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C. R. Acad. Sci. Paris, Ser. I 346 (2008) 691–696
COMPTES RENDUS MATHEMATIQUE
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Mathematical Physics/Probability Theory

Cut-off and exit from metastability: two sides of the same coin

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Received 15 January 2008; accepted after revision 15 April 2008

Available online 8 May 2008

Presented by Marc Yor

Abstract

We present a general framework linking cut-off and exit excursions for birth-and-death processes on a countable alphabet. Under suitable hypotheses, we prove that cut-off convergence towards a (local) equilibrium is accompanied by exponentially distributed out-of-equilibrium excursions. Furthermore, atypical trajectories leading to these excursions and final cut-off trajectories are related by time inversion; in particular their time lengths have identical laws. ***To cite this article: O. Bertoncini et al., C. R. Acad. Sci. Paris, Ser. I 346 (2008).***

Résumé

Cut-off et sortie de la métastabilité : les deux faces de la même pièce. Nous présentons un cadre général qui relie cut-off et excursions de sortie pour des processus de naissance et de mort sur un alphabet dénombrable. Sous des hypothèses adaptées, nous montrons que le cut-off vers un équilibre (local) est accompagné par une distribution exponentielle des temps de sortie de l'équilibre. De plus, les trajectoires atypiques menant à ces excursions sont les renversées temporelles de trajectoires de cut-off ; en particulier leurs durées suivent la même loi. ***Pour citer cet article : O. Bertoncini et al., C. R. Acad. Sci. Paris, Ser. I 346 (2008).***

Version française abrégée

Le phénomène de *cut-off* correspond à une convergence *abrupte* vers l'équilibre pour une famille de chaînes de Markov à des instants *déterministes* asymptotiques. Soit $X^{(n)}$ une famille de processus de Markov ergodiques indexés par un paramètre n, et soient $P_t^{(n)}$ leurs lois au temps t et $\pi^{(n)}$ les mesures invariantes correspondantes. La famille $X^{(n)}$ admet un cut-off s'il existe une fonction (croissante) t_n et une « distance » D (pas nécessairement une métrique, mais non-nulle pour des mesures différentes) telles que la fonction $d^{(n)}(t) = D(P_t^{(n)}, \pi^{(n)})$ est proche, dans une échelle de temps macroscopique, d'une fonction avec saut en t_n lorsque $n \to \infty$ (Fig. 1(a)). Ce phénomène a été étudié à l'aide des propriétés spectrales des matrices de transition et de techniques d'analyse fonctionnelle et de Fourier (voir [9,10,

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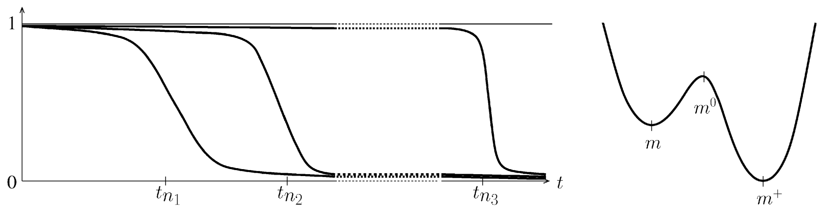
1631-073X/$ – see front matter
doi:10.1016/j.crma.2008.04.007



(a) (b)

Fig. 1. (a) Abrupt asymptotic convergence ($n_1 < n_2 < n_3$); (b) The local minimum at m^- introduces the metastability.

Fig. 1. (a) Convergence abrupte asymptotique ($n_1 < n_2 < n_3$) ; (b) Le minimum local en m^- induit la métastabilité.

15,16]). Dans ce travail nous utilisons une approche probabiliste développée dans [11] (voir aussi [19] et le chapitre correspondant dans [20]).

La sortie de la métastabilité implique aussi une convergence *abrupte*, mais celle-ci a lieu à des instants très *aléatoires*. Physiquement, cela correspond à la relaxation finale d'un système « piégé » dans une situation de non-équilibre (liquide en surfusion par exemple). Mathématiquement, cela correspond à la sortie d'un minimum local pour des évolutions dont le profil énergétique est tel que dans la Fig. 1(b).

Des études récentes de la métastabilité (voir [14]) suivent l'approche "pathwise" introduite dans [8] qui s'interesse aux réalisations individuelles. Elle montre que les lois des temps de sortie d'un puits d'attraction d'un minimum local convergent vers une loi exponentielle lorsque la « barrière d'énergie » croît. Les distances aux points de sortie suivent typiquement des courbes similaires à celles de la Fig. 1, mais avec des sauts à des instants aléatoires.

