Gibbs point processes : modelling and inference

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Outline

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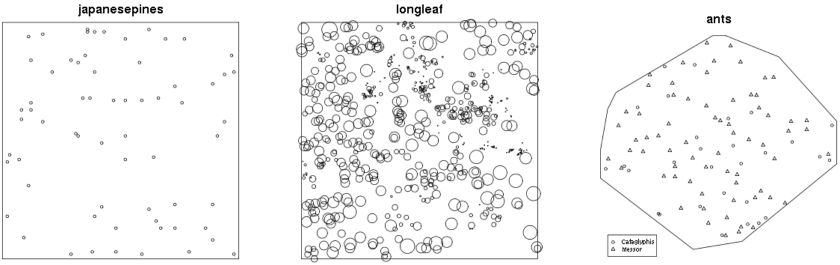
Type of data

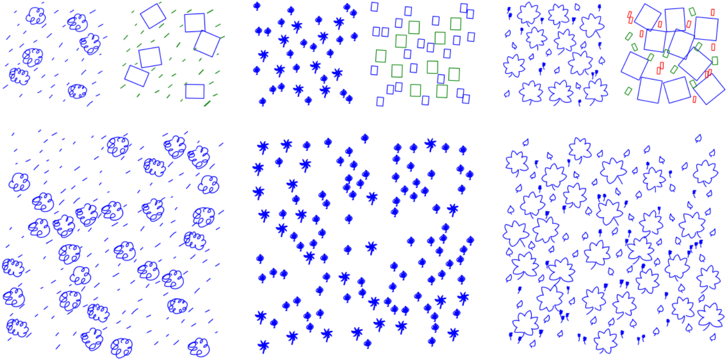


Scientific questions :

1. Independence or interaction ? regular or clustered distribution ?
2. Spatial variation in the density and marks ?
3. Interaction in each sub-pattern, between sub-patterns...

Another example in computer graphics

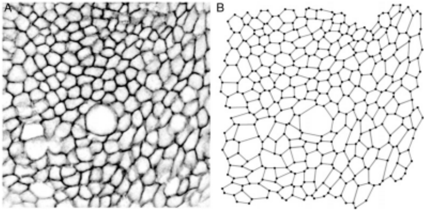
(Hurtut, Landes, Thollot, Gousseau, Drouilhet, C.'09.)



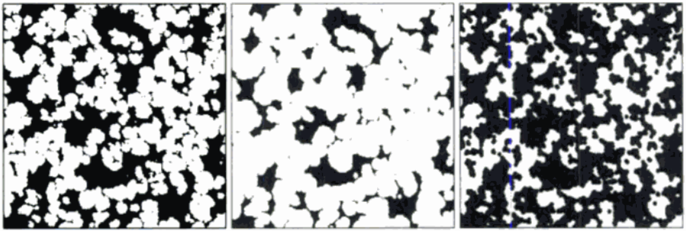
Problem : simulation at large scale of a pattern drawn in a small window.

Examples with geometrical structures

1. Epithelial cells



2. Materials interface



Outline

1. Type of data of interest
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   - Examples
3. Identification
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   - Pseudo-likelihood method
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   - Variational Principle method
4. Validations through residuals
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   - Measures of departures to the true model
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Marked point processes

- State space : $\mathbb{S} = \mathbb{R}^d \times \mathbb{M}$ associated to $\mu = \lambda \otimes \lambda^{\mathrm{m}}$.
- Let $x^m = (x, m)$ an element of $\mathbb{S}$, i.e. a marked point.
- Ω is the space of locally finite point configurations φ in $\mathbb{S}$
- For $\Lambda \Subset \mathbb{R}^d$: Λ bounded borelian set of $\mathbb{R}^d$.
- φ_Λ is the restriction of φ on Λ and $|\varphi_\Lambda|$ is the number of points φ_Λ.

Definition (marked point process)

A marked point process is a random variable, Φ, on Ω.

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Poisson process

For $z > 0$, the standard (non-marked) poisson point process π^z with intensity $z\lambda$ is defined by

$$\begin{cases} \forall\ \Lambda, \quad |\pi^z_\Lambda| := \pi^z(\Lambda) \sim \mathcal{P}(z\lambda(\Lambda)) \\ \forall\ \Lambda, \Lambda' \text{ with } \Lambda \cap \Lambda' = \emptyset, \quad \pi^z_\Lambda \text{ and } \pi^z_{\Lambda'} \text{ are independent.} \end{cases}$$

Stationary Gibbs models on $\mathbb{R}^d$

Consider a parametric family of energies $(V_\Lambda(\cdot;\theta))_{\Lambda \Subset \mathbb{R}^d}$ for $\theta \in \mathbb{R}^p$ defined on Ω and with value on $\mathbb{R} \cup \{+\infty\}$.

Definition

A probability measure P_θ on Ω is a stationary marked Gibbs measure for the compatible and invariant by translation family of energies $(V_\Lambda(.;\theta))_{\Lambda \Subset \mathbb{R}^d}$ if for every $\Lambda \Subset \mathbb{R}^d$, for P_θ-a.e. outside configuration φ_{Λ^c}, the distribution of P_θ conditionally to φ_{Λ^c} admits the following conditional density with respect to π_Λ $(:= \pi_\Lambda^1)$:

$$f_\Lambda(\varphi_\Lambda | \varphi_{\Lambda^c};\theta) = \frac{1}{Z_\Lambda(\varphi_{\Lambda^c};\theta)} e^{-V_\Lambda(\varphi;\theta)},$$

where $Z_\Lambda(\varphi_{\Lambda^c};\theta)$ is the normalizing constant called partition function.

Compatibility for all $\Lambda \subset \Lambda' \Subset \mathbb{R}^d$, there exists a measurable function $\psi_{\Lambda,\Lambda'}$ from Ω to $\mathbb{R} \cup \{+\infty\}$ such that

$$\forall \varphi \in \Omega, \quad V_{\Lambda'}(\varphi;\theta) = V_\Lambda(\varphi;\theta) + \psi_{\Lambda,\Lambda'}(\varphi_{\Lambda^c};\theta).$$

Existence/unicity problem

The choice of $(V_\Lambda(\cdot;\theta))_{\Lambda\Subset\mathbb{R}^d}$ entirely defines the Gibbs measure P_θ.
But, given a family : does there exist a Gibbs measure P_θ ? Is it unique (phase transition problem) ?

- Ruelle(69), Preston(76) : Superstable and lower regular potentials (*e.g.* Lennard-Jones model).
- BBD(99) : local stability and finite range (actually quasilocality) assumptions.
- D(05) : non hereditary energies. [A family $(V_\Lambda(\cdot;\theta))_{\Lambda\Subset\mathbb{R}^d}$ is **hereditary** if $\forall\Lambda\Subset\mathbb{R}^d,\ V_\Lambda(\varphi;\theta)=+\infty\Rightarrow V_\Lambda(\varphi\cup x^m;\theta)=+\infty.$]
- DDG(10) : stability and locality (to the configuration) assumptions.

Existence assumption [Mod]

we observe a realization of Φ with marked Gibbs measure $P_{\theta^\star}$, where $\theta^\star\in\mathring{\Theta}$, Θ is a compact set of $\mathbb{R}^p$ and for all $\theta\in\Theta$, there exists a stationary marked Gibbs measure P_θ for the family $(V_\Lambda(.;\theta))_{\Lambda\Subset\mathbb{R}^d}$ assumed to be invariant by translation, compatible.

Local energy function

Definition

The energy required to insert x^m in φ is defined for every $\Lambda \ni x$ by

$$V\left(x^m|\varphi;\theta\right) := V_\Lambda(\varphi \cup x^m;\theta) - V_\Lambda(\varphi;\theta),$$

which from the compatibility assumption is independent of Λ.

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For every mark m, every configuration φ and for all $\theta \in \Theta$

[LS] Local stability : $\exists\ K > 0$ such that $V\left(0^m|\varphi;\theta\right) \geq -K$.

[FR] Finite range : $\exists\ D > 0$ such that $V\left(0^m|\varphi;\theta\right) = V\left(0^m|\varphi_{\mathcal{B}(0,D)};\theta\right)$.

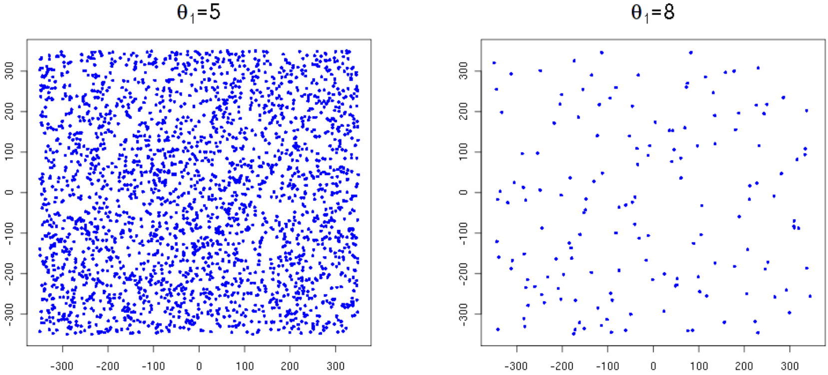
D, K independent of θ, m, φ.

BBD(99)

$$\textbf{[LS]} + \textbf{[FR]} \Longrightarrow \textbf{[Mod]}$$

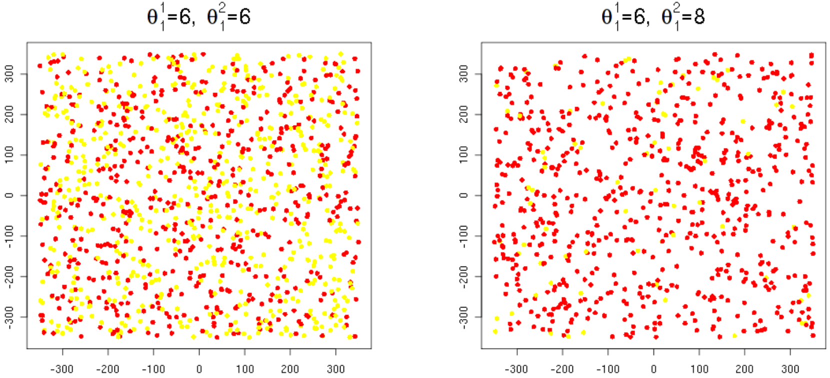
Poisson point process, $\mathbb{M} = \{0\}$

$$V_\Lambda(\varphi;\theta) = \theta_1 |\varphi_\Lambda|$$



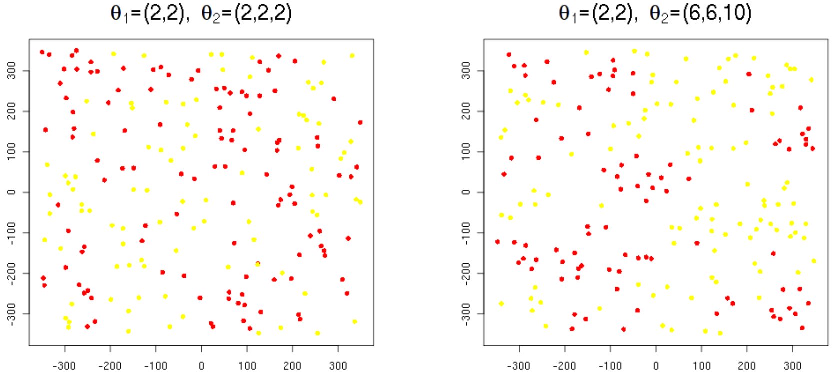
Multi-type Poisson point process, $\mathbb{M} = \{1, 2\}$

$$V_\Lambda(\varphi; \theta) = \theta_1^1 |\varphi_\Lambda^1| + \theta_1^2 |\varphi_\Lambda^2|$$



Strauss marked point process, $\mathbb{M} = \{1, 2\}$

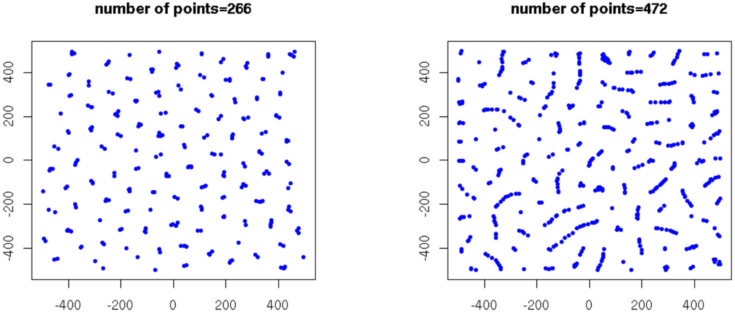
$$V_\Lambda(\varphi;\theta) = \sum_{m=1}^{2} \theta_1^m |\varphi_\Lambda^m| + \sum_{1\le m\le m'\le 2} \theta_2^{m,m'} \sum_{\substack{\{x^m, y^{m'}\}\in\mathcal{P}_2(\varphi)\\ \{x^m,y^{m'}\}\cap\Lambda\neq\emptyset}} \mathbf{1}_{[0,D^{m,m'}]}(\|y-x\|),$$



Multi-Strauss point process, $\mathbb{M} = \{0\}$ on a planar structured graph

$$V_\Lambda(\varphi;\theta) = \theta_1|\varphi_\Lambda| + \sum_{k=1}^{K} \theta_2^k \sum_{\substack{\{x,y\}\in G_2(\varphi)\\ \{x,y\}\cap\Lambda\neq\emptyset}} \mathbf{1}_{[D_{k-1},D_k]}(\|y-x\|),$$

$G_2(\varphi) = \mathcal{P}_2(\varphi)$ $\qquad$ $G_2(\varphi) = Del_2(\varphi)$

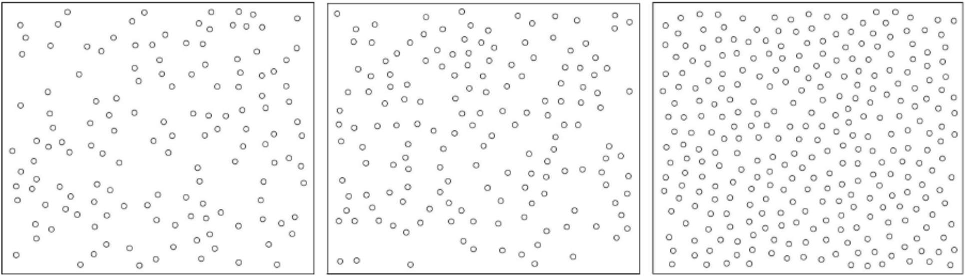


$$D_0 = 0, D_1 = 20, D_2 = 80, \ \theta = (1,2,4)$$

Lennard-Jones model

$$V_\Lambda^{LJ}(\varphi;\theta) := \theta_1|\varphi_\Lambda| + 4\theta_2 \sum_{\substack{\{x,y\}\in P_2(\varphi)\\ \{x,y\}\cap\Lambda\neq\emptyset}} \left(\left(\frac{\theta_3}{\|y-x\|}\right)^{12} - \left(\frac{\theta_3}{\|y-x\|}\right)^{6} \right)$$

with $\theta = (\theta_1,\theta_2,\theta_3) \in \mathbb{R}\times(\mathbb{R}^+)^2$.

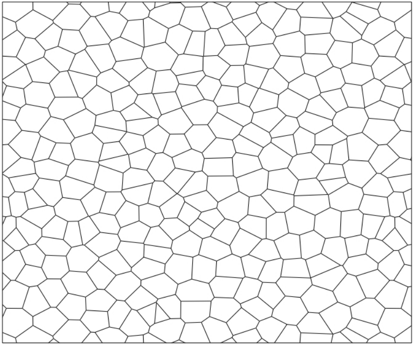


$\theta_2 = 0$ $\qquad$ $\theta_2 = 0.1$ $\qquad$ $\theta_2 = 2$

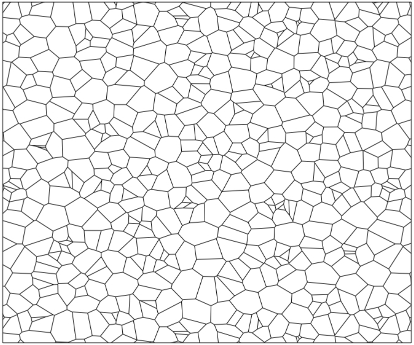
Gibbs Voronoi tessellation

$$V_\Lambda(\varphi) = \sum_{\substack{C \in \mathrm{Vor}(\varphi) \\ C \cap \Lambda \neq \emptyset}} V_1(C) + \sum_{\substack{C, C' \in \mathrm{Vor}(\varphi) \\ C \text{ and } C' \text{are neighbors} \\ (C \cup C') \cap \Lambda \neq \emptyset}} V_2(C, C')$$

$V_1(C)$: deals with the shape of the cell and $V_2(C, C') = \theta \; d(vol(C), vol(C'))$.



$\theta > 0$



$\theta < 0$

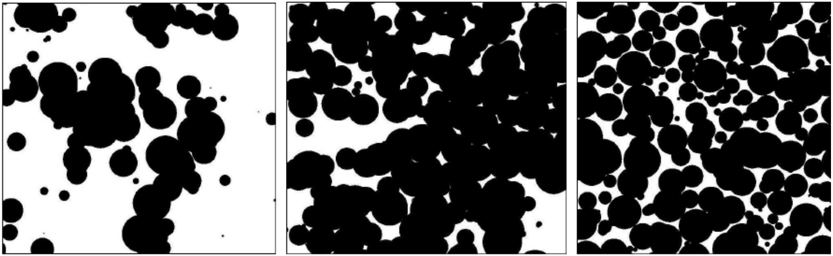
Quermass model $\mathbb{M} = [0, \overline{R}]$

For finite configuration φ

$$V(\varphi; \theta) = \theta_1 |\varphi| + \theta_2 \, \mathcal{P}(\Gamma) + \theta_3 \, \mathcal{A}(\Gamma) + \theta_4 \, \mathcal{E}(\Gamma) \quad \text{where } \Gamma = \bigcup_{(x,R) \in \varphi} \mathcal{B}(x, R)$$

where $\mathcal{P}(\Gamma)$, $\mathcal{A}(\Gamma)$ and $\mathcal{E}(\Gamma)$ respectively denote the perimeter, the volume and the Euler-Poincaré characteristic of Γ.

Simulation for a uniform distribution on $[0, 2]$ on the radius : θ_1 constant



$(\theta_2, \theta_3, \theta_4) = (0, 0.2, 0)$ $\quad$ $(\theta_2, \theta_3, \theta_4) = (0, 0, 1)$ $\quad$ $(\theta_2, \theta_3, \theta_4) = (-1, -1, 0)$

Outline

Maximum likelihood method

We observe φ_{Λ_n}, a realization of a **hereditary** marked point process satisfying **[Mod]** in Λ_n.

$$\hat{\theta}_n^{MLE} = \underset{\theta \in \Theta}{argmax} \frac{1}{Z_{\Lambda_n}(\varphi;\theta)} e^{-V(\varphi_{\Lambda_n};\theta)}$$

where

$$Z_\Lambda(\varphi;\theta) = \sum_{k \geq 0} \frac{1}{k!} \int_\Lambda \ldots \int_\Lambda e^{-V_\Lambda(\{x_1,\ldots,x_k\};\theta)} dx_1 \ldots dx_k.$$

$Z_{\Lambda_n}(\varphi;\theta)$ is untractable ! !

Remarks

- Intensive Monte-Carlo based simulations (Møller(07)) have to be used to estimate $Z(\theta)$.
- Only few theoretical results are available for $\hat{\theta}_n^{MLE}$ (e.g. consistency in general ?)

Pseudo-likelihood method (1)

Idea on the lattice (Besag (68), Ripley (88) : consider the product of the conditional densities in each site conditionally on the other ones.

For point processes JM(94) extended the definition of log-pseudolikelihood function

$$LPL_{\Lambda_n}(\varphi;\theta) = -\int_{\Lambda_n \times \mathbb{M}} e^{-V(x^m|\varphi;\theta)} \mu(dx^m) - \sum_{x^m \in \varphi_{\Lambda_n}} V\left(x^m|\varphi \setminus x^m;\theta\right).$$

Define $\widehat{\theta}_n^{MPLE} := \underset{\theta \in \Theta}{argmax}\ LPL_{\Lambda_n}(\varphi;\theta)$.

Remarks

- "computable" estimate, quick and easy implementation.
- Seems less accurate than the MLE (when available).
- Asymptotic results available for a large class of energies BCD(08),CD(10),DL(09)

Pseudo-likelihood method (2)

Let Λ_n be a cube with volume growing to $+\infty$.

Proposition BCD(08),CD(10),DL(09)

Under **[Mod]** and **[FR]**, the assumption **[Id-MPLE]**

$$\forall \theta \neq \theta^\star, \quad P\left(V\left(0^M|\Phi;\theta\right) \neq V\left(0^M|\Phi;\theta^\star\right)\right) > 0,$$

regularity and integrability assumptions on the local energy function

(i) $\widehat{\theta}_{MPLE}(\Phi) \stackrel{a.s.}{\to} \theta^\star$.

(ii) if $P_{\theta^\star}$ is ergodic, $\exists\ \Sigma_{MPLE} \geq 0 : |\Lambda_n|^{1/2}\left(\widehat{\theta}_{MPLE}(\Phi) - \theta^\star\right) \stackrel{d}{\to} \mathcal{N}(0, \Sigma_{MPLE})$.

(iii) If $P_{\theta^\star}$ is not ergodic but with additional assumptions on Σ_{MPLE}, one can define a consistent estimate of $\widehat{\Sigma}_{MPLE}^{-1/2}$ of $\Sigma_{MPLE}^{-1/2}$ and derive a normalized CLT.

Takacs-Fiksel method (1)

Theorem (Georgii-Nguyen-Zessin)

For any $h(\cdot,\cdot;\theta) : \mathbb{S} \times \Omega \to \mathbb{R}$, *for any* $\theta \in \Theta$,

$$E_{\theta^\star}\left(\sum_{x^m \in \varphi} h\left(x^m, \varphi \setminus x^m; \theta\right) \right) = E_{\theta^\star}\left(\int_{\mathbb{R}^d \times \mathbb{M}} h\left(x^m, \varphi; \theta\right) e^{-V(x^m|\varphi;\theta^\star)} \mu(dx^m) \right)$$

Define

$$I_\Lambda(\varphi; h, \theta) = \int_{\Lambda \times \mathbb{M}} h\left(x^m, \varphi; \theta\right) e^{-V(x^m|\varphi;\theta)} \mu(dx^m) - \sum_{x^m \in \varphi_\Lambda} h\left(x^m, \varphi \setminus x^m; \theta\right).$$

Idea of TF method : ergodic theorem and GNZ formula $\Rightarrow I_{\Lambda_n}(\varphi; \theta^\star) \simeq 0$.

Let us give K test functions $h_k(\cdot,\cdot;\theta) : \mathbb{S} \times \Omega \to \mathbb{R}$ (for $k = 1, \dots, K$).

$$\widehat{\theta}_{TF}(\varphi) := \underset{\theta \in \Theta}{\arg\min} \sum_{k=1}^{K} I_{\Lambda_n}(\varphi; h_k, \theta)^2,$$

Takacs-Fiksel method (2)

$$\widehat{\theta}_{TF}(\varphi) := \arg\min_{\theta\in\Theta} \sum_{k=1}^{K} \left(\int_{\Lambda_n\times\mathbb{M}} h_k\left(x^m,\varphi;\theta\right) e^{-V(x^m|\varphi;\theta)}\mu(dx^m) - \sum_{x^m\in\varphi_{\Lambda_n}} h_k\left(x^m,\varphi\setminus x^m;\theta\right)\right)^2$$

Remarks and interest of the TF method :

- when $\mathbf{h} = \mathbf{V}^{(1)}$, $\widehat{\theta}_{TF}(\varphi) = \widehat{\theta}_{MPLE}(\varphi)$.
- quick estimator : for example $h_k(x^m,\varphi;\theta) := 1_{\mathcal{B}(0,r_k)}(\|x\|)e^{V(x^m|\varphi;\theta^\star)}$.
- allows the identification of the Quermass model with a pertinent choice of test functions allowing to compute the sum term.

Takacs-Fiksel method (2)

$$\widehat{\theta}_{TF}(\varphi) := \arg\min_{\theta\in\Theta} \sum_{k=1}^{K} \left(\int_{\Lambda_n\times\mathbb{M}} h_k\left(x^m,\varphi;\theta\right) e^{-V(x^m|\varphi;\theta)}\mu(dx^m) - \sum_{x^m\in\varphi_{\Lambda_n}} h_k\left(x^m,\varphi\setminus x^m;\theta\right) \right)^2$$

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- allows the identification of the Quermass model with a pertinent choice of test functions allowing to compute the sum term.
- The consistency and the CLT may be obtained (CDDL(10)) under **[Mod]**, **[FR]**, regularity and integrability assumptions and the identifiability condition **[Id-TF]**

$$\sum_{k=1}^{K} E\left(h_k(0^M,\Phi;\theta)\left(e^{-V(0^M|\Phi;\theta)} - e^{-V(0^M|\Phi;\theta^\star)}\right)\right)^2 = 0 \quad \Longrightarrow \theta = \theta^\star.$$

- Problem with the choice of test functions, **[Id-TF]** may fail ! More practical criterion have been proposed in CDDL(10).

Variational principle method (non-marked) Baddeley and Dereudre (10)

VP equation : $\forall$ function $h : \mathbb{S} \times \Omega \to \mathbb{R}$

$$E_{\theta^\star}\left(\sum_{x\in\Phi} \nabla h(x|\varphi \setminus \Phi)\right) = E_{\theta^\star}\left(\sum_{x\in\Phi} h(x|\Phi \setminus x)\nabla V(x|\Phi;\theta^\star)\right).$$

- If $V(x|\varphi;\theta^\star) \to V(x|\varphi;\theta^\star) + c$: same VP equ. $\Rightarrow$ cannot estimate $\theta_1^\star$.
- Assume $V(x|\varphi;\theta^\star) = \theta_1 + \widetilde{\theta}^T\widetilde{\mathbf{V}}(x|\varphi)$, VP equ. leads to

$$E_{\theta^\star}\left(\sum_{x\in\Phi} div\ h(x|\varphi \setminus x)\right) = \widetilde{\theta}^T\left(\sum_{x\in\Phi} h(x|\varphi \setminus x) div\ \widetilde{V}_i(x|\varphi \setminus x)\right)_{i=1,\dots,p}$$

- Let us give $h_1,\dots,h_p$ and define the vector G and the matrix D by

$$G_k := \sum_{x\in\varphi_{\Lambda_n}} div\ h_k(x|\varphi \setminus x) \quad \text{and } D_{k,i} := \sum_{x\in\varphi_{\Lambda_n}} h_k(x|\varphi \setminus x)\ div\ \widetilde{V}_i(x|\varphi \setminus x)$$

$$\widehat{\widetilde{\theta}} := D^{-1}G.$$

Rmk : $h_k = div\ \widetilde{V}_k \Rightarrow D \geq 0$, and asymptotic results can be obtained.

Outline

Validation through residuals

Baddeley et al (05,08) have proposed to use the GNZ formula as a diagnostic tool :

1. Let us give a model and define an estimate $\widehat{\theta}$ of $\theta^\star$.
2. Let us give a test function and define the h-residuals $R_{\Lambda_n}(\varphi;h) = I_{\Lambda_n}(\varphi;h,\widehat{\theta})$, i.e.

$$R_{\Lambda_n}(\varphi;h) := \int_{\Lambda_n \times \mathbb{M}} h\left(x^m,\varphi;\widehat{\theta}\right) e^{-V\left(x^m|\varphi;\widehat{\theta}\right)}\mu(dx^m) - \sum_{x^m \in \varphi_{\Lambda_n}} h\left(x^m,\varphi\setminus x^m;\widehat{\theta}\right)$$

If the model is valid, then one may expect that $R_{\Lambda_n}(\varphi;h)/|\Lambda_n| \simeq 0$!

