_{A,p}$ on $\eta(\mathbf{r})$ which is a realization of (4.4)–(4.5). The measure $\mu_{A,p}$ is, however, no longer a product measure, since in general $g_k(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_k) \neq 1$ for $k \geq 3$; for example, with the choice $A = \{e_1, 2e_1\}$ above,

$$\langle \eta(e_1)\eta(2e_1)\eta(3e_1) \rangle_{\mu_{A,p}} = \frac{1 + p^2(1 - p)}{8}, \tag{4.7}$$

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which is not equal to $1/8$ unless p is zero or 1.

Because the set A and the value p are here essentially arbitrary, there will be a non-denumerable number of inequivalent measures realizing (4.4)–(4.5); all these are ergodic since their correlations are finite range. Since $\nu_{1/2} = \mu_0 = \mu_1$ is Gibbsian, the measure $\nu_{1/2}$ maximizes $s(\mu|\mu_0)$ among all measures realizing (4.4)–(4.5), and in particular among all the $\mu_{A,p}$. In this case it is known, in fact, that $\nu_{1/2}$ is the unique maximizer, so that none of the $\mu_{A,p}$ for $p \neq 0, 1$ can be Gibbsian with only one and two body potentials.

By applying the thinning process discussed in section 2 to $\mu_{A,p}$ we obtain, for $0 < \rho \leq 1/2$, an infinite collection of measures realizing

$$\langle \eta(\mathbf{r}) \rangle = \rho \qquad \text{and} \qquad g(\mathbf{r}) = 1, \quad \mathbf{r} \neq 0. \tag{4.8}$$

By interchanging particles and holes (and replacing ρ by $1 - \rho$) we obtain also solutions of (4.8) for $\rho > 1/2$.

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