Point Processes with Specified Correlation Functions

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I. Introduction

(A) A point process in $\mathbb{R}^d$ is a random set of points $\{x_1, x_2, \cdots\} \subset \mathbb{R}^d$

- a finite number of points in any bounded region
- we assume a translation invariant distribution

Examples:

- Poisson process
- Configurational ensemble for a continuous statistical mechanical system in equilibrium (Gibbs)

Notation: describe process by a random field (here a random measure)

$$\eta(x) = \sum_i \delta(x - x_i)$$

<u>Correlation</u> <u>functions</u>:

$$\rho_1(x) = \langle \eta(x) \rangle \equiv \rho \quad \underline{\text{density}}$$

$$\rho_2(x,y) = \left\langle \sum_{i \neq j} \delta(x - x_i)\, \delta(y - x_j) \right\rangle$$

($\rightarrow$ probability density for finding particles at x and y)

$$= \langle \eta(x)\, \eta(y) \rangle - \rho\, \delta(x-y)$$

Write $$\boxed{\rho_2(x,y) = \rho^2 g(x-y)}$$

<u>Poisson</u> <u>process</u>: $g \equiv 1$

Similarly $\rho_k(x_1, \cdots, x_k)$, $k = 1, 2, 3, \cdots$

(B) <u>Problem</u>: given ρ and $g(x)$, does there exist a point process η with

$$\rho_1(x) = \rho, \quad \rho_2(x,y) = \rho^2 g(x-y) \,?$$

If so, we say η <u>realizes</u> (ρ, g).

(C) Remarks:

(1) Applications:

- classical theory of fluids
- sphere packing (Torquato + Stillinger)
- Amusement

(2) Could also try to realize specified $\rho_1 \rho_2, \cdots, \rho_k$

(3) Lenard (1975) studied problem with $\rho_1, \rho_2, \cdots$

(4) Can also formulate on $\mathbb{Z}^d$

- $\eta(x) = 1$ or 0, $x \in \mathbb{Z}^d$
- $\rho_k(x_1, \dots, x_k)$ = probability of points at the distinct lattice sites $x_1, \dots, x_k$.

(D) Outline

- Some simple necessary conditions, and one sufficient condition, for realizability
- Examples
- A general realizability result at low density
- Realizability by Gibbs measures

II. Conditions for realizability

Ⓐ Necessary conditions

① Positivity: $\rho, g \geq 0$.

② Positive definiteness (PDC)

The quadratic form

$$S(x,y) = \langle \eta(x)\eta(y)\rangle - \langle \eta(x)\rangle\langle \eta(y)\rangle$$

is positive definite:

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} S(x,y)\, f(x) f(y)\, dx\, dy \geq 0$$

$$\left(= \mathrm{Var}\left(\int \eta(x) f(x)\, dx \right)\right)$$

or

$$\hat{S}(k) \equiv \rho + \rho^2 \int_{\mathbb{R}^d} e^{ik\cdot x} (g(x) - 1)\, dx \geq 0.$$

($\Rightarrow$ Gaussian realizability)

③ Yamada condition:

If $N_\Lambda \equiv \int_\Lambda \eta(x)\, dx$ and $\langle N_\Lambda \rangle = k + \theta$,

$k \in \mathbb{Z}$, then $\mathrm{Var}(N_\Lambda) \geq \theta(1-\theta)$.

$$\mathrm{Var}(N_\Lambda) = \langle (N_\Lambda - k - \theta)^2 \rangle$$

$$= \theta(1-\theta) + \langle (N_\Lambda - k)(N_\Lambda - k - 1)\rangle \geq \theta(1-\theta)$$

(B) A sufficient condition

If (ρ, g) is realizable and $\rho' < \rho$ then (ρ', g) is realizable.