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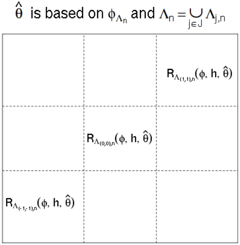
Examples :

- Classical examples $h = 1, e^V, e^{V/2}$ leading to the raw, the inverse and the Pearson residuals.
- A more evolved one : let $h_r(x^m,\varphi;\theta) := \mathbf{1}_{[0,r]}(d(x^m,\varphi))\, e^{V(x^m|\varphi;\theta)}$ where $d(x^m,\varphi) = \inf_{y^m\in\varphi}\|y-x\|$, $R_{\Lambda_n}(\varphi;h_r)$ corresponds to a difference of two estimates of the empty space function $F(r) := P\left(d(0^M,\Phi)\le r\right)$

Measures of departures to the true model

1. Objective 1 : fix some test function h (ex : $h = 1$) and split $\Lambda_n = \cup_{j \in \mathcal{J}} \Lambda_j$



   1. compute the h-residuals in each Λ_j
   2. construct $\|\mathbf{R}_1\|^2$ where

$$\mathbf{R}_1 := \left(R_{\Lambda_j}(\varphi, h, \widehat{\theta}_n) \right)_{j \in \mathcal{J}} .$$

2. Objective 2 : fix $\mathbf{h} = (h_1, \ldots, h_s)^T$ (ex : $h_j = h_{r_j}$, $r_1 < r_2 < \cdots < r_s$)

   $\hat{\theta}$ is based on φ_{Λ_n}

$$\begin{cases} R_{\Lambda_n}(\Phi, h_1, \widehat{\theta}_n) \\ \vdots \\ R_{\Lambda_n}(\Phi, h_j, \widehat{\theta}_n) \\ \vdots \\ R_{\Lambda_n}(\Phi, h_s, \widehat{\theta}_n) \end{cases}$$

   1. compute the s h_j-residuals in Λ_n
   2. construct $\|\mathbf{R}_2\|^2$ where

$$\mathbf{R}_2 := \left(R_{\Lambda_n}(\varphi, h_j, \widehat{\theta}_n) \right)_{j=1,\ldots,s} .$$

Towards goodness-of-fit tests

Under similar assumptions as previously and with general assumptions on $\widehat{\theta}$ (essentially consistency and CLT)

Proposition (CL(10))

(i) As $n \to +\infty$, $\mathbf{R}_1(\Phi; h)/|\Lambda_{0,n}|$ and $\mathbf{R}_2(\Phi; \mathbf{h})/|\Lambda_n|$ converge a.s. to 0.
(ii) If $P_{\theta^\star}$ is not ergodic (but with additional assumptions) a normalized CLT holds for $\mathbf{R_1}$ and $\mathbf{R_2}$, leading to

$$|\Lambda_{0,n}|^{-1} \|\widehat{\Sigma}_1^{-1/2} \mathbf{R}_1(\Phi; h)\|^2 \xrightarrow{d} \chi^2_{|\mathcal{J}|} \quad \text{and} \quad |\Lambda_n|^{-1} \|\widehat{\Sigma}_2^{-1/2} \mathbf{R}_2(\Phi; \mathbf{h})\|^2 \xrightarrow{d} \chi^2_s.$$

- $\Sigma_1 = \lambda_{Inn} \, \underline{\mathbf{I}}_{|\mathcal{J}|} + |\mathcal{J}|^{-1}(\lambda_{Res} - \lambda_{Inn}) \, \underline{\mathbf{J}}$ with $\underline{\mathbf{J}} = \mathbf{e}\mathbf{e}^T$ and $\mathbf{e} = (1, \ldots, 1)^T$.
- $\lambda_{Inn} = f(P^\star_\theta, V, h)$ and $\lambda_{Res} = f(\theta^\star, V, h, \widehat{\theta})$.
- This form suggested us to study the centered residuals for which we may prove

$$|\Lambda_{0,n}|^{-1} \, \widehat{\lambda}_{Inn}^{-1} \, \|\mathbf{R}_1(\Phi; h) - \overline{\mathbf{R}}_1(\Phi; h)\|^2 \xrightarrow{d} \chi^2_{|\mathcal{J}|-1}.$$