Available online at www.sciencedirect.com
ScienceDirect
C. R. Acad. Sci. Paris, Ser. I 345 (2007) 583–586
Comptes Rendus Mathematique
http://france.elsevier.com/direct/CRASS1/

Probability Theory

Ergodic properties of geometrical crystallization processes

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Received 1 December 2006; accepted after revision 2 October 2007

Available online 7 November 2007

Presented by Paul Deheuvels

Abstract

We consider a birth and growth process with germs being born according to a Poisson point process whose intensity measure is invariant under translations in space. The germs can be born in unoccupied space and then start growing until they occupy the available space. In this general framework, the crystallization process can be characterized by a random field which, for any point in the state space, assigns the first time at which this point is reached by a crystal. Under general conditions on the growth speed and geometrical shape of free crystals, we prove that the random field is mixing in the sense of ergodic theory, and we also obtain estimates for the absolute regularity coefficient. ***To cite this article: Y. Davydov, A. Illig, C. R. Acad. Sci. Paris, Ser. I 345 (2007).***

Résumé

Propriétés d'ergodicité des processus géométriques de cristallisation. Nous nous intéressons à la cristallisation d'un domaine par des germes apparaissant selon un processus ponctuel de Poisson d'intensité invariante par translation spatiale. Les germes se fixent uniquement en zone libre et se mettent ensuite à croître pour former des cristaux qui occupent progressivement l'espace. Ce procédé peut être décrit par le champ aléatoire donnant en tout point de l'espace le premier instant de recouvrement par un cristal. Nous démontrons sous des hypothèses générales sur la vitesse de croissance et la forme des cristaux libres que le processus est mélangeant au sens de la théorie ergodique et obtenons des estimations du coefficient de régularité absolue. ***Pour citer cet article : Y. Davydov, A. Illig, C. R. Acad. Sci. Paris, Ser. I 345 (2007).***

1. Introduction

We consider the crystallization process which deals with points, called germs, $g = (x_g, t_g)$ in the space $\mathbb{R}^d \times \mathbb{R}^+$, where t_g denotes random time and x_g random location. The germ birth process $\mathcal{N}$ is a Poisson point process on $\mathbb{R}^d \times \mathbb{R}^+$ with intensity measure Λ. Once germs, or crystallization centers, are born, crystals grow if their location is not yet occupied by another crystal. When two crystals meet, the growth stops at the meeting point.

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1631-073X/$ – see front matter
doi:10.1016/j.crma.2007.10.017

To describe crystal expansion in unoccupied space, for a germ $g = (x_g, t_g)$ and a point x in $\mathbb{R}^d$, let $A_g(x)$ be the time when the point x is reached by the crystal born in the location x_g at the time t_g. The crystallization process is then characterized by the random field (r.f.) ξ, which, for any location x in $\mathbb{R}^d$, assigns its crystallization time

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

Consequently, at time t, a free crystal is the set $C_g(t) = \{x \mid A_g(x) \leqslant t\}$.

The above model was introduced by Kolmogorov [3] and, independently, by Johnson and Mehl [2]. It has been intensively studied by many authors, including Møller [5–7], Micheletti and Capasso [4], who represent the main approaches. In these publications one can also find exhaustive lists of references. A very large part of these investigations deals with geometrical structures of mosaics after all the germs have been grown. In contrast, our main attention in the current work is on the ergodic properties of the crystallization process, thus providing a base for efficient estimation of model parameters and subsequent analysis of limit theorems such as asymptotical normality.

The rest of the paper is organized as follows. Under general assumptions, we demonstrate in Section 2 that the r.f. ξ is mixing in the sense of ergodic theory. In Section 3 we provide estimates of the absolute regularity coefficient for the r.f. ξ.

2. Assumptions on the birth and growth process and mixing

Germs are born according to a Poisson point process $\mathcal{N}$ on $E = \mathbb{R}^d \times \mathbb{R}^+$. That is, germs are random points $g = (x_g, t_g)$ in E, where x_g is the location in the growth space $\mathbb{R}^d$ and t_g is the birth time on the time axis $\mathbb{R}^+$. We suppose that the intensity measure of $\mathcal{N}$ has the expression

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

where λ^d is the Lebesgue measure on $\mathbb{R}^d$ and m is a measure on $\mathbb{R}^+$ such that $m([0, a]) < \infty$ for all $a > 0$. The cases to be considered below (cf. [5]) are those with a discrete measure m and with a density measure $m(dt) = \alpha t^{\beta-1}\lambda(dt)$, where $\alpha, \beta > 0$ are parameters. Since the Lebesgue measure is invariant under translations on $\mathbb{R}^d$, we have that $\mathcal{N}$ is space homogeneous.

For time t, we consider the so called *causal cone* $K_t = \{g \in E \mid A_g(0) \leqslant t\}$, which consists of all possible germs that can reach the origin before t. The measure $\Lambda(K_t)$ of the causal cone K_t is denoted by $F(t)$. These set and function play important roles in the sequel.

We assume that, for any germ $g = (x_g, t_g)$, the associated free crystal at time $t \geqslant t_g$ is equal to $C_g(t) = x_g \bigoplus [V(t) - V(t_g)]K$, where K is a convex compact set such that $0 \in K^\circ$ with $\bigoplus$ denoting the Minkowski sum, and $V(t)$ is an absolutely continuous function of t whose value is the distance achieved with positive speed $v(t)$. Finally, let M be a constant such that $v \leqslant M$, and let $A = D_K/d_K$, where d_K is the diameter of the greatest ball centered at zero and contained in K, whereas D_K is the diameter of the smallest ball centered at zero and containing K. Note that when $K = B(0, 1)$ and $v = M$, then we have the well-known model which corresponds to the linear expansion in all directions at a constant speed.

We next consider the mixing of the r.f. ξ. To start with, we assume without loss of generality that ξ is a canonical r.f. on $(\Omega, \mathcal{F}, \mathbb{P})$. Namely, we suppose that $\Omega = \mathbb{R}^T$ with $T = \mathbb{R}^d$, $\mathcal{F}$ is the σ-field generated by the cylinders, and $\mathbb{P}$ is the distribution of ξ so that for all $\omega \in \Omega$, $\xi(x, \omega) = \omega(x)$. Since the Lebesque measure on $\mathbb{R}^d$ is invariant under translations, the r.f. ξ is homogeneous, that is, $\mathbb{P}$ is invariant under the translations $S_h(\omega)(x) = \omega(x + h)$ for all h in $\mathbb{R}^d$. We say that the canonical r.f. is mixing if, for all A and $B \in \mathcal{F}$,

$$\mathbb{P}\{A \cap S_h^{-1}(B)\} \underset{|h| \to \infty}{\longrightarrow} \mathbb{P}\{A\}\mathbb{P}\{B\}.$$

Note that every mixing r.f. in the above sense is ergodic. We have the following theorem:

Theorem 2.1. *For $d \geqslant 1$, the r.f. $\xi = (\xi(x))_{x \in \mathbb{R}^d}$ is mixing.*

3. Absolute regularity property

Keeping in mind that in our context the process ξ is (strictly) stationary, when $d = 1$, the strong mixing coefficient $\alpha(r)$ is defined, for all $r \geqslant 0$, by the equation

$$\alpha(r) = \sup_{A \in \mathcal{F}_{(-\infty,0]}, B \in \mathcal{F}_{[r,+\infty)}} \left|\mathbb{P}(A \cap B) - \mathbb{P}(A)\mathbb{P}(B)\right|,$$

where $\mathcal{F}_{(-\infty,0]} = \sigma\{\xi(x), x \leqslant 0\}$ and $\mathcal{F}_{[r,+\infty)} = \sigma\{\xi(x), x \geqslant r\}$ are the σ-fields generated by the random variables inside the corresponding braces. The absolute regularity coefficient is

$$\beta(r) = \|\mathcal{P}_{(-\infty,0] \cup [r,+\infty)} - \mathcal{P}_{(-\infty,0]} \times \mathcal{P}_{[r,+\infty)}\|_{var},$$

where $\|\mu\|_{var}$ is the total variation norm of a signed measure μ, and $\mathcal{P}_T$ is the distribution of the restriction $\xi_{|T}$ in the set $\mathcal{C}(T)$ of continuous real-valued functions defined on T. Note that $\mathcal{C}(T_1 \cup T_2)$ is canonically identified with $\mathcal{C}(T_1) \times \mathcal{C}(T_2)$ when $T_1 \cap T_2 = \emptyset$. Since $\alpha(r) \leqslant 2^{-1}\beta(r)$, the absolute regularity of the r.f. ξ implies its α-mixing.

Theorem 3.1. *If $d = 1$, then the r.f.* (*or random process*) *ξ is absolutely regular and*

$$\beta(r) \leqslant C_1 e^{-F(C_2 r)},$$

where C_1 and C_2 are constants, e.g., $C_1 = 16$ and $C_2 = 1/(2M)$.

We next elaborate on the coefficient of absolute regularity when $d \geqslant 2$. Let $\mathcal{F}_T$ be the σ-field generated by the random variables $\xi(x)$ for all x in a subset T of $\mathbb{R}^d$. For two disjoint subsets T_1 and T_2, and for two σ-fields $\mathcal{F}_{T_1}$ and $\mathcal{F}_{T_2}$, the absolute regularity coefficient is

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

where $\mathcal{P}_T$ denotes the distribution of the restriction $\xi_{|T}$. Note that $\beta(T_1, T_2)$ can also by written as the expectation $E\|\mathcal{P}_{\{\xi_{|T_1}|\mathcal{F}_{T_2}\}} - \mathcal{P}_{T_1}\|_{var}$, where $\mathcal{P}_{\{\xi_{|T_1}|\mathcal{F}_{T_2}\}}$ is the conditional distribution of $\xi_{|T_1}$ given $\mathcal{F}_{T_2}$ In the following theorem we obtain an upper bound for $\beta(T_1, T_2)$ when the two quadrants T_1 and T_2 are separated by a $2r$-width band. Since the r.f. ξ is homogeneous, we can choose $T_1 = \prod_{i=1}^d (-\infty, 0]$ and $T_2 = \prod_{i=1}^d [a_i, +\infty)$, supposing that $\sum_1^d a_i = 2r\sqrt{d}$.

Theorem 3.2. *When $d \geqslant 2$, then*

$$\beta(T_1, T_2) \leqslant C_1 \sum_{k=1}^{\infty} k^{d-1} e^{-F(C_2 k)},$$

where we can choose $C_1 = 16$, $C_2 = 2R/(dH)$, $H = 2(A + M)$ and $R = r/H$.

Our next theorem gives an upper bound for the two enclosed domains $T_1 = [-a, a]^d$ and $T_2 = ([-b, b]^d)^c$ separated by a $2r$-width polygonal band, assuming $r = \frac{(b-2a)\sqrt{d}}{4} > 0$.

Theorem 3.3. *When $d \geqslant 2$, then*

$$\beta(T_1, T_2) \leqslant C_1 \sum_{k=1}^{\infty} k^{d-1} e^{-F(C_2 k)},$$

where we can choose $C_1 = 8(d2^d + 1)$, $C_2 = 2R/(dH)$, $H = 2(A + M)$ and $R = r/H$.

The main idea of proof is based on substituting the original process ξ by the process

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

This relies on the fact that, with a probability as close to 1 as desired, we have the equality $\xi(x) = \xi_T(x)$ for all $|x| \leqslant r(T)$, where $r(T) \to \infty$ when $T \to \infty$. Hence, we can utilize the independence of ξ_T and $S_h\xi_T$ for all h such that $|h| > 2r(T)$.

We conclude this section with two estimates of the majorizing series in Theorems 3.2 and 3.3. First, if $F(t) \geqslant (d+\delta)\ln t - \ln\gamma$ with $\delta, \gamma > 0$, then we obtain a polynomial estimate

$$\sum_{k=1}^{\infty} k^{d-1} \mathrm{e}^{-F(Ck)} \leqslant \gamma' C^{-(d+\delta)} \quad \text{with } \gamma' = \gamma \sum_{k=1}^{\infty} k^{-(1+\delta)}.$$

Second, if $F(t) \geqslant \gamma t^{\delta} - c$ with $\delta, \gamma, c > 0$, then we have a super-exponential estimate

$$\sum_{k=1}^{\infty} k^{d-1} \mathrm{e}^{-F(Ck)} \leqslant c_2 \mathrm{e}^{-\gamma C^{\delta}} \quad \text{with } c_2 = c_1 \sum_{k=1}^{\infty} k^{d-1} \mathrm{e}^{-\gamma C^{\delta}(k^{\delta}-1)}.$$

4. Conclusion

Theorem 2.1 can be directly applied to establish consistency of different functionals (such as volume fraction, mean number of crystals in the unit volume) and parameters of the model (see [1]). Theorems 3.2 and 3.3 provide a natural way to apply known limit theorems concerning β-mixing fields to establish asymptotical normality of these estimates.

Acknowledgements

The authors are grateful to R. Zitikis for discussions and interest in this work, and to an anonymous referee for useful remarks and suggestions.

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