Proof by "thinning":

- $\{x_1, x_2, \cdots\}$ a point set for the (ρ, g)-process
- Keep or discard each x_i independently, keeping a point with probability $\frac{\rho'}{\rho}$.
- New process η'

$$\langle \eta'(x) \rangle = \rho'$$

$$\rho_2'(x,y) = \frac{\rho'}{\rho}\frac{\rho'}{\rho}\rho_2(x,y)$$

$$= (\rho')^2 g(x,y).$$

So for fixed g there is a critical density ρ_c with realizability for $0 \le \rho < \rho_c$

III Examples

Ⓐ Step-function correlation in $\mathbb{R}^d$

(from Torquato - Stillinger)

$$g(x) = \begin{cases} 0, & |x| < 1, \quad \text{hard core} \\ 1, & |x| \geq 1, \quad \text{no correlation} \end{cases}$$

What is ρ_c?

PDC: $S(0) = \rho + \rho^2 \int_{\mathbb{R}^d} [g-1] = \rho - \rho^2 v_d 2^d \geq 0$

so $$\rho_c \leq \frac{1}{2^d v_d}$$

(v_d: volume of sphere, diameter 1, in $\mathbb{R}^d$)

General result below gives

$$\rho_c \geq \frac{1}{e\, 2^d v_d}$$

d = 1 ($v_d = 1$, $\rho_c \leq \frac{1}{2}$ by PDC)

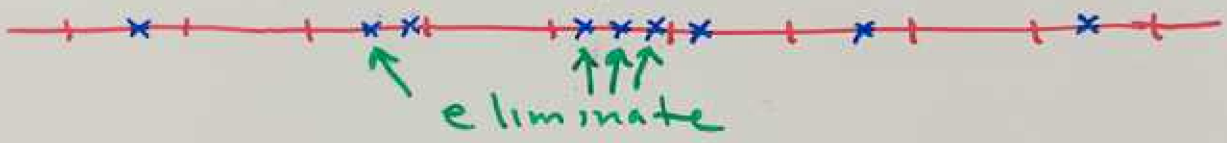
Special construction gives

$$\rho_c \geq \frac{1}{e}$$

<u>Construction</u>: eliminate points from a Poisson process, density λ:

$$\cdots x_{-1} < x_0 < x_1 < x_2 \cdots$$

If $x_i > x_{i+1} - 1$, eliminate x_i



Density $\rho = \lambda e^{-\lambda}$ maximized at

$\rho = e^{-1}$ for $\lambda = 1$.

(T + S believe $\rho_c = 1/2$ on basis of computer simulations)

(B) A lattice version on $\mathbb{Z}$ $(d=1)$

$$g_\alpha(x) = \begin{cases} \alpha, & x = \pm 1 \\ 1, & x = \pm 2, \pm 3, \cdots \end{cases}$$

$\rho_c \to \rho_\alpha$

(1) <u>$\alpha = 0$</u>:

$$\text{PDC} \Rightarrow \rho_0 \leq 1/3$$

Construction as above $\Rightarrow \rho_0 \geq \frac{1}{4}$.

But in fact we can show

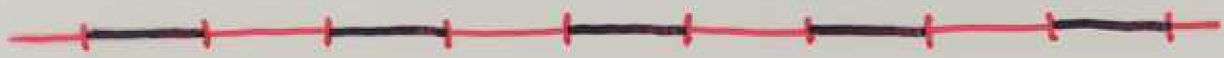
$$\rho_0 \leq \frac{326 - \sqrt{3115}}{822} \simeq 0.3287\ldots$$

$$\rho_0 \geq 0.264$$ (with E. Cagliotti)

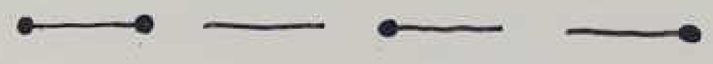
(2) $\alpha \geq 1$

$$\rho_\alpha = \frac{1}{2\alpha - 1}$$ (From PDC and a different construction)

Pairing construction



- pair sites; distinct pairs independent
- On a pair:

configuration 

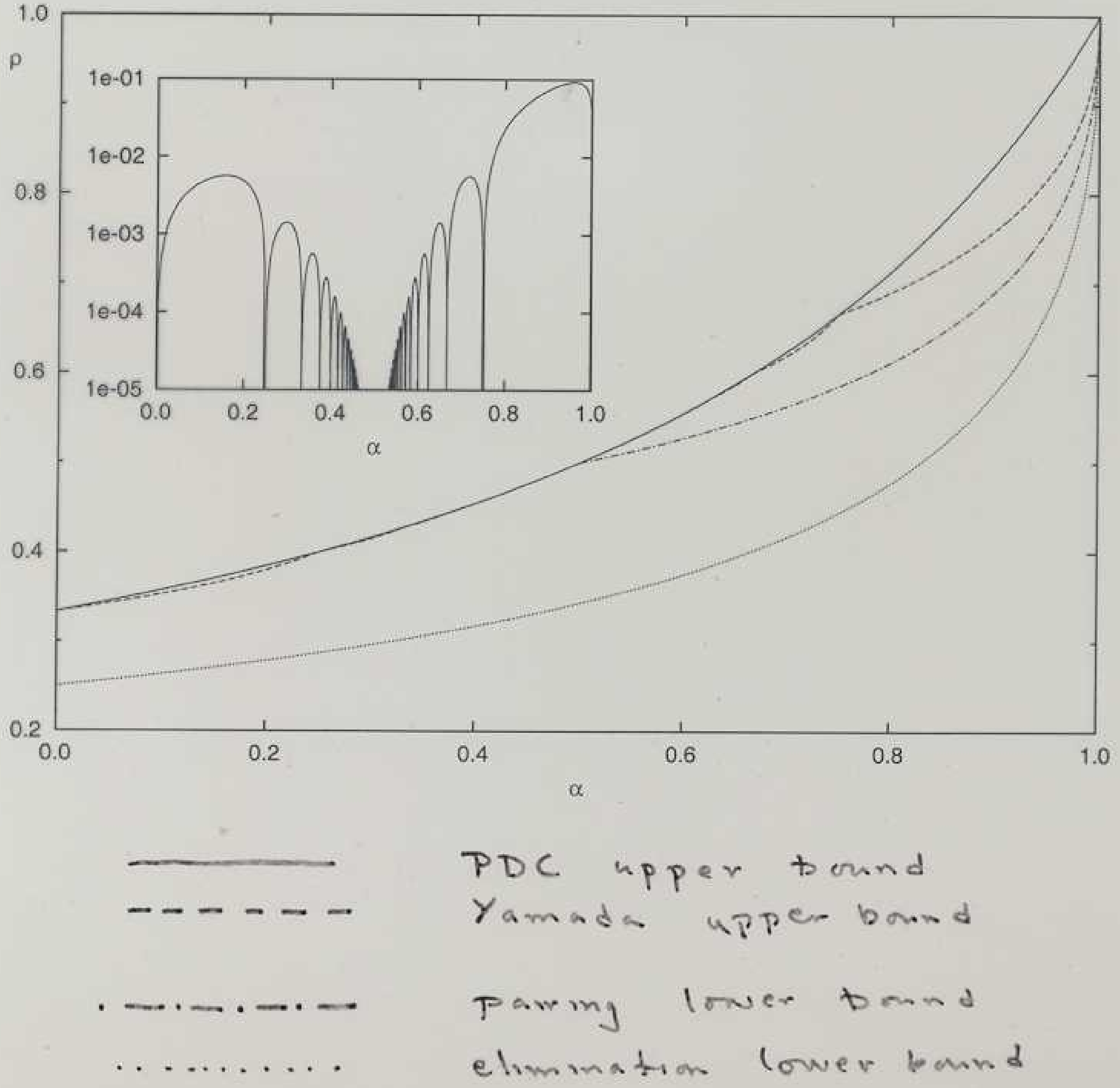
probability p q $\frac{1-p-q}{2}$

- average with translate

(3) $\alpha = \frac{1}{2}$, $\rho_\alpha = \frac{1}{2}$ (PDC; pairing)

(4) $0 \leq \alpha \leq 1$

$$\rho_\alpha \leq \frac{1}{3 - 2\alpha}$$ (PDC)



PDC upper bound
Yamada upper bound
pairing lower bound
elimination lower bound

(c) Sphere packing problem

(Torquato + Stillinger)

- Pack identical spheres (say diameter 1) into $\mathbb{R}^d$

  volume density ϕ

- Find $\phi_{max}(d)$.

Approaches

(1) Lattice packing

Minkowski (1905) $\phi_{max}(d) \geq \frac{\zeta(d)}{2^{d-1}}$

Lower bound has been improved but still $\sim 2^{-d}$.

(2) Disordered packing

- Find a point process in $\mathbb{R}^d$ with density ρ and

$$g(x) = 0 \quad \text{if} \quad |x| < 1.$$

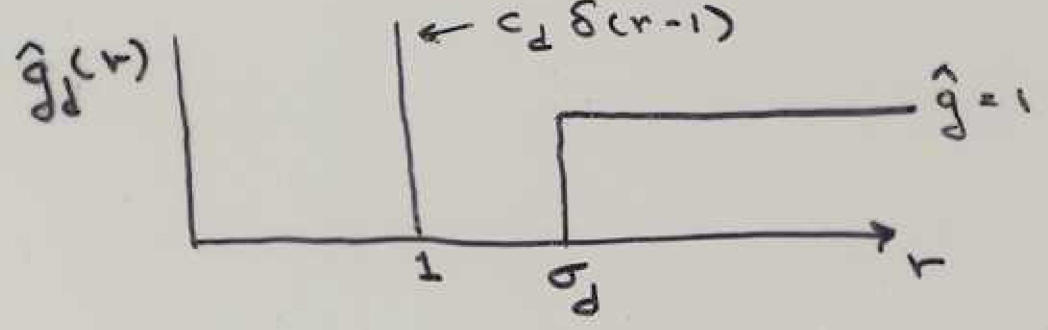
- (Almost) any realization gives sphere packing.

So $\boxed{\phi_{max}(d) \geq \rho v_d}$ (v_d: volume of sphere in $\mathbb{R}^d$, diameter 1)

To find the point process

Conjecture (TS): If d is sufficiently large then any (ρ, g) with $\rho \geq 0$, $g \geq 0$, and satisfying PDC is realizable.

So take $g_d(x) = \hat{g}_d(|x|)$



Calculation (TS): (ρ_d, g_d) satisfies PDC for some ρ_d with

$$\rho_d v_d \sim 2^{-(0.77865\ldots)d}$$

IV Realizability at small density

Given $g(x)$, $x \in \mathbb{R}^d$, satisfying certain conditions, prove realizability of (ρ, g) for sufficiently small ρ.

Extension of an argument of Ambartzumian + Sukiasian (1991).

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We have $\rho_2(x_1, x_2) = \rho^2 g(x_1 - x_2)$

Ansatz: for all $n \geq 2$,

$$\rho_n(x_1, \cdots, x_n) = \rho^n \prod_{1 \leq i < j \leq n} g(x_j - x_i)$$

Now fix $\Lambda \subset \mathbb{R}^d$ and define

$$P_n^{\Lambda}(x_1, \cdots, x_n)$$

to be the probability density for finding exactly n points in Λ, at positions $x_1, \cdots, x_n$.

Then by the inclusion-exclusion formula

$$p_n^{\wedge}(x_1,\dots,x_n) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int_{\Lambda^k} \rho_{n+k}(x_1,\dots,x_n,y_1,\dots,y_k)\, dy_1 \cdots dy_k$$

- This series converges (under our hypotheses on g)
- If we show $p_n^{\wedge} \geq 0$ for $\rho \leq \rho^*$, with ρ^* independent of Λ, we are done.

$$= \rho^n \prod_{1 \leq i < j \leq n} g(x_j - x_i) \sum_{k=0}^{\infty} \frac{(-\rho)^k}{k!} \cdot$$

$$\cdot \int_{\Lambda^k} \prod_{1 \leq i < j \leq k} g(y_j - y_i) \prod_{\substack{1 \leq i \leq n \\ 1 \leq j \leq k}} g(y_j - x_i)\, dy_1 \cdots dy_k$$

Define $V(y) = -\log g(y)$

so $g(y_j - y_i) = e^{-V(y_j - y_i)}$

$$V^{(1)}(y) = \sum_{i=1}^{n} V(y - x_i)$$

so $\prod_{i=1}^{n} g(y_j - x_i) = e^{-V^{(1)}(y)}$

So

$$\rho_n^\Lambda (x_1, \dots, x_n) = \rho^n \prod_{1 \le i < j \le n} g(x_j - x_i) \, \Xi_\Lambda(-\rho, V^{(1)}, V)$$

where $\Xi_\Lambda(z, V^{(1)}, V)$ is the standard grand canonical partition function for a particle system in Λ, interaction potential V, one-body external potential $V^{(1)}$.

Appeal (almost directly) to standard results (Ruelle's book) based on Kirkwood-Salsburg equations. (Modify proof slightly due to form of $V^{(1)}$).

Conclusion: Suppose that <u>either</u>

- $g \le 1$ ($V \ge 0$ repulsive)

<u>or</u>

- hard core ($g(x) = 0$, $|x| < D$) and $|g(x) - 1| \to 0$ sufficiently fast as $|x| \to \infty$.

Then there is a (computable) constant $b > 0$ such that $\hat{p_n} \geq 0$ if

$$\rho \leq e b \int_{\mathbb{R}^d} |g(x) - 1| \, dx$$

($b = 1$ if $g \leq 1$.)

(so e.g. for

$$g(x) = \begin{cases} 0, & x < 1, \\ 1, & x \geq 1, \end{cases}$$

$$\frac{1}{e\, 2^d v_d} \leq \rho_c \leq \frac{1}{2^d v_d}$$)

V. Gibbsian realizations

Ask: can a given (ρ, g) be realized by a Gibbs ensemble with two-body interactions?

$$e^{-V(x-y)}$$

(or if not translation invariant, $e^{-V^{(1)}(x)}$, $e^{-V(x,y)}$)

(A) Result of L. Koralov:

Yes on $\mathbb{Z}^d$, ρ small,

$$\sum_{\substack{x \in \mathbb{Z}^d \\ x \neq 0}} |g(x) - 1| \leq 1.$$

(B) Maximizing entropy

Suppose (ρ, g) is realizable; look for realization which <u>maximizes</u> <u>entropy</u>

At least formally, this is Gibbsian.

Consider problem on finite set X.

Given $\rho(x)$, $x \in X$; $g(x,y)$, $x, y \in X, x \neq y$.

Want to find probabilities P_η:

$$\sum_\eta P_\eta = 1$$

$$\sum_\eta \delta_{\eta(x),1} P_\eta = \rho(x)$$

$$\sum_\eta \delta_{\eta(x),1}\, \delta_{\eta(y),1}\, P_\eta = \rho(x)\rho(y)g(x,y)$$

Maximize

$$S = \sum_\eta P_\eta \log P_\eta$$

subject to these constraints

Use Lagrange multipliers, find

$$P_\eta = Z\, e^{-\sum_{\eta(x)=1} \lambda_1(x)}\, e^{-\sum_{\eta(x)=\eta(y)=1} \lambda_2(x,y)}$$

with $\lambda_1(x)$, $\lambda_2(x,y)$ Lagrange mult.

Lagrange multiplier method can be justified if $\rho < \rho_c$.