Crystallization processes : ergodic properties and statistical inference

Joint work with Youri Davydov

Aude ILLIG

University of Versailles Saint-Quentin

14th December 2012

1. Crystallization model
    - Description
    - Assumptions

2. β-mixing coefficients
    - Definitions
    - Mixing properties of the crystallization r.f.

3. Parameters estimation
    - Parameters and estimators
    - Asymptotic properties
    - Absolutely continuous case
    - Case of a discrete measure

- Germs: $g = (x_g, t_g) \in \mathbf{R}^d \times \mathbf{R}^+$
  - $x_g \in \mathbf{R}^d$ crystallization center location in the growth space
  - $t_g \in \mathbf{R}^+$ crystallisation center birth time
- Birth process: Poisson point process $\mathcal{N}$ on $\mathbf{R}^d \times \mathbf{R}^+$ with intensity measure:

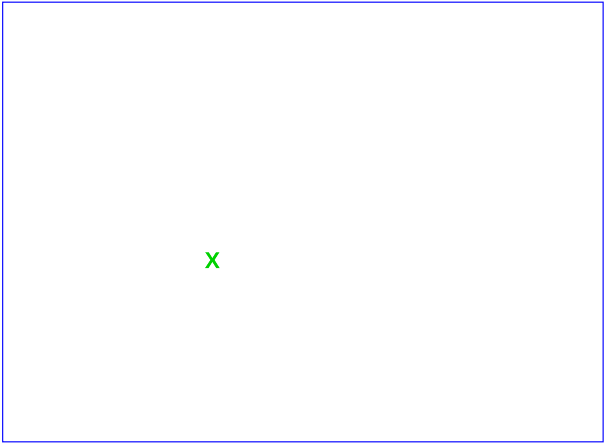
$$\Lambda(dx \times dt) = \lambda^d(dx) \times m(dt)$$

  - λ^d Lebesgue measure on $\mathbf{R}^d$
  - m locally finite measure on $\mathbf{R}^+$
- Crystals growth: Θ_t = Portion of $\mathbf{R}^d$crystallized at time t
  - If $x_g \in \Theta_{t_g}$: no crystal starts growing at x_g
  - If $x_g \notin \Theta_{t_g}$: instantaneous growth of a crystal at x_g (shape/speed to be defined)
  - Growth stops at the meeting points

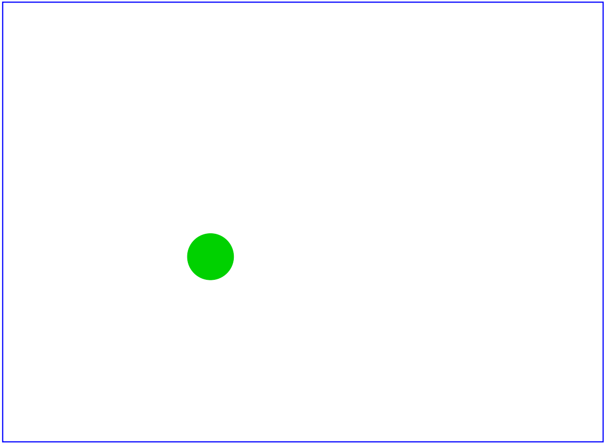
Model intoduced by [5, Kolmogorov (37)] and [4, Johnson & Mehl (39)]

Dimension 2

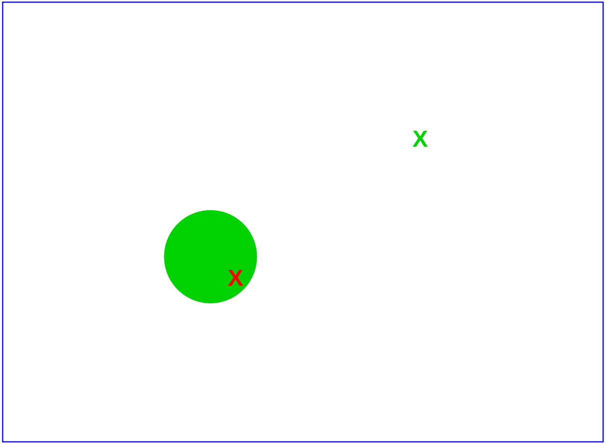
Dimension 2



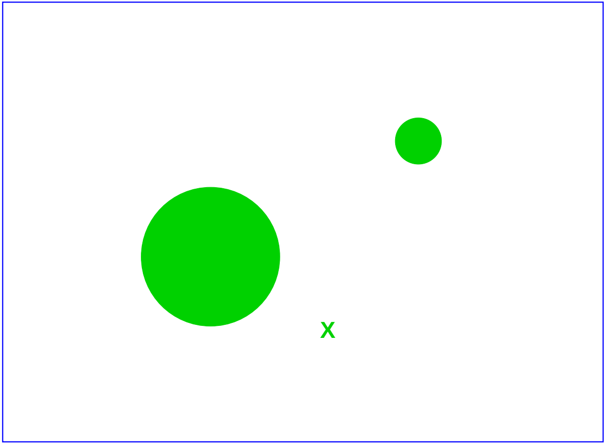
Dimension 2



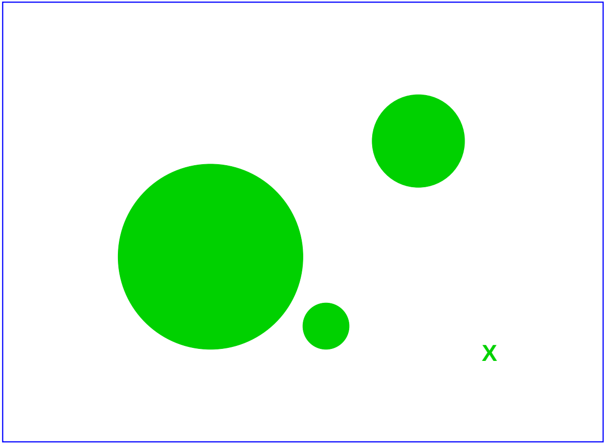
Dimension 2



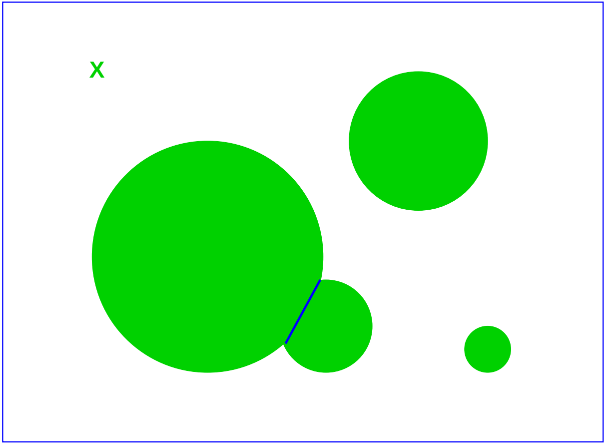
Dimension 2



Dimension 2



Dimension 2



- Exact germination process:

$$\Theta_t = \text{Portion of } \mathbf{R}^d \text{crystallized at time } t$$

The set $\mathcal{N}_c$ of germs g_c giving birth to a crystal is a point process with intensity measure:

$$(1 - \mathbf{1}_{\Theta_{t^-}})\Lambda(dx \times dt)$$

This corresponds to the approach in [6, Micheletti & Capasso (97)]

- Møller approach:

We proceed in the same way as in [7, 8, 9, Møller (89,92,95)].