La distribution exponentielle des temps de sortie provient de la distribution du nombre d'excursions que le système doit réaliser pour quitter le minimum local. Dans ce travail, nous montrons que les trajectoires de sortie et de cut-off sont des phénomènes complémentaires : pour des processus avec une dérive suffisante, l'évolution vers un équilibre (local) est de type cut-off, alors que dans l'autre direction, les excursions de sortie ont lieu à des instants exponentiels. Ces faits sont démontrés pour des familles de chaînes de naissance et de mort incluant le modèle d'Ehrenfest.

Dans notre cadre, les évolutions de type cut-off, et les excursions de sortie exponentielles nous permettent de décrire complètement l'évolution du système. Par exemple, la sortie du puits de m^- de la Fig. 1(b) se décompose en une excursion atypique vers m^0, qui dure un temps exponentiel, et une tombée de type cut-off vers m^+ qui a lieu dans une échelle de temps beaucoup plus courte. Le caractère exponentiel de la trajectoire est donc dû à la première excursion. En outre, l'existence d'un cut-off *explique* le caractère exponentiel de la métastabilité : une excursion qui n'atteint pas m^0, est presque toujours suivie d'une descente de type cut-off. Il faut donc un grand nombre de tentatives (indépendantes par la propriété de Markov) pour réussir à atteindre m^0 et c'est cette distribution géométrique qui induit la loi exponentielle. Pour compléter le tableau, nous montrons par réversibilité que les excursions typiques $m^- \to m^0$ sont les renversées temporelles des trajectoires typiques de cut-off $m^0 \to m^-$ dans un sens probabiliste précis (voir (6)). Ceci explique la similarité entre les caractères abrupts du cut-off et de la métastabilité.

Ces considérations nous amènent à se placer dans le cas d'un puits *unique* pour mieux comprendre la relation entre les deux phénomènes. Nous montrons (Theorem 2.2) qu'asymptotiquement en la hauteur du puits : (i) la trajectoire de descente admet un cut-off ; alors que (ii) celle de sortie est exponentielle. Le modèle que nous considérons est une famille de chaînes de naissance et de mort sur $[\![0, a]\!] := \{0, \ldots, a\} \subset \mathbb{N}$ avec une dérive vers zéro (5). C'est cette condition sur la vitesse relative entre la quantité K_a (2) et le temps moyen pour atteindre 0 en partant de a qui traduit la pente du profil énergétique. Nous montrons de plus (Theorem 2.2(iii)) que la loi du temps d'atteinte de a après la dernière visite en 0 ($\widetilde{T}^{(a)}_{0\to a}$) est égale à celle de $\widetilde{T}^{(a)}_{a\to 0}$, le temps d'atteinte de zéro après le dernier passage en a.

1. Introduction

The *cut-off* phenomenon [2], also called *threshold phenomenon* [3] or *abrupt switch* [1], refers to the *sudden* convergence to equilibrium of a family of Markov chains at asymptotically *deterministic* times. Let $X^{(n)}$ be a family of ergodic Markov processes labeled by a parameter n, and denote by $P_t^{(n)}$ the evolved distributions at time t and $\pi^{(n)}$ the corresponding invariant measures. The family $X^{(n)}$ exhibits cut-off if there exists a (increasing) function t_n and a "distance" D (need not be a metric, but must be non-zero for different measures) such that the function $d^{(n)}(t) =$

$D(P_t^{(n)}, \pi^{(n)})$ becomes, in macroscopic time scale, closer to a step function with jump at t_n as $n \to \infty$ (Fig. 1). This phenomenon has been studied using Fourier techniques, spectral properties of transition matrices, and functional analysis techniques (see [9,10,15,16] for reviews). In this work we adopt the probabilistic approach advocated in [11] (see also [19] and the relevant chapter in [20]).

Exit from metastability also involves a *sudden* convergence but at extremely *random* times. Physically, it corresponds to the final relaxation of systems "trapped" in a non-equilibrium situation (e.g. supercooled or overheated liquids). Mathematically, it corresponds to an escape from a local minimum for evolutions driven by an energy profile such as in Fig. 1(b). Present rigorous studies of metastability (see [14] for an account) follow the "pathwise approach" introduced in [8] in which individual realizations are followed. The approach shows that exit times from traps become exponentially distributed as the "barrier heights" grow. Distances to equilibrium typically follow curves similar to those of Fig. 1, but with jumps at random times. An efficient alternative approach has recently been introduced, see [6,7].

The exponential law of exit times comes, in fact, from the distribution of the number of excursions needed to take the system out of the local minimum. In the present work we show that escape excursions and cut-off can be intertwined phenomena: For processes with sufficient drift, the evolution towards a (local) equilibrium is cut-off like, while in the opposite direction exit excursions occur at exponential times. We show these facts for a family of birth-and-death chains that include the Ehrenfest model.

Within our framework, cut-off evolutions and exponential excursions become the building blocks to describe the overall evolution. For instance, the exit of the m^--trap of Fig. 1(b) decomposes into an "exceptional" excursion up to m^0, which takes an exponential time, followed by a cut-off fall down to m^+. The latter happens in a much shorter time scale, hence the former is responsible for the exponential character of the time to reach equilibrium. Furthermore, the existence of cut-off *explains* the exponential character of metastability: An excursion unable to reach m^0 is almost unavoidably followed by a cut-off-like descent to m^-. A successful exit trajectory happens, thus, only after a large number of tries, which are independent by the Markov property. This geometric distribution of successes leads to an exponential law. To complete the picture, we observe that, by reversibility, typical excursions $m^- \to m^0$ are the time reversed of typical cut-off trajectories $m^0 \to m^-$ in some precise probabilistic sense (see (6) below). This explains the similar sudden character of cut-off and escape phenomena.

2. Definitions and results

The discussion of last paragraph shows that, to understand the relation between cut-off and metastability, it is enough to consider evolutions down and up a certain height in a *single* well. We set out to prove that, asymptotically in its height, the downhill trajectory exhibits cut-off while the uphill one exhibit metastability features. The complete evolution in presence of several wells involves, then, sequences of exponential "climbing times" and abrupts fall into wells. Its study is a mathematical problem of a different nature that has already been addressed, for instance, within the theory developed in [12,13,18].

As simple but representative models we consider birth-and-death chains on intervals $[\![0, a]\!] := \{0, \dots, a\} \subset \mathbb{N}$. These are characterized by non-zero transition probabilities $p(x, x+1) =: p_x$, $0 \leqslant x \leqslant a-1$, $p(a, a) =: p_a$, $p(x, x-1) =: q_x$, $1 \leqslant x \leqslant a$, $p(0, 0) =: q_0$. Both p_x and q_x may depend on a. The parameter a plays the role of n in the previous section; our results are asymptotic for $a \to \infty$. These chains have a unique invariant measure, which is also reversible, with

$$\pi^{(a)}(x) = \prod_{i=1}^{x} \frac{p_{i-1}}{q_i} \pi_a(0). \tag{1}$$

The associated energy profile $H(x)$, defined by writing $p(x, y) \propto \exp\{-[H(y) - H(x)]\}$, satisfies $2[H(x) - H(x-1)] = -\log(p_{x-1}/q_x)$. By (1) this implies $\pi_a(x)/\pi_a(0) = \exp\{-2[H(x) - H(0)]\}$. This energy profile, thus, resembles a wedge with a vertical left wall at 0^- and a right wall whose steepness can be gauged through the quantity

$$K_a := \sup_{x \in [\![0,a]\!]} \frac{\pi_a([\![x, a]\!])}{\pi_a(x)}. \tag{2}$$

Indeed, by (1) $\pi_a(x) \leqslant \exp(-\alpha_a x)$ with $\alpha_a = -\log(1 - K_a^{-1})$; hence $H(x) - H(0) \geqslant \alpha_a x/2$.

The relation between cut-off and escape trajectories is achieved at the level of *hitting times*. If $X_x^{(a)} = (X_x^{(a)}(t))_{t\in\mathbb{N}}$ denotes the chain started at x, we define $T_{x\to y}^{(a)} = \inf\{t > 0\colon\ X_x^{(a)}(t) = y\}$ the hitting time of y, $\tau_{x\to x,y}^{(a)} = \sup\{0 < t < T_{x\to y}^{(a)}\colon\ X_x^{(a)}(t) = x\}$ the last visit to x before hitting y, and $\widetilde{T}_{x\to y}^{(a)} = T_{x\to y}^{(a)} - \tau_{x\to x,y}^{(a)}$ the time to hit y after the last visit to x.

Definition 2.1.

(i) A family of random variables $T^{(a)}$ *exhibits cut-off behavior at their mean times* if

$$\frac{T^{(a)}}{\mathbb{E}[T^{(a)}]} \xrightarrow[a\to\infty]{\text{Proba}} 1. \tag{3}$$

(equivalently, $\lim_{a\to\infty} \mathbb{P}(T^{(a)} > c\mathbb{E}[T^{(a)}]) = 1$ for $c < 1$ and 0 for $c > 1$).

(ii) A family of random variables $\widehat{T}^{(a)}$ *exhibits escape-time behavior at their mean times* if

$$\frac{\widehat{T}^{(a)}}{\mathbb{E}[\widehat{T}^{(a)}]} \xrightarrow[a\to\infty]{\mathcal{L}} \exp(1). \tag{4}$$

The following theorem summarizes our results:

Theorem 2.2. *Let $X^{(a)}$ be a family of birth-and-death chains on $[\![0, a]\!]$ such that*

$$\inf_{a\in\mathbb{N}} \inf_{x\in[\![0,a]\!]} q_x > 0 \quad \text{and} \quad \frac{K_a^2}{\mathbb{E}[T_{a\to 0}^{(a)}]} \xrightarrow[a\to\infty]{0}. \tag{5}$$

Then,

(i) *The random variables $T_{a\to 0}^{(a)}$ exhibit cut-off behavior at their mean times.*

(ii) *The random variables $T_{0\to a}^{(a)}$ exhibit escape-time behavior at their mean times.*

(iii) *Let $v^k = (v_1, \ldots, v_k)$ be a trajectory of length k, $\mathcal{V}_a^k = \{v^k\colon\ v_1 = a, v_k = 0,$ and $v_i \neq a, 0, \forall 1 < i < k\}$ and $\mathcal{U}_a = \bigcup_{k<\infty} \mathcal{V}_a^k$. If $\mathcal{R}$ is the time-reversal operator, $\mathcal{R}(v^k) = \{v_k, \ldots, v_1\}$, then*

$$\mathbb{P}\big(X_a^{(a)} \text{ starts in } \mathcal{V}_a^k \mid X_a^{(a)} \text{ starts in } \mathcal{U}_a\big) = \mathbb{P}\big(X_0^{(a)} \text{ starts in } \mathcal{R}\big(\mathcal{V}_a^k\big) \mid X_a^a \text{ starts in } \mathcal{R}(\mathcal{U}_a)\big). \tag{6}$$

As a consequence, $\widetilde{T}_{a\to 0}^{(a)} \stackrel{\mathcal{L}}{=} \widetilde{T}_{0\to a}^{(a)}$.

Requirements (5) are satisfied if $\sup_a K_a =: K < \infty$, for example if p_x and q_x are independent of a and define a positively recurrent chain on $\mathbb{N}$. This happens, for instance, for the heat-bath evolution of the magnetization for the Curie–Weiss model. The condition $K < \infty$ corresponds to a well with fixed steepness and diverging depth. In contrast, in the metastability results reviewed in [14] the steepness tends to infinity ($m^0 \to m^-$ in Fig. 1, or $K_a \to_a 0$ in our setting). Moreover, the previous theorem allows $K_a \to_a \infty$, though at a smaller pace than $\mathbb{E}[T_{a\to 0}^{(a)}]$. This generality makes the result applicable to the Ehrenfest model. In this model one follows the number of balls of one of two urns containing a total of N balls. At each time-unit one of the balls is chosen at random and changed of urn. Shifting $N/2 \to 0$ and calling $a = N/2$ the model is equivalent to a birth-and-death chain with $p_x = (a - x)/(2a)$, $q_x = (a + x)/(2a)$, $K_a \sim \sqrt{a}$ and $\mathbb{E}[T_{a\to 0}^{(a)}] \sim a \log a$ [5].

3. Sketch of the proofs

Let us briefly present the highlights of the proof of Theorem 2.2. Full details can be found in [5,4].

Cut-off behavior. As pointed out in [11], a family $T^{(a)}$ exhibits cut-off behavior if $\mathbb{E}[T^{(a)}] \to_a \infty$ and $\mathrm{Var}(T^{(a)}/\mathbb{E}[T^{(a)}]) \to_a 0$. To prove (i) we estimate this expectation and variance for $T_{a\to 0}^{(a)}$, starting from available explicit expressions.

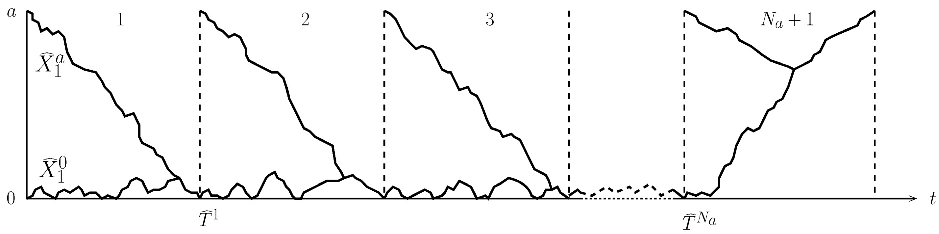


Fig. 2. Coupling to prove $\mathbb{E}[T^{(a)}_{a\to 0}]/\mathbb{E}[T^{(a)}_{0\to a}] \underset{a\to\infty}{\longrightarrow} 0$.

Fig. 2. Couplage pour la démonstation $\mathbb{E}[T^{(a)}_{a\to 0}]/\mathbb{E}[T^{(a)}_{0\to a}] \underset{a\to\infty}{\longrightarrow} 0$.

Escape-time behavior. As shown in [8], an exponential law is a consequence of downwards excursions involving a much shorter time scale than upwards excursions. To prove the exponential character of $T^{(a)}_{0\to a}$ is sufficient to show that

$$\mathbb{E}\big[T^{(a)}_{a\to 0}\big]/\mathbb{E}\big[T^{(a)}_{0\to a}\big] \to_a 0. \tag{7}$$

To prove this, we define a coupling $(\widehat{X}^a, \widehat{X}^0)$ between two chains starting respectively at a and 0. The copies start in an independent fashion until they intersect at which point they merge ($\widehat{X}^a = \widehat{X}^0$). This common trajectory is continued until either 0 or a is reached. In the former case, we call it a regeneration, restart $\widehat{X}^a$ independently at a and repeat the construction (Fig. 2). The number N_a of regeneration times is a geometric random variable with $\mathbb{E}[N_a] = 1/\mathbb{P}(T^{(a)}_{a\to 0} > T^{(a)}_{0\to a}) \underset{a\to\infty}{\longrightarrow} \infty$.

The limit is a consequence of conditions (5) *and*, in particular, of the cut-off behavior for $T^{(a)}_{a\to 0}$. Hence N_a converges to an exponential random variable and (7) follows. The argument formalizes the expected behavior: there is a geometric number of tries before a final excursion reaches a.

Reversed trajectories. As in [17] we observe that, by reversibility,

$$\pi^{(a)}(a)\mathbb{P}\big(X^{(a)}_a \text{ starts as } v^k\big) = \pi^{(a)}(0)\mathbb{P}\big(X^{(a)}_0 \text{ starts as } \mathcal{R}(v^k)\big).$$

This yields (6).

The left- and right-hand side of this equation are respectively equal to $\mathbb{P}(\widetilde{T}^{(a)}_{a\to 0} = k)$ and $\mathbb{P}(\widetilde{T}^{(a)}_{0\to a} = k)$.

4. Final comments

Our results suggest that cut-off and escape excursions should be studied as complementary aspects of evolutions in presence of drifts associated to local energy minima. We believe that, in great generality, the occurrence of cut-off should imply exponential laws for the reversed evolution. The converse is false: Metastable behavior arises from "downhill" evolutions that are faster but not necessarily cut-off-like. Energy wells with rugged walls should lead quite naturally to counterexamples. In this sense, the occurrence of cut-off conveys more precise information than that contained in exit times.

References

[1] D. Aldous, Random walks on finite groups and rapidly mixing Markov chains, in: Seminar on Probability, XVII, in: Lecture Notes in Math., vol. 986, Springer, Berlin, 1983, pp. 243–297.

[2] D. Aldous, P. Diaconis, Shuffling cards and stopping times, Amer. Math. Monthly 93 (5) (1986) 333–348.

[3] D. Aldous, P. Diaconis, Strong uniform times and finite random walks, Adv. Appl. Math. 8 (1) (1987) 69–97.

[4] J. Barrera M., O. Bertoncini, R. Fernández, Abrupt convergence and metastability for birth and death chains, in preparation.

[5] O. Bertoncini, Convergence abrupte et métastabilité, Thesis, Université de Rouen, 2007.

[6] A. Bovier, M. Eckhoff, V. Gayrard, M. Klein, Metastability in stochastic dynamics of disordered mean-field models, Probab. Theory Related Fields 119 (1) (2001) 99–161.

[7] A. Bovier, M. Eckhoff, V. Gayrard, M. Klein, Metastability and low lying spectra in reversible Markov chains, Commun. Math. Phys. 228 (2) (2002) 219–255.

[8] M. Cassandro, A. Galves, E. Olivieri, M.E. Vares, Metastable behavior of stochastic dynamics: a pathwise approach, J. Statist. Phys. 35 (5–6) (1984) 603–634.

[9] P. Diaconis, Group Representations in Probability and Statistics, Institute of Mathematical Statistics Lecture Notes—Monograph Series, vol. 11, Institute of Mathematical Statistics, Hayward, CA, 1988.
[10] P. Diaconis, The cutoff phenomenon in finite Markov chains, Proc. Natl. Acