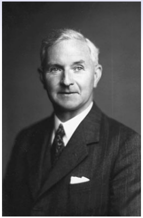
Lennard-Jones potential estimation [1]

Jean-François Coeurjolly

Joint work with Frédéric Lavancier

1. based on C-L, Parametric estimation of pairwise Gibbs point processes with infinite range interaction, Bernoulli, 2016



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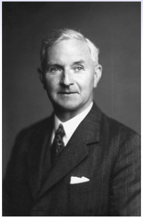

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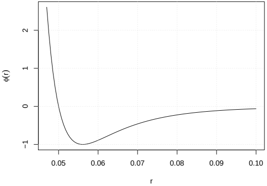

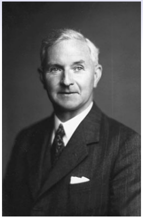

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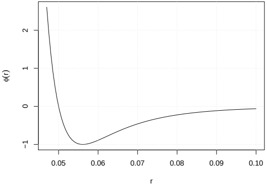

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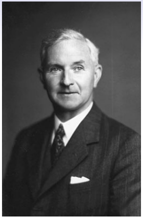

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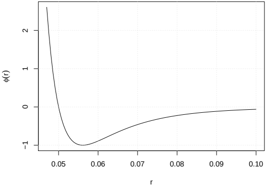

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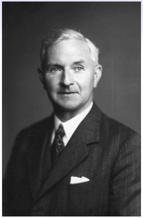

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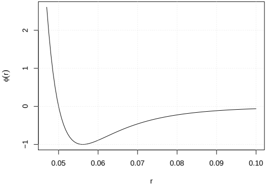

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Thank you for your attention

A few notation

- Let π_Λ^β, $\Lambda \Subset \mathbb{R}^d$ (bounded Borel set of $\mathbb{R}^d$), $\beta > 0$: Poisson point process in Λ with intensity β.
- Let $\Phi : \mathbb{R}^d \to \mathbb{R} \cup \{\infty\}$ be a potential function and $H_\Lambda : \Omega_T \to \mathbb{R} \cup \{\infty\}$ be the Hamiltonian given by

$$H_\Lambda(\mathbf{x}) = \frac{1}{2} \sum_{\substack{u,v \in \mathbf{x},\, u \neq v, \\ \{u,v\} \cap \mathbf{x}_\Lambda \neq \emptyset}} \Phi(u-v)$$

$\mathbf{\Omega} = \{\mathbf{x} \in \mathbf{\Omega}_T, \forall \Lambda \Subset \mathbb{R}^d, H_\Lambda(\mathbf{X}) < \infty\}$, $\mathbf{\Omega}_T$ set of tempered configurations.

Dobrushin-Landford-Ruelle formalism

P is a Gibbs measure if $P(\mathbf{\Omega}) = 1$ and for P-a.e. $\mathbf{x}$ and any Λ the cond. law of P given x_{Λ^c} is absolutely continuous w.r.t. π_Λ^β with density

$$\exp\left(-H_\Lambda(\mathbf{x})\right) / Z_\Lambda(\mathbf{x}_{\Lambda^c}).$$

Papangelou conditional intensity

Let $\lambda : \mathbb{R}^d \times \Omega \to \mathbb{R}_+$ defined for any $u \in \Lambda$ by

$$\lambda(u, \mathbf{x}) = \beta \, \frac{e^{-H_\Lambda(\mathbf{x} \cup u)}}{e^{-H_\Lambda(\mathbf{x})}} = \beta \, e^{-\sum_{v \in \mathbf{x}} \Phi(v-u)}.$$

= can be viewed as the conditional probability to have a point in a vicinity of u, given that the rest of the configuration is $\mathbf{x}$.

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Statistical model : $\Phi \to \Phi_\theta$, $\lambda \to \lambda_\theta$, where $\theta \in \mathbb{R}^p$, $p \geq 1$

Exponential family model :

$$\lambda_\theta(u, \mathbf{x}) = \beta e^{-\sum_{v \in \mathbf{x}} \Phi_\theta(v-u)} = e^{-\theta^\top t(u,\mathbf{x})}$$

with $\theta_1 = -\log \beta$ and $t = (t_1, \ldots, t_p)^\top$ where $t_1(u, \mathbf{x}) = 1$and

$$t_m(u, \mathbf{x}) = \sum_{v \in \mathbf{x}} g_m(v - u), \quad m = 2, \ldots, p.$$

$\Rightarrow \Phi_\theta = \sum_{m=2}^{p} \theta_m g_m.$

Existence of a Gibbs measure, Ruelle (1969)

If the potential Φ_θ is bounded from below and there exist $0 < r_1 < r_2 < \infty$, $c > 0$ and $\gamma_1, \gamma_2 > d$ such that

$$\Phi_\theta(u) \geq c\|u\|^{-\gamma_1} \text{ for } \|u\| \leq r_1 \text{ and } |\Phi_\theta(u)| \leq c\|u\|^{-\gamma_2} \text{ for } \|u\| \geq r_2,$$

then $\exists$ at least one stationary Gibbs measure.

Examples

- Hard-core with finite range potential!!
- $\Phi(u) = \|u\|^{-\gamma}$ with $\gamma > d$; $\Phi(u) = e^{-\|u\|}\|u\|^{-\gamma}$ with $\gamma > d$.
- Lennard-Jones type pair potential defined for some $d < \gamma_2 < \gamma_1$ and some $A, B > 0$ by $\Phi(u) = A\|u\|^{-\gamma_1} - B\|u\|^{-\gamma_2}$.
- Standard LJ-model= $d = 2$, $\gamma_1 = 12$ and $\gamma_2 = 6$.

We assume **[g]** in the following

a collection of technical conditions on the g_m's which (among other) imply that Φ_θ satisfies Ruelle conditions. (stisfied by previous examples)

Domain of observation

$\mathbf{X}$ is observed in W_n, where (W_n) is an increasing sequence of convex domains, such that $W_n \to \mathbb{R}^d$ as $n \to \infty$.

PL and LR

Popular alternatives to the ML (no normalizing constant). In particular, the PL estimator is defined as the maximum of

$$\mathsf{LPL}_{W_n}(\mathbf{X};\theta) = \sum_{u \in \mathbf{X} \cap W_n} \log \lambda_\theta(u, \mathbf{X} \setminus u) - \int_{W_n} \lambda_\theta(u, \mathbf{X}) \mathrm{d}u.$$

<u>Problem</u> : $\lambda_\theta(u, \mathbf{X})$ depends on $\mathbf{X} \cap W_n^c$ which is not observed.

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Border-correction (Møller and Jensen (91), Jensen and Künsch (94), Billiot et al. (08), C and Drouilhet (10), Baddeley et al (14))

$$\begin{aligned} \mathbf{X} \text{ has a finite range } &\Leftrightarrow \Phi_\theta \text{ is compactly supported in } B(0,R),\ R < \infty \\ &\Leftrightarrow \lambda_\theta(u, \mathbf{x}) = \lambda_\theta(u, \mathbf{x}_{u,R}),\ \text{where } \mathbf{x}_{u,R} = \mathbf{x} \cap B(u,R) \end{aligned}$$

$$\Rightarrow \mathsf{LPL}_{W_n \ominus R}(\mathbf{X};\theta) = \sum_{u \in \mathbf{X} \cap W_n \ominus R} \log \lambda_\theta(u, \mathbf{X}_{u,R} \setminus u) - \int_{W_n \ominus R} \lambda_\theta(u, \mathbf{X}_{u,R}) \mathrm{d}u$$

Pseudolikelihood for infinite range models

Let (α_n) and (R_n) be two sequences of real numbers. We define

$$\widetilde{\mathsf{LPL}}_{W_n \ominus \alpha_n, R_n}(\mathbf{X};\theta) = \sum_{u \in \mathbf{X} \cap W_n \ominus \alpha_n} \log \lambda_\theta(u, \mathbf{X}_{u,R_n} \setminus u) - \int_{W_n \ominus \alpha_n} \lambda_\theta(u, \mathbf{X}_{u,R_n}) \mathrm{d}u$$

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Interesting choices (further investigated)

- $\alpha_n = R_n \Leftrightarrow$ border correction for finite range interaction models with range R taking $R_n = R$;
- $R_n = \infty \Leftrightarrow$ accounting for the maximal possible range of interaction ;
- $R_n = \infty$ and $\alpha_n = 0 \Leftrightarrow$ maximal possible range of interaction **and** no erosion is considered.

Consistency result

If $\alpha_n|W_n|^{-1/d} \to 0$ and $R_n \to \infty$ as $n \to \infty$ and if for any $y \in \mathbb{R} \setminus \{0\}$, $P\left\{y^\top t(0,\mathbf{X}) \neq 0\right\} > 0$, then as $n \to \infty$, $\widehat{\theta} \to \theta^\star$ a.s.

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Asymptotic normality result

Let α_n and R_n be such that $\alpha_n |W_n|^{-1/d} \to 0$, ${\alpha_n}^{-\gamma'} |W_n|^{1/2} \to 0$ and ${R_n}^{-\gamma'} |W_n|^{1/2} \to 0$ for some $0 < \gamma' < \gamma_2 - d$.

Assume $U_\infty, \Sigma_\infty > 0$ and $\boxed{\gamma_2 > 2d}$, then

$$|W_n|^{1/2} \left(\widehat{\theta} - \theta^\star\right) \xrightarrow{d} \mathcal{N}\left(0, U_\infty^{-1} \Sigma_\infty U_\infty^{-1}\right)$$

- U_∞ : asymptotic normalized sensitivity matrix.
- Σ_∞ : asymptotic covariance matrix of the score function.

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Remarks

- $\gamma_2 > 2d$ is the more important condition (satisfied for LJ).
- for the asymptotic normality result, α_n must tend to ∞.

A few explanations of the difficulties : consistency

(for ease, assume $\alpha_n = R_n$)

- for finite range models, $\mathsf{LPL}_{W_n \ominus R}(\mathbf{X}, \cdot)$ is a concave function and the score function is unbiased.
- for inifinite range models, $\widetilde{\mathsf{LPL}}_{W_n \ominus R_n, R_n}(\mathbf{X}, \cdot)$ can still be shown to be a concave function.
- But its score (at $\theta^\star$) writes

$$s_{W_n \ominus R_n}(\mathbf{X}, \theta^\star) = \int_{W_n \ominus R_n} t(u, \mathbf{X}_{u,R_n}) \lambda_{\theta^\star}(u, \mathbf{X}_{u,R_n}) \mathrm{d}u - \sum_{u \in \mathbf{X} \cap W_n \ominus R_n} t(u, \mathbf{X}_{u,R_n})$$

$$\Rightarrow \ \mathrm{E} s_{W_n \ominus R_n}(\mathbf{X}, \theta^\star) \overset{GNZ}{=} \int_{W_n \ominus R_n} t(u, \mathbf{X}_{u,R_n}) \left(\lambda_{\theta^\star}(u, \mathbf{X}_{u,R_n}) - \lambda_{\theta^\star}(u, \mathbf{X}) \right) \mathrm{d}u \neq 0$$

A few explanations of the difficulties : CLT

- CLT for $\widehat{\theta}$ (mainly) ensues from a CLT for the score function.
- Assume $W_n \ominus R_n = \cup_{j \in \mathcal{J}_n} \Delta_j$ where the Δ_j's are unit cubes centered at $j \in \mathbb{Z}^d$.
- Let $Z_{n,j} = s_{\Delta_j}(\mathbf{X}, \theta^\star) - \mathrm{E}(s_{\Delta_j}(\mathbf{X}, \theta^\star))$

$$s_{W_n \ominus R_n}(\mathbf{X}, \theta^\star) = \sum_{j \in \mathcal{J}_n} s_{\Delta_j}(\mathbf{X}, \theta^\star) = \sum_{j \in \mathcal{J}_n} Z_{n,j} + \underbrace{\sum_{j \in \mathcal{J}_n} \mathrm{E} s_{\Delta_j}(\mathbf{X}, \theta^\star)}_{= o_P(|W_n|^{-1/2})}$$

- The $Z_{n,j}$'s are not α-mixing!! For finite-range models, typically, they are conditionally centered, i.e.

$$\mathrm{E}\left(Z_{n,j} \mid \mathbf{X} \cap \Delta_j^c\right) = 0 \qquad \textbf{[conditional GNZ]}$$

$\Rightarrow$ CLT for sums of conditonally centered for functionals of Markov random fields.

Theorem (Jensen and Künsch (1994), Comets and Janzura (1998), Guyon and Gaetan (2004), Coeurjolly and Lavancier (2012))

$X_{n,j}$ be a triangular array field in a measurable space S ; For $n \in \mathbb{N}$, let $\mathcal{I}_n \subset \mathbb{Z}^d$ and $\alpha_n \in \mathbb{R}_+$ such that $|\mathcal{I}_n| \to \infty$ and $\alpha_n \to \infty$ as $n \to \infty$. Define $S_n = \sum_{j \in \mathcal{I}_n} Z_{n,j}$ where $Z_{n,j} = f_{n,j}(X_{n,k}, k \in K_j)$ with $\mathcal{K}_j = \{k \in \mathbb{Z}^d, |k-j| \leq A\}$ and where $f_{n,j} : S^{\mathcal{K}_{n,j}} \to \mathbb{R}^p$ is a measurable function. We define $\widehat{\Sigma}_n$ and Σ_n by

$$\widehat{\Sigma}_n = \sum_{j \in \mathcal{I}_n} \sum_{\substack{k \in \mathcal{I}_n \\ |k-j| \leq A}} Z_{n,j} Z_{n,k}^\top \qquad \text{and} \qquad \Sigma_n = \mathrm{E}\widehat{\Sigma}_n.$$

(a) $\mathrm{E} Z_{n,j} = 0$ and $\sup_{n \geq 1} \sup_{j \in \mathcal{I}_n} \mathrm{E}\|Z_{n,j}\|^4 < \infty$.

Then, $|\mathcal{I}_n|^{-1}(\widehat{\Sigma}_n - \Sigma_n) \to 0 \quad$ in L^2. If in addition

(c) $\exists Q > 0$ such that $|\mathcal{I}_n|^{-1}\Sigma_n \geq Q$ for n sufficiently large,

(d) $\mathrm{E}\left(Z_{n,j} \mid X_{n,k}, k \neq j\right) = 0$

then

$$\Sigma_n^{-1/2} S_n \xrightarrow{d} \mathcal{N}(0, I_p). \tag{1}$$

Theorem (Coeurjolly and Lavancier (2016))

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(a) $\mathrm{E}Z_{n,j} = 0$ and there exists $q \ge 1$ such that $\sup_{n \ge 1} \sup_{j \in \mathcal{I}_n} \mathrm{E}\|Z_{n,j}\|^{4q} < \infty$,

(b) for any sequence $\mathcal{J}_n \subset \mathcal{I}_n$ such that $|\mathcal{J}_n| \to \infty$ as $n \to \infty$, $|\mathcal{J}_n|^{-1} \sum_{j,k \in \mathcal{J}_n} \left\|\mathrm{E}(Z_{n,j} Z_{n,k}^\top)\right\| = \mathcal{O}(1)$.

Then if $\alpha_n^{\frac{4q-1}{2q-1}d} = o(|\mathcal{I}_n|)$ as $n \to \infty$, $|\mathcal{I}_n|^{-1}(\widehat{\Sigma}_n - \Sigma_n) \to 0$ in L^{2q}. If in addition

(c) $\exists Q > 0$ such that $|\mathcal{I}_n|^{-1}\Sigma_n \ge Q$ for n sufficiently large,

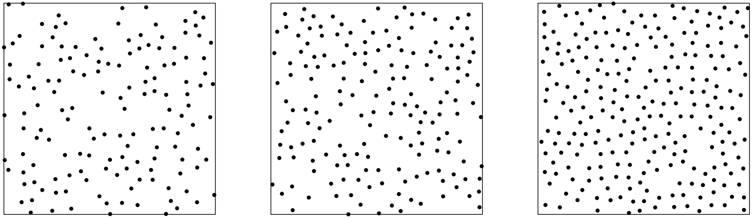
(d) as $n \to \infty$

$$|\mathcal{I}_n|^{-1/2} \sum_{j \in \mathcal{I}_n} \mathrm{E}\left\|\mathrm{E}\left(Z_{n,j} | X_{n,k}, k \ne j\right)\right\| \to 0,$$

then

$$\Sigma_n^{-1/2} S_n \xrightarrow{d} \mathcal{N}(0, I_p). \tag{2}$$

- LJ model with parameters : $\beta = 100$, $\sigma = 0.1$ and $\varepsilon = 0.1, 0.5, 1$ (low, moderate and high rigidity models).
- $W_n = [-1/2, 1/2]^2, [-1, 1]^2$ and $[-2, 2]^2$.



$\varepsilon = 0.1$ $\varepsilon = 0.5$ $\varepsilon = 1$

- RWMSE = $\sqrt{\text{WMSE}}$ = root-weighted empirical mean squared error, where

$$\text{WMSE} = \frac{\widehat{E}\left\{\left(\widehat{\log\beta} - \log\beta\right)^2\right\}}{(\log\beta)^2} + \frac{\widehat{E}\left\{(\widehat{\sigma} - \sigma)^2\right\}}{\sigma^2} + \frac{\widehat{E}\left\{(\widehat{\varepsilon} - \varepsilon)^2\right\}}{\varepsilon^2}$$

	RWMSE		
	$[-1/2, 1/2]^2$	$[-1, 1]^2$	$[-2, 2]^2$
Low ($\varepsilon = 0.1$)			
$\alpha_n = R_n \in [0.05, 0.3]$	3.26 (0.13)	1.25 (0.13)	0.62 (0.12)
$\alpha_n \in [0.05, 0.3],\ R_n = \infty$	3.72 (0.05)	1.79 (0.05)	0.63 (0.06)
$\alpha_n = 0,\ R_n = \infty$	3.5	1.66	0.69
Moderate ($\varepsilon = 0.5$)			
$\alpha_n = R_n \in [0.05, 0.3]$	0.65 (0.12)	0.34 (0.14)	0.2 (0.15)
$\alpha_n \in [0.05, 0.3],\ R_n = \infty$	0.68 (0.05)	0.38 (0.05)	0.19 (0.05)
$\alpha_n = 0,\ R_n = \infty$	0.59	0.33	0.18
High ($\varepsilon = 1$)			
$\alpha_n = R_n \in [0.05, 0.3]$	1.04 (0.08)	0.42 (0.16)	0.13 (0.16)
$\alpha_n \in [0.05, 0.3],\ R_n = \infty$	1.34 (0.05)	0.36 (0.05)	0.16 (0.05)
$\alpha_n = 0,\ R_n = \infty$	1.23	0.27	0.17

- 100 replications
- α_n and/or $R_n \in [0.05, 0.3] \Leftrightarrow$ 30 values regularly sampled.
- When an interval is considered, we report the optimal α_n value between brackets.

No further question ? Mine : what's the social event ?

(Level imposed by Aalborg was amazingly high)

Assumption [g]

For convenience we let $g_1 = 0$ and we denote by g the p-dimensional vector $g = (0, g_2, \dots, g_p)^\top$. We make the following assumption on g.
[g] For all $m \geq 2$, g_m is bounded from below and there exist $\gamma_1, \gamma_2 > d$ and $c_g, r_0 > 0$ such that

(i) $\forall \|x\| < r_0$ and $\forall \theta \in \boldsymbol{\Theta}$, $\theta_2\, g_2(x) \geq c_g \|x\|^{-\gamma_1}$

(ii) $\forall m \geq 3,\ g_m(x) = o(\|x\|^{-\gamma_1})$ as $\|x\| \to 0$

(iii) $\forall m \geq 2$ and $\forall \|x\| \geq r_0$, $|g_m(x)| \leq c\|x\|^{-\gamma_2}$.