1. First, assume that all germs give birth to a crystal: the germination process is the Poisson point process denoted by $\mathcal{N}$ with intensity measure:

$$\Lambda(dx \times dt)$$

2. Then, all germs appeared in occupied zone are deleted.

- Exact germination process:

$$\Theta_t = \text{Portion of } \mathbf{R}^d \text{crystallized at time } t$$

The set $\mathcal{N}_c$ of germs g_c giving birth to a crystal is a point process with intensity measure:

$$(1 - \mathbf{1}_{\Theta_{t^-}})\Lambda(dx \times dt)$$

This corresponds to the approach in [6, Micheletti & Capasso (97)]

- Møller approach:

We proceed in the same way as in [7, 8, 9, Møller (89,92,95)].

1. First, assume that all germs give birth to a crystal: the germination process is the Poisson point process denoted by $\mathcal{N}$ with intensity measure:

$$\Lambda(dx \times dt)$$

2. Then, all germs appeared in occupied zone are deleted.

Free crystal

A free crystal is a crystal which grows freely and originates from a germ born in a location not yet occupied by other crystals at the time of its birth ($x_g \notin \Theta_{t_g}$).

For all germ $g \in \mathbf{R}^d \times \mathbf{R}^+$,

- for all $x \in \mathbf{R}^d$, $A_g(x)$ is the *crystallization time* of x by the crystal associated to the germ g and assumed to be free
- for all $t \in \mathbf{R}^+$, $C_g(t) = \{x \in \mathbf{R}^d \,|\, A_g(x) \leq t\}$ is the *free crystal* associated to the germ g.

Crystallization random field

For all $x \in \mathbf{R}^d$,

$$\xi(x) = \inf_{g \in \mathcal{N}} A_g(x)$$

is the crystallization time of the location x. The crystallization process is then caracterized by the random field $(\xi(x))_{x \in \mathbf{R}^d}$.

Free crystal

A free crystal is a crystal which grows freely and originates from a germ born in a location not yet occupied by other crystals at the time of its birth ($x_g \notin \Theta_{t_g}$).

For all germ $g \in \mathbf{R}^d \times \mathbf{R}^+$,

- for all $x \in \mathbf{R}^d$, $A_g(x)$ is the *crystallization time* of x by the crystal associated to the germ g and assumed to be free
- for all $t \in \mathbf{R}^+$, $C_g(t) = \{x \in \mathbf{R}^d \mid A_g(x) \leq t\}$ is the *free crystal* associated to the germ g.

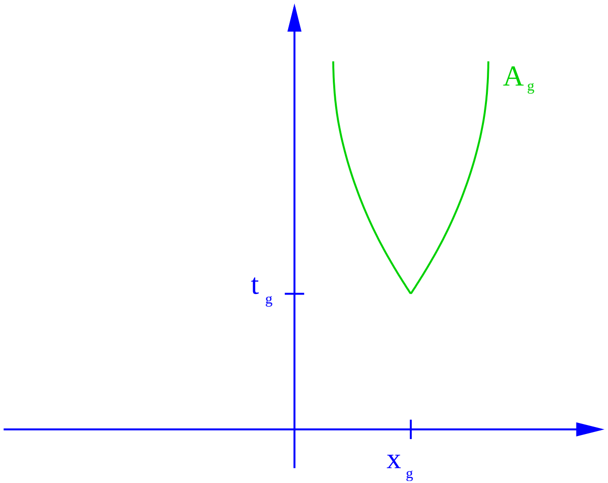
Crystallization random field

For all $x \in \mathbf{R}^d$,

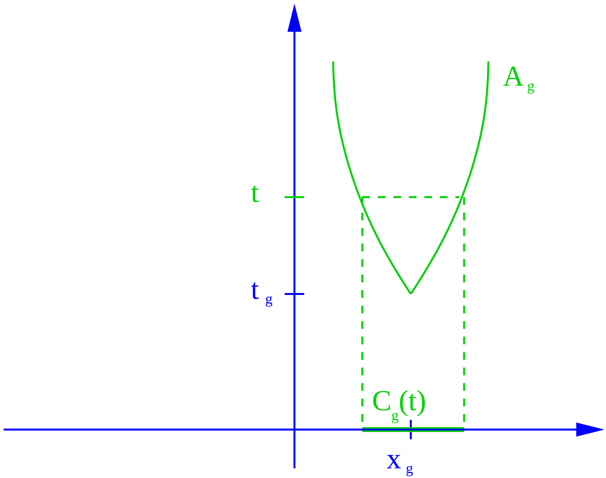
$$\xi(x) = \inf_{g \in \mathcal{N}} A_g(x)$$

is the crystallization time of the location x. The crystallization process is then caracterized by the random field $(\xi(x))_{x \in \mathbf{R}^d}$.

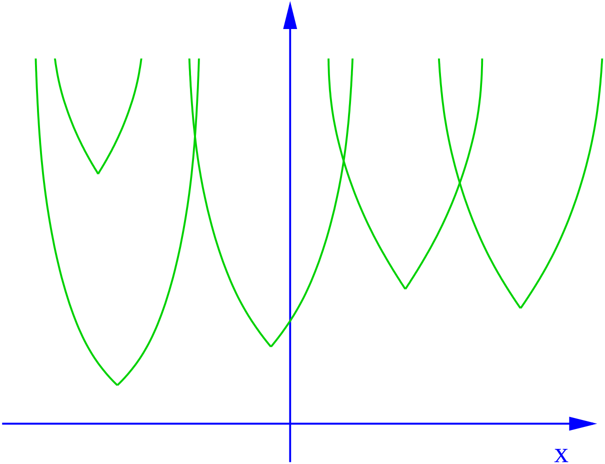
Dimension 1



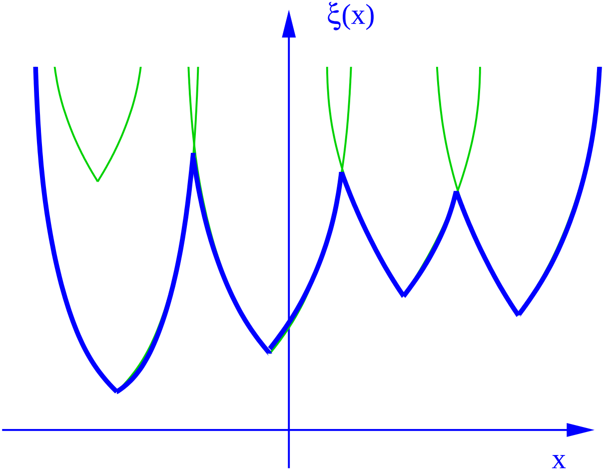
Dimension 1



Dimension 1



Dimension 1



- Assumptions: For all germ $g = (x_g, t_g) \in \mathbf{R}^d \times \mathbf{R}^+$, we assume that

$$\forall t \geq t_g, \qquad C_g(t) = x_g \oplus [V(t) - V(t_g)]K.$$

  - K convex and compact set, $0 \in K^\circ$. We denote by D_K the diameter $\inf\{D > 0 \,|\, K \subset B(0, D/2)\}$.
  - V absolutely continuous function, $V(t) = \int_0^t v(s)ds$ with speed $0 < v \leq M$.

- Consequences: If $t = A_g(x)$, then:

$$\begin{aligned} [V(t) - V(t_g)]p_{x-x_g,K} &= |x - x_g| \\ A_g(x) &= V^{-1}\left[\frac{|x-x_g|}{p_{x-x_g,K}} + V(t_g)\right] \end{aligned}$$

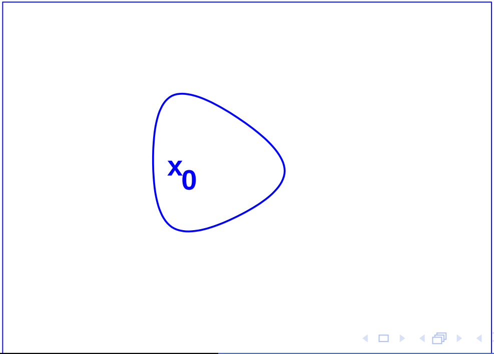
- Example: Linear expansion in all directions for $K = B(0,1)$, $v = M$:

$$A_g(x) = t_g + \frac{|x - x_g|}{M}$$

- Assumptions: For all germ $g = (x_g, t_g) \in \mathbf{R}^d \times \mathbf{R}^+$, we assume that

$$\forall t \geq t_g, \qquad C_g(t) = x_g \oplus [V(t) - V(t_g)]K.$$

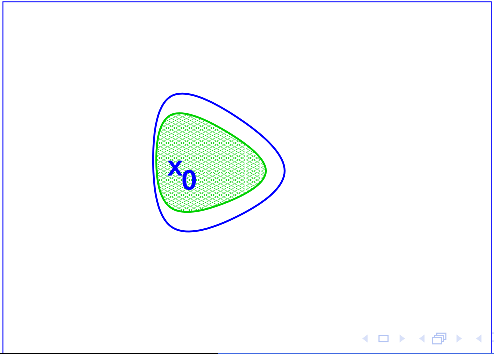
  - K convex and compact set, $0 \in K^\circ$. We denote by D_K the diameter $\inf\{D > 0 \,|\, K \subset B(0, D/2)\}$.
  - V absolutely continuous function, $V(t) = \int_0^t v(s)ds$ with speed $0 < v \leq M$.



- Assumptions: For all germ $g = (x_g, t_g) \in \mathbf{R}^d \times \mathbf{R}^+$, we assume that

$$\forall t \geq t_g, \qquad C_g(t) = x_g \oplus [V(t) - V(t_g)]K.$$

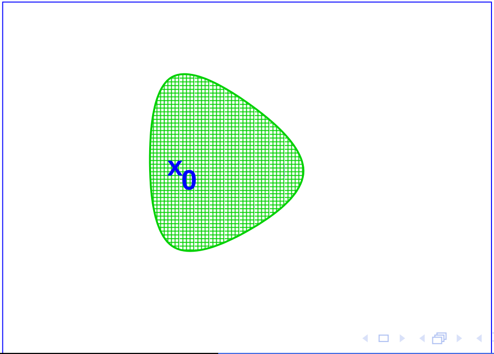
  - K convex and compact set, $0 \in K^\circ$. We denote by D_K the diameter $\inf\{D > 0 \,|\, K \subset B(0, D/2)\}$.
  - V absolutely continuous function, $V(t) = \int_0^t v(s)ds$ with speed $0 < v \leq M$.



- Assumptions: For all germ $g = (x_g, t_g) \in \mathbf{R}^d \times \mathbf{R}^+$, we assume that

$$\forall t \geq t_g, \qquad C_g(t) = x_g \oplus [V(t) - V(t_g)]K.$$

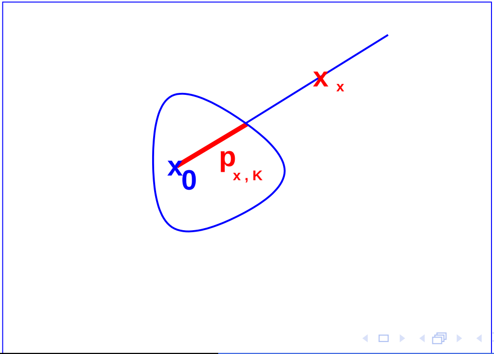
  - K convex and compact set, $0 \in K^\circ$. We denote by D_K the diameter $\inf\{D > 0 \,|\, K \subset B(0, D/2)\}$.
  - V absolutely continuous function, $V(t) = \int_0^t v(s)ds$ with speed $0 < v \leq M$.



- Assumptions: For all germ $g = (x_g, t_g) \in \mathbf{R}^d \times \mathbf{R}^+$, we assume that

$$\forall t \geq t_g, \qquad C_g(t) = x_g \oplus [V(t) - V(t_g)]K.$$

  - K convex and compact set, $0 \in K^\circ$. We denote by D_K the diameter $\inf\{D > 0 \,|\, K \subset B(0, D/2)\}$.
  - V absolutely continuous function, $V(t) = \int_0^t v(s)ds$ with speed $0 < v \leq M$.



- Assumptions: For all germ $g = (x_g, t_g) \in \mathbf{R}^d \times \mathbf{R}^+$, we assume that

$$\forall t \geq t_g, \qquad C_g(t) = x_g \oplus [V(t) - V(t_g)]K.$$

  - K convex and compact set, $0 \in K^\circ$. We denote by D_K the diameter $\inf\{D > 0 \,|\, K \subset B(0, D/2)\}$.
  - V absolutely continuous function, $V(t) = \int_0^t v(s)ds$ with speed $0 < v \leq M$.

- Consequences: If $t = A_g(x)$, then:

$$\begin{aligned} [V(t) - V(t_g)]p_{x-x_g,K} &= |x - x_g| \\ A_g(x) &= V^{-1}\left[\frac{|x-x_g|}{p_{x-x_g,K}} + V(t_g)\right] \end{aligned}$$

- Example: Linear expansion in all directions for $K = B(0,1)$, $v = M$:

$$A_g(x) = t_g + \frac{|x - x_g|}{M}$$

β-mixing coefficients

Theorem 1

$\forall d \geq 1$, ξ is mixing.

For two disjoint subsets T_1 and T_2 of $\mathbf{R}^d$, the *absolute regularity coefficient* is:

$$\beta(T_1, T_2) = \|\mathcal{P}_{T_1 \cup T_2} - \mathcal{P}_{T_1} \times \mathcal{P}_{T_2}\|_{var}$$

where $\mathcal{P}_T$ is the distribution of the restriction $\xi_{|T} = (\xi(x))_{x \in T}$.

1. As ξ is homogeneous, it is sufficient to know $\beta(T_1, T_2)$ up to translations on T_1 and T_2.
2. When $d \geq 2$, we consider sets separated in the sense of *Bulinskii (1987)*.

β-mixing coefficients

Theorem 1

$\forall d \geq 1$, ξ is mixing.

For two disjoint subsets T_1 and T_2 of $\mathbf{R}^d$, the *absolute regularity coefficient* is:

$$\beta(T_1, T_2) = \|\mathcal{P}_{T_1 \cup T_2} - \mathcal{P}_{T_1} \times \mathcal{P}_{T_2}\|_{var}$$

where $\mathcal{P}_T$ is the distribution of the restriction $\xi_{|T} = (\xi(x))_{x \in T}$.

1. As ξ is homogeneous, it is sufficient to know $\beta(T_1, T_2)$ up to translations on T_1 and T_2.
2. When $d \geq 2$, we consider sets separated in the sense of *Bulinskii (1987)*.

β-mixing coefficients

Theorem 1

$\forall d \geq 1$, ξ is mixing.

For two disjoint subsets T_1 and T_2 of $\mathbf{R}^d$, the *absolute regularity coefficient* is:

$$\beta(T_1, T_2) = \|\mathcal{P}_{T_1 \cup T_2} - \mathcal{P}_{T_1} \times \mathcal{P}_{T_2}\|_{var}$$

where $\mathcal{P}_T$ is the distribution of the restriction $\xi_{|T} = (\xi(x))_{x \in T}$.

1. As ξ is homogeneous, it is sufficient to know $\beta(T_1, T_2)$ up to translations on T_1 and T_2.
2. When $d \geq 2$, we consider sets separated in the sense of *Bulinskii (1987)*.

β-mixing coefficients

Theorem 1

$\forall d \geq 1$, ξ is mixing.

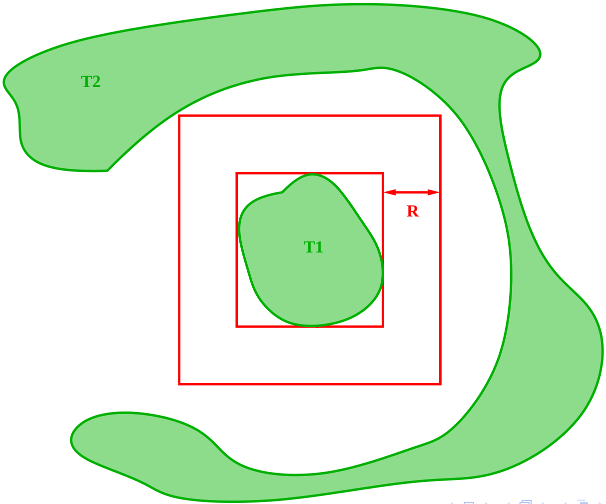
For two disjoint subsets T_1 and T_2 of $\mathbf{R}^d$, the *absolute regularity coefficient* is:

$$\beta(T_1, T_2) = \|\mathcal{P}_{T_1 \cup T_2} - \mathcal{P}_{T_1} \times \mathcal{P}_{T_2}\|_{var}$$

where $\mathcal{P}_T$ is the distribution of the restriction $\xi_{|T} = (\xi(x))_{x \in T}$.

1. As ξ is homogeneous, it is sufficient to know $\beta(T_1, T_2)$ up to translations on T_1 and T_2.
2. When $d \geq 2$, we consider sets separated in the sense of *Bulinskii (1987)*.

Dimension 2



α-mixing coefficients

For two disjoint subsets T_1 and T_2 of $\mathbf{R}^d$, the *strong mixing coefficient* is:

$$\alpha(T_1, T_2) = \sup_{A \in \mathcal{F}_{T_1}, B \in \mathcal{F}_{T_2}} |\mathbf{P}(A \cap B) - \mathbf{P}(A)\mathbf{P}(B)|$$

where $\mathcal{F}_{T_i} = \sigma\{\xi(x), x \in T_i\}$ for $i = 1, 2$.

Hence,

Mixing coefficients inequality

$$\alpha(T_1, T_2) \leq \beta(T_1, T_2)$$

Dimension 1

Causal cone

For all $t > 0$, the so-called *causal cone* $K_t = \{g \in \mathbf{R}^+ \times \mathbf{R} \,|\, A_g(0) \leq t\}$ consists of all possible germs that can capture the origin before time t. The measure $\Lambda(K_t)$ is denoted by $\mathcal{G}(t)$.

Remark 1: $\lim_{t \to +\infty} \mathcal{G}(t) = +\infty$.

Theorem 2

If $d = 1$, for two intervals $T_1 = (-\infty, 0]$ and $T_2 = [r, +\infty)$, the coefficient $\beta(T_1, T_2)$ is denoted by $\beta(r)$ and satisfies:

$$\beta(r) \leq C_1 \, \mathrm{e}^{-\mathcal{G}(C_2\, r)}$$

where $C_1 = 8$, $C_2 = \frac{1}{2\, M'}$ and $M' = MD_K$.

Dimension 1

Causal cone

For all $t > 0$, the so-called *causal cone* $K_t = \{g \in \mathbf{R}^+ \times \mathbf{R} \,|\, A_g(0) \leq t\}$ consists of all possible germs that can capture the origin before time t. The measure $\Lambda(K_t)$ is denoted by $\mathcal{G}(t)$.

Remark 1: $\lim_{t\to+\infty}\mathcal{G}(t) = +\infty$.

Theorem 2

If $d = 1$, for two intervals $T_1 = (-\infty, 0]$ and $T_2 = [r, +\infty)$, the coefficient $\beta(T_1, T_2)$ is denoted by $\beta(r)$ and satisfies:

$$\beta(r) \leq C_1 \, \mathrm{e}^{-\mathcal{G}(C_2\, r)}$$

where $C_1 = 8$, $C_2 = \frac{1}{2\,M'}$ and $M' = MD_K$.

Dimension 1

Causal cone

For all $t > 0$, the so-called *causal cone* $K_t = \{g \in \mathbf{R}^+ \times \mathbf{R} \,|\, A_g(0) \leq t\}$ consists of all possible germs that can capture the origin before time t. The measure $\Lambda(K_t)$ is denoted by $\mathcal{G}(t)$.

Remark 1: $\lim_{t \to +\infty} \mathcal{G}(t) = +\infty$.

Theorem 2

If $d = 1$, for two intervals $T_1 = (-\infty, 0]$ and $T_2 = [r, +\infty)$, the coefficient $\beta(T_1, T_2)$ is denoted by $\beta(r)$ and satisfies:

$$\beta(r) \leq C_1 \, \mathrm{e}^{-\mathcal{G}(C_2 \, r)}$$

where $C_1 = 8$, $C_2 = \frac{1}{2\,M'}$ and $M' = MD_K$.

Dimension 1

Sketch of the proof:

Lemme 1

Let $(\eta(x))_{x\in\mathbf{R}}$ be a random process and T_1 and T_2 two disjoint subsets of $\mathbf{R}$. If there exists two *independent processes* $(\eta_1(x))_{x\in\mathbf{R}}$, $(\eta_2(x))_{x\in\mathbf{R}}$ and two positive constants δ_1, δ_2 such that

$$\mathbf{P}\{\eta(x) = \eta_i(x), \ \ \forall x \in T_i\} \geq 1 - \delta_i \text{ for } i = 1, 2$$

then

$$\beta(T_1, T_2) \leq 4\,(\delta_1 + \delta_2).$$

Let us introduce, for all $T \subset \mathbf{R}$,

$$\xi_T(x) = \inf_{\substack{g \in \mathcal{N} \\ x_g \in T}} A_g(x).$$

Dimension 1

Sketch of the proof:

Lemme 1

Let $(\eta(x))_{x\in\mathbf{R}}$ be a random process and T_1 and T_2 two disjoint subsets of $\mathbf{R}$. If there exists two *independent processes* $(\eta_1(x))_{x\in\mathbf{R}}$, $(\eta_2(x))_{x\in\mathbf{R}}$ and two positive constants δ_1, δ_2 such that

$$\mathbf{P}\{\eta(x)=\eta_i(x),\ \ \forall x\in T_i\}\geq 1-\delta_i \text{ for } i=1,2$$

then

$$\beta(T_1,T_2)\leq 4\,(\delta_1+\delta_2).$$

Let us introduce, for all $T\subset\mathbf{R}$,

$$\xi_T(x)=\inf_{\substack{g\in\mathcal{N}\\ x_g\in T}} A_g(x).$$

Dimension 1

Lemme 2

$$\forall R > 0, \quad \mathbf{P}\{\xi(x) = \xi_{(-\infty, M'R]}(x), \forall x \leq 0\} \geq 1 - \mathrm{e}^{-\mathcal{G}(R)}$$

Lemme 3

$$\forall R > 0, \quad \mathbf{P}\{\xi(x) = \xi_{[M'R, +\infty)}(x), \forall x \geq 2\,M'R\} \geq 1 - \mathrm{e}^{-\mathcal{G}(R)}$$

Proof of Lemma 2: We first note that

$$\mathbf{P}\{\xi(0) \leq R\} = \mathbf{P}\{\mathcal{N} \cap K_R \neq \emptyset\} = 1 - \mathrm{e}^{-\mathcal{G}(R)}.$$

Then, we prove that

$$\{\xi(0) \leq R\} \subset \{\xi(x) = \xi_{(-\infty, M'R]}(x), \forall x \leq 0\}.$$

Dimension 1

Lemme 2

$$\forall R > 0, \quad \mathbf{P}\{\xi(x) = \xi_{(-\infty, M'R]}(x), \forall x \leq 0\} \geq 1 - \mathrm{e}^{-\mathcal{G}(R)}$$

Lemme 3

$$\forall R > 0, \quad \mathbf{P}\{\xi(x) = \xi_{[M'R, +\infty)}(x), \forall x \geq 2\,M'R\} \geq 1 - \mathrm{e}^{-\mathcal{G}(R)}$$

Proof of Lemma 2: We first note that

$$\mathbf{P}\{\xi(0) \leq R\} = \mathbf{P}\{\mathcal{N} \cap K_R \neq \emptyset\} = 1 - \mathrm{e}^{-\mathcal{G}(R)}.$$

Then, we prove that

$$\{\xi(0) \leq R\} \subset \{\xi(x) = \xi_{(-\infty, M'R]}(x), \forall x \leq 0\}.$$

Dimension 1

Lemme 2

$$\forall R > 0, \quad \mathbf{P}\{\xi(x) = \xi_{(-\infty, M'R]}(x), \forall x \leq 0\} \geq 1 - \mathrm{e}^{-\mathcal{G}(R)}$$

Lemme 3

$$\forall R > 0, \quad \mathbf{P}\{\xi(x) = \xi_{[M'R, +\infty)}(x), \forall x \geq 2\,M'R\} \geq 1 - \mathrm{e}^{-\mathcal{G}(R)}$$

Proof of Lemma 2: We first note that

$$\mathbf{P}\{\xi(0) \leq R\} = \mathbf{P}\{\mathcal{N} \cap K_R \neq \emptyset\} = 1 - \mathrm{e}^{-\mathcal{G}(R)}.$$

Then, we prove that

$$\{\xi(0) \leq R\} \subset \{\xi(x) = \xi_{(-\infty, M'R]}(x), \forall x \leq 0\}.$$

Dimension 1

Suppose that $\xi(0) \leq R$ and prove that

$$\inf_{\substack{g \in \mathcal{N} \\ x_g \leq M'R}} A_g(x) \leq \inf_{\substack{g \in \mathcal{N} \\ x_g > M'R}} A_g(x) \quad \forall x \leq 0.$$

If $g \in \mathcal{N}$ is such that $x_g > M'R$, we derive that

$$A_g(0) \geq \frac{|x_g|}{Mp_{x-x_g,K}} + t_g > R.$$

But $\xi(0) \leq R$, so there exists $g_0 \in \mathcal{N}$ such that $x_{g_0} \leq M'R$ and

$$\xi(0) = A_{g_0}(0) \leq R.$$

For all $g \in \mathcal{N}$ such that $x_g > M'R$, we finally derive that

$$A_{g_0}(x) \leq A_g(x) \quad \forall x \leq 0.$$

Dimension $d \geq 2$

Causal cone

For all $t > 0$, the so-called *causal cone* $K_t = \{g \in \mathbf{R}^+ \times \mathbf{R}^d \mid A_g(0) \leq t\}$ consists of all possible germs that can capture the origin before time t.
The measure $\Lambda(K_t)$ is denoted by $\mathcal{G}(t)$.

Crystals shape

The crystals shape are defined by the convex compact K:

- D_K is the diameter of the smallest ball centered at zero and containing K
- d_K is the diameter of the greatest ball centered at zero and contained in K
- $A = \frac{D_K}{d_K}$

Dimension $d \geq 2$

Causal cone

For all $t > 0$, the so-called *causal cone* $K_t = \{g \in \mathbf{R}^+ \times \mathbf{R}^d \,|\, A_g(0) \leq t\}$ consists of all possible germs that can capture the origin before time t. The measure $\Lambda(K_t)$ is denoted by $\mathcal{G}(t)$.

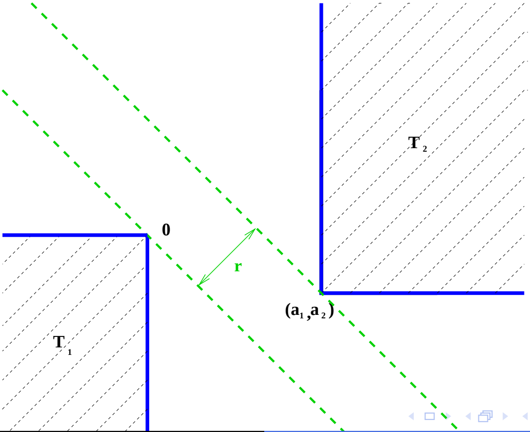
Crystals shape

The crystals shape are defined by the convex compact K:

- D_K is the diameter of the smallest ball centered at zero and containing K
- d_K is the diameter of the greatest ball centered at zero and contained in K
- $A = \frac{D_K}{d_K}$

Dimension $d \geq 2$

Let $T_1 = \prod_{i=1}^{d}(-\infty, 0]$ and $T_2 = \prod_{i=1}^{d}[a_i, +\infty)$ be two quadrants (Q) separated by a r-width band with $r = \frac{\sum_{i=1}^{d} a_i}{\sqrt{d}} > 0$.



Dimension $d \geq 2$

Theorem 3

If $d \geq 2$, for two quadrants (Q) $T_1 = \prod_{i=1}^d (-\infty, 0]$ and $T_2 = \prod_{i=1}^d [a_i, +\infty)$, the coefficient $\beta(T_1, T_2)$ is denoted by $\beta_Q(a, r)$ where a stands for $(a_1, \dots, a_d)$. If

$$\beta_Q(r) = \sup_{a \in \mathbf{R}^d \mid \sum_{i=1}^d a_i = \sqrt{d}\, r} \beta_Q(a, r),$$

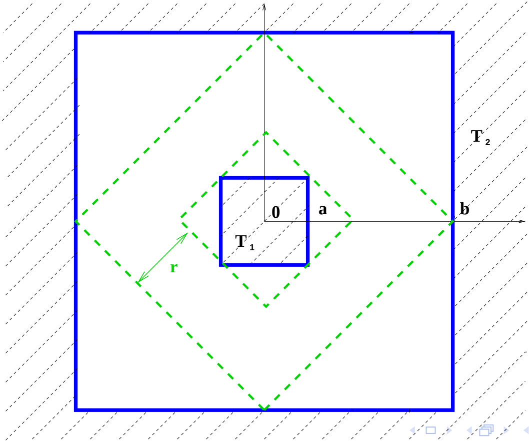
then

$$\beta_Q(r) \leq C_1 \sum_{k=1}^{\infty} k^{d-1} \mathrm{e}^{-\mathcal{G}(C_2(d)\, r\, k)}$$

where $C_1 = 8$ and $C_2(d) = \frac{1}{d\, H^2}$ with $H = 2\,(A + M')$ and $M' = MD_K$.

Dimension $d \geq 2$

Let $T_1 = [-a, a]^d$ and $T_2 = ([-b, b]^d)^c$ be two enclosed domains (ED) separated by a r-width polygonal band with $r = \frac{(b-2a)\sqrt{d}}{2} > 0$



Dimension $d \geq 2$

Theorem 4

If $d \geq 2$, for two enclosed domains (ED) $T_1 = [-a, a]^d$ and $T_2 = ([-b, b]^d)^c$ separated by a r-width polygonal band, the coefficient $\beta(T_1, T_2)$ is denoted by $\beta_{ED}(a, r)$. If

$$\beta_{ED}(r) = \sup_{a>0} \beta_{ED}(a, r),$$

then

$$\beta_Q(r) \leq C_1(d) \sum_{k=1}^{\infty} k^{d-1} \mathrm{e}^{-\mathcal{G}(C_2(d)\, r\, k)}$$

where $C_1(d) = 4(1 + d\, 2^d)$ and $C_2(d) = \frac{1}{d\, H^2}$ with $H = 2\,(A + M')$ and $M' = D_K M$.

Intensity measure parameters estimation

The *intensity measure* of the Poisson point process is:

$$\Lambda = \lambda^d \times m.$$

Two cases:

1. The measure m is absolutely continuous and $m(dt) = a\, t^{b-1} dt$ with $a, b > 0$.
   Parameters a, b are to be estimated.
2. The measure m is discrete and $m = \sum_{i=1}^{q} p_i\, \delta_{a_i}$ with $\sum_{i=1}^{q} p_i = 1$, $p_i > 0$ for all $i = 1 \dots q$ and $0 < a_1 < \cdots < a_q$.
   Parameters $p_i, \quad i = 1 \dots q$ are to be estimated.

Framework

1. We assume that $v = 1$ and $K = B(0, 1)$.
2. We suppose that we observe *only one realisation* ξ_{obs} of the random field $\xi = (\xi(x))_{x \in \mathbf{R}^d}$ on a large domain

$$D_n = [0, n]^d \subseteq \mathbf{R}^d.$$

Thus, at each time t, we observe the crystallized zone

$$(\Theta_t)_{obs} \cap D_n = \{x \in D_n \,|\, \xi_{obs}(x) \in [0, t]\}.$$

Estimators

We consider

$$\begin{aligned} \mathcal{F}(t) &= \mathbf{P}\{\xi(0) \leq t\} \\ &= 1 - \mathrm{e}^{-\Lambda(K_t)} \\ &= 1 - \mathrm{e}^{-\mathcal{G}(t)} \end{aligned}$$

We estimate $\mathcal{F}(t)$ by

$$\hat{\mathcal{F}}_n(t) := \frac{1}{n^d} \int_{[0,n]^d} \mathbb{1}_{[0,t]}(\xi(x))\, \lambda^d(dx)$$

Estimators

We also consider the measure of the causal cone:

$$\mathcal{G}(t) = -\log(1 - \mathcal{F}(t))$$

We estimate $\mathcal{G}(t)$ by

$$\hat{\mathcal{G}}_n(t) := -\log(1 - \hat{\mathcal{F}}_n(t))$$

Consistency

Since ξ is mixing, we derive the following Proposition 1.

Proposition 1

$$\begin{aligned}\hat{\mathcal{F}}_n(t) &:= \frac{1}{n^d}\int_{[0,n]^d} \mathbb{1}_{[0,t]}(\xi(x))\,\lambda^d(dx)\\ \hat{\mathcal{G}}_n(t) &:= -\log(1-\hat{\mathcal{F}}_n(t))\end{aligned}$$

are strongly consistant estimtors for $\mathcal{F}(t)$ and $\mathcal{G}(t)$:

$$\begin{aligned}\hat{\mathcal{F}}_n(t) &\xrightarrow[n\to\infty]{p.s.} \mathcal{F}(t)\\ \hat{\mathcal{G}}_n(t) &\xrightarrow[n\to\infty]{p.s.} \mathcal{G}(t)\end{aligned}$$

Asymptotic normality

Let $(\eta(x))_{x\in\mathbf{R}^d}$ be a homogeneous random field:

- $\mathbf{E}(\eta(x)) = \mu$
- $R(u) = \mathrm{Cov}(\eta(0), \eta(u))$
- $S_n = \int_{[0,n]^d} (\eta(x) - \mu)\, dx$

We are interested in the asymptotic behaviour of $\frac{S_n}{\sigma n^{\frac{d}{2}}}$ under α-mixing conditions:

- when $d = 1$:

$$\alpha(\rho) = \sup_{A\in\mathcal{F}_{(-\infty,0]},B\in\mathcal{F}_{[\rho,+\infty)}} |\mathbf{P}(A\cup B) - \mathbf{P}(A)\mathbf{P}(B)|$$

- when $d \geq 2$:

$$\alpha_{ED}(\rho) = \sup_{a>0} \alpha_{ED}(a, \rho)$$

Asymptotic normality

Theorem 5

If for some $\delta > 0$,

$$\|\eta(x)\|_{2+\delta} < \infty \tag{1}$$

and

$$\int_0^\infty \rho^{d-1}\,\alpha(\rho)^{\frac{\delta}{2+\delta}}\,d\rho < \infty \tag{2}$$

then $\int_{\mathbf{R}^d} |R(u)|\,du < \infty$. Moreover, if $\sigma^2 = \int_{\mathbf{R}^d} R(u)\,du > 0$, then

$$\frac{S_n}{\sigma n^{\frac{d}{2}}} \xrightarrow[n\to\infty]{\mathcal{D}} \mathcal{N}(0,1).$$

Analogue of Bolthausen's theorem (1982) for continuous-parameter random fields

Asymptotic normality

Theorem 5

If

$$\sup_{x \in \mathbf{R}^d} |\eta(x)| < \infty \tag{1}$$

and

$$\int_0^{\infty} \rho^{d-1} \alpha(\rho) \, d\rho < \infty \tag{2}$$

then $\int_{\mathbf{R}^d} |R(u)| \, du < \infty$. Moreover, if $\sigma^2 = \int_{\mathbf{R}^d} R(u) \, du > 0$, then

$$\frac{S_n}{\sigma n^{\frac{d}{2}}} \xrightarrow[n \to \infty]{\mathcal{D}} \mathcal{N}(0, 1).$$

Analogue of Bolthausen's theorem (1982) for continuous-parameter random fields

Asymptotic normality

Corollary 1

Let $(\xi(x))_{x\in\mathbf{R}^d}$ be a stationary random field *satisfying the α-mixing condition*. For all $t \in \mathbf{R}^+$, write

$$\eta_t(x) = \mathbf{1}_{\{\xi(x)\leq t\}} \quad \forall x \in \mathbf{R}^d.$$

Let h be fixed in $\mathbf{N}^*$. If, for $(t_1,\ldots,t_h)' \in (\mathbf{R}^+)^d$, the matrix $\Gamma = \ (\gamma_{i,j})_{i,j=1\ldots h}$ which (i,j)-th entry equals

$$\gamma_{i,j} = \int_{\mathbf{R}^d} \mathrm{Cov}\left(\eta_{t_i}(0), \eta_{t_j}(x)\right)\, dx$$

is *positive-definite*, then,

$$n^{\frac{d}{2}}\left((\hat{\mathcal{F}}_n(t_1),\ldots,\hat{\mathcal{F}}_n(t_h))' - (\mathcal{F}(t_1),\ldots,\mathcal{F}(t_h))'\right) \xrightarrow[n\to\infty]{\mathcal{D}} \mathcal{N}(0,\Gamma).$$

Asymptotic normality

Corollary 2

If $(\xi(x))_{x\in\mathbf{R}^d}$ is a stationary random field *satisfying the α-mixing condition* and the matrix Γ of Corollary 1 is *positive definite*, then

$$n^{\frac{d}{2}}\left((\hat{\mathcal{G}}_n(t_1),\ldots,\hat{\mathcal{G}}_n(t_h))' - (\mathcal{G}(t_1),\ldots,\mathcal{G}(t_h))'\right) \xrightarrow[n\to\infty]{\mathcal{D}} \mathcal{N}(0,V)$$

where the (i,j)-th entry of the covariance matrix $V=(v_{i,j})_{i,j=1\ldots h}$ equals

$$e^{\mathcal{G}(t_i)}\, e^{\mathcal{G}(t_j)}\, \gamma_{i,j}.$$

$m(dt) = a\,t^{b-1}dt$

$$\begin{aligned}
\mathcal{G}(t) &= \Lambda(K_t) \\
&= \int_0^t \lambda^d(B(0, t-s))a\,s^{b-1}ds \\
&= c_d\,a\,t^{d+b}\,I_d(b)
\end{aligned}$$

where

$$c_d = \lambda^d(B(0,1))$$

and

$$I_d(b) = \frac{d!}{b\,(b+1)\ldots(b+d)}.$$

For $t = t_1$ and $t = t_2$, we obtain the following system:

$$\begin{cases} b = \dfrac{\log\left(\frac{\mathcal{G}(t_1)}{\mathcal{G}(t_2)}\right)}{\log t_1 - \log t_2} - d \\ \\ a = \dfrac{\mathcal{G}(t_1)}{c_d\, l_d(b)\, t_1^{d+b}} \end{cases}$$

We introduce the continuous functions

$$g(x_1, x_2) = \frac{\log(\frac{x_1}{x_2})}{\log t_1 - \log t_2} - d$$

and

$$f(x_1, x_2) = \frac{x_1}{c_d\, l_d(g(x_1, x_2))\, t_1^{d+g(x_1,x_2)}}$$

The system can be summerized under the following form:

$$\begin{cases} a = f(\mathcal{G}(t_1), \mathcal{G}(t_2)) \\ b = g(\mathcal{G}(t_1), \mathcal{G}(t_2)) \end{cases}$$

Proposition 2

The following statistics are strongly consistent estimators for parameters a and b:

$$\hat{b}_n := g(\hat{\mathcal{G}}_n(t_1), \hat{\mathcal{G}}_n(t_2)) \xrightarrow[n\to\infty]{p.s.} b$$

$$\hat{a}_n := f(\hat{\mathcal{G}}_n(t_1), \hat{\mathcal{G}}_n(t_2)) \xrightarrow[n\to\infty]{p.s.} a.$$

- When $d = 1$, we get that

$$\alpha(r) \leq C_1 \, e^{-\gamma \, r^{1+b}}$$

with $\gamma = c_d \, a \, C_2^{1+b} \, I_d(b)$.

$$\Longrightarrow \int_0^\infty \alpha(r) \, dr < \infty$$

- When $d \geq 2$, we obtain that

$$\alpha_{ED}(r) \leq C_1(d) \left(\sum_{k=1}^{\infty} k^{d-1} e^{-\gamma(d) \, r^{d+b} (k^{d+b} - 1)} \right) e^{-\gamma(d) \, r^{d+b}}$$

with $\gamma(d) = c_d \, a \, I_d(b) C_2(d)^{d+b}$

and for $A > 0$, $\sup_{r \geq A} \sum_{k=1}^{\infty} k^{d-1} e^{-\gamma(d) \, r^{d+b} (k^{d+b} - 1)} < \infty$.

$$\Longrightarrow \int_0^\infty r^{d-1} \alpha_{ED}(r) \, dr < \infty$$

- When $d = 1$, we get that

$$\alpha(r) \leq C_1\, e^{-\gamma\, r^{1+b}}$$

with $\gamma = c_d\, a\, C_2^{1+b}\, I_d(b)$.

$$\Longrightarrow \int_0^\infty \alpha(r)\, dr < \infty$$

- When $d \geq 2$, we obtain that

$$\alpha_{ED}(r) \leq C_1(d) \left(\sum_{k=1}^{\infty} k^{d-1} e^{-\gamma(d)\, r^{d+b}(k^{d+b}-1)} \right) e^{-\gamma(d)\, r^{d+b}}$$

with $\gamma(d) = c_d\, a\, I_d(b) C_2(d)^{d+b}$

and for $A > 0$, $\sup_{r \geq A} \sum_{k=1}^{\infty} k^{d-1} e^{-\gamma(d)\, r^{d+b}(k^{d+b}-1)} < \infty$.

$$\Longrightarrow \int_0^\infty r^{d-1} \alpha_{ED}(r)\, dr < \infty$$

Theorem 6

Assume, for $h = 2$, that the matrix Γ of Corollary 1 is *positive definite*. Then,

$$n^{\frac{d}{2}} \left((\hat{a}_n, \hat{b}_n) - (a, b) \right) \xrightarrow[n \to \infty]{\mathcal{D}} \mathcal{N}(0, MVM')$$

where V is the matrix defined in Corollary 2 and $M = (m_{i,j})_{i,j=1,2}$ with for $j = 1, 2$,

$$m_{1,j} = \frac{\delta f}{\delta x_j}(\mathcal{G}(t_1), \mathcal{G}(t_2))$$

$$m_{2,j} = \frac{\delta g}{\delta x_j}(\mathcal{G}(t_1), \mathcal{G}(t_2))$$

$$m = \sum_{i=1}^{q} p_i \, \delta_{a_i}$$

$$\begin{aligned} \mathcal{G}(t) &= \Lambda(K_t) \\ &= c_d \sum_{i=1}^{q} p_i \, (t - a_i)^d 1_{\{a_i \leq t\}}. \end{aligned}$$

where

$$c_d = \lambda^d(B(0,1))$$

For $t = a_i$ with $i = 2 \dots q$, we obtain the following equations:

$$\mathcal{G}(a_i) = c_d \sum_{j=1}^{i-1} p_j \, (a_i - a_j)^d \qquad \forall i = 2 \dots q.$$

Equivalently, we have that

$$\begin{cases} p_1 = \dfrac{1}{(a_2 - a_1)^d} \dfrac{\mathcal{G}(a_2)}{c_d} \\[2ex] p_i = \dfrac{1}{(a_{i+1} - a_i)^d} \left(\dfrac{\mathcal{G}(a_{i+1})}{c_d} - \displaystyle\sum_{j=1}^{i-1} p_j (a_{i+1} - a_j)^d \right) \quad \forall i = 2 \dots q-1 \end{cases}$$

Introducing the following continuous functions,

$$f_1(x_2,\ldots,x_q) = \frac{1}{(a_2-a_1)^d}\frac{x_2}{c_d}$$

$$f_i(x_2,\ldots,x_q) = \frac{1}{(a_{i+1}-a_i)^d}\left(\frac{x_{i+1}}{c_d} - \sum_{j=1}^{i-1} f_j(x_2,\ldots,x_q)(a_{i+1}-a_j)^d\right)$$

$\forall i = 2\ldots q-1$.
The previous equations can be rewritten as follows

$$p_i = f_i(\mathcal{G}(a_2),\ldots,\mathcal{G}(a_q)) \;\; \forall i = 1\ldots q-1.$$

Proposition 3

The following statistics are strongly consistent estimators for parameters p_i :

$$\hat{p}_{i,n} := f_i(\hat{\mathcal{G}}_n(a_2), \ldots, \hat{\mathcal{G}}_n(a_q)) \xrightarrow[n\to\infty]{p.s.} p_i \quad \forall i = 1 \ldots q-1.$$

Moreover,

$$\hat{p}_{q,n} := 1 - \sum_{j=1}^{q-1} \hat{p}_{i,n} \xrightarrow[n\to\infty]{p.s.} p_q.$$

We have that

$$\mathcal{G}(t) = c_d \sum_{i=1}^{q} p_i \, (t - a_i)^d \quad \forall t > a_q.$$

As a consequence,

$$\mathcal{G}(t) \sim_\infty c_d \, t^d$$

For $d \geq 1$ and r sufficiently large, we get that

$$\beta(r) \leq C \, e^{-\gamma \, r^d},$$

where C and γ are some positive constants.

$$\Rightarrow \int_0^\infty r^{d-1} \alpha(r) \, dr < \infty$$

Theorem 7

Assume, when $h = q - 1$, $t_i = a_{i+1}$ for all $i = 1 \dots q-1$, that the matrix Γ of Corollary 1 is *positive definite*. Then,

$$n^{\frac{d}{2}} \left((\hat{p}_{1,n}, \dots, \hat{p}_{q-1,n})' - (p_1, \dots, p_{q-1})' \right) \xrightarrow[n\to\infty]{\mathcal{D}} \mathcal{N}(0, MVM')$$

where V is the matrix defined in Corollary 2 and M is the matrix which (i,j)-th entry equals

$$m_{i,j} = \frac{\delta f_i}{\delta x_{j+1}} (\mathcal{G}(a_2), \dots, \mathcal{G}(a_q))$$

Example

We assume that:

1. $d = 1$
2. $m = p_1\delta_{a_1} + p_2\delta_{a_2}$ with $0 < a_1 < a_2 = a_1 + 1$

We obtain that:

1. $(\hat{p}_{1,n}, \hat{p}_{2,n}) = (\frac{\hat{\mathcal{G}}_n(a_2)}{2}, 1 - \hat{p}_{1,n}) \xrightarrow[n\to\infty]{p.s.} (p_1, p_2)$.
2. $$\begin{aligned} \sigma^2(p_1) &= \int_{\mathbf{R}} \mathrm{Cov}\left(\mathbf{1}_{\{\xi(0)\le a_2\}}, \mathbf{1}_{\{\xi(x)\le a_2\}}\right)\, dx \\ &= e^{-4\,p_1} \int_0^2 e^{-p_1\,(1-\frac{x}{2})} - 1\, dx = e^{-4\,p_1}\, f(p_1) > 0 \end{aligned}$$
3.

Example

We assume that:

1. $d = 1$
2. $m = p_1 \delta_{a_1} + p_2 \delta_{a_2}$ with $0 < a_1 < a_2 = a_1 + 1$

We obtain that:

1. $(\hat{p}_{1,n}, \hat{p}_{2,n}) = (\frac{\hat{\mathcal{G}}_n(a_2)}{2}, 1 - \hat{p}_{1,n}) \xrightarrow[n\to\infty]{p.s.} (p_1, p_2)$.
2. $$\begin{aligned} \sigma^2(p_1) &= \int_{\mathbb{R}} \mathrm{Cov}\left(\mathbf{1}_{\{\xi(0)\leq a_2\}}, \mathbf{1}_{\{\xi(x)\leq a_2\}}\right)\, dx \\ &= e^{-4\,p_1} \int_0^2 e^{-p_1\,(1-\frac{x}{2})} - 1\, dx = e^{-4\,p_1} f(p_1) > 0 \end{aligned}$$
3.

Example

We assume that:

1. $d = 1$
2. $m = p_1 \delta_{a_1} + p_2 \delta_{a_2}$ with $0 < a_1 < a_2 = a_1 + 1$

We obtain that:

1. $(\hat{p}_{1,n}, \hat{p}_{2,n}) = \left(\dfrac{\hat{\mathcal{G}}_n(a_2)}{2}, 1 - \hat{p}_{1,n}\right) \xrightarrow[n\to\infty]{p.s.} (p_1, p_2).$
2. $$\begin{aligned} \sigma^2(p_1) &= \int_{\mathbf{R}} \operatorname{Cov}\left(\mathbf{1}_{\{\xi(0)\leq a_2\}}, \mathbf{1}_{\{\xi(x)\leq a_2\}}\right) dx \\ &= e^{-4\,p_1} \int_0^2 e^{-p_1\,(1-\frac{x}{2})} - 1\,dx = e^{-4\,p_1} f(p_1) > 0 \end{aligned}$$
3.

Example

We assume that:

1. $d = 1$
2. $m = p_1\delta_{a_1} + p_2\delta_{a_2}$ with $0 < a_1 < a_2 = a_1 + 1$

We obtain that:

1. $(\hat{p}_{1,n}, \hat{p}_{2,n}) = (\frac{\hat{\mathcal{G}}_n(a_2)}{2}, 1 - \hat{p}_{1,n}) \xrightarrow[n\to\infty]{p.s.} (p_1, p_2)$.
2. $$\begin{aligned} \sigma^2(p_1) &= \int_{\mathbf{R}} \mathrm{Cov}\left(\mathbf{1}_{\{\xi(0)\le a_2\}}, \mathbf{1}_{\{\xi(x)\le a_2\}}\right)\, dx \\ &= e^{-4\,p_1} \int_0^2 e^{-p_1\,(1-\frac{x}{2})} - 1\, dx = e^{-4\,p_1}\, f(p_1) > 0 \end{aligned}$$
3. $\sqrt{n}(\hat{p}_{1,n} - p_1) \xrightarrow[n\to\infty]{\mathcal{D}} \mathcal{N}(0, (e^{4\,p_1}/4)\,\sigma^2(p_1))$.

Example

We assume that:

1. $d = 1$
2. $m = p_1\delta_{a_1} + p_2\delta_{a_2}$ with $0 < a_1 < a_2 = a_1 + 1$

We obtain that:

1. $(\hat{p}_{1,n}, \hat{p}_{2,n}) = (\frac{\hat{\mathcal{G}}_n(a_2)}{2}, 1 - \hat{p}_{1,n}) \xrightarrow[n\to\infty]{p.s.} (p_1, p_2)$.
2. $$\begin{aligned} \sigma^2(p_1) &= \int_{\mathbf{R}} \mathrm{Cov}\left(\mathbf{1}_{\{\xi(0)\leq a_2\}}, \mathbf{1}_{\{\xi(x)\leq a_2\}}\right) dx \\ &= e^{-4\,p_1} \int_0^2 e^{-p_1\,(1-\frac{x}{2})} - 1\,dx = e^{-4\,p_1}\, f(p_1) > 0 \end{aligned}$$
3. $\sqrt{n}(\hat{p}_{1,n} - p_1)/[(e^{2\,\hat{p}_{1,n}}/2)\sigma(\hat{p}_{1,n})] \xrightarrow[n\to\infty]{\mathcal{D}} \mathcal{N}(0,1)$.

- Yu. Davydov, A. Illig, "Ergodic properties of crystallization processes", Preprint `arXiv:math/0610966` (2006).
- Yu. Davydov, A. Illig, "Ergodic properties of geometrical cristallization processes", C. R., Math., Acad. Sci. Paris 345, No. 10 (2007) pp. 583-586.
- Yu. Davydov, A. Illig, "Ergodic properties of crystallization processes", Journal of Mathematical Sciences, V. 163, **4** (2009) pp. 375-381.
- W. A. Johnson, and R. F. Mehl, "Reaction Kinetics in Processes of Nucleation and Growth", Trans. Amer. Inst. Min. Metal. Petro. Eng. **135** (1939), pp. 416-458.
- A. N. Kolmogorov, "Statistical theory of crystallization of metals", Bull. Acad. Sci. USSR Mat. Ser. 1 (1937) pp. 355-359.
- A. Micheletti, and V. Capasso, "The stochastic geometry of polymer crystallization processes", Stochastic Anal. Appl. **15** no. 3 (1997) pp. 355-373.
- J. Møller, "Random tessellations in $\mathbf{R}^d$", Adv. in Appl. Probab. **21** (1989) pp. 37-73.
- J. Møller, "Random Johnson-Mehl tessellations", Adv. in Appl. Probab. **24** (1992) pp. 814-844.
- J. Møller, "Generation of Johnson-Mehl crystals and comparative analysis of models for random nucleation", Adv. in Appl. Probab. **27** (1995) pp. 367-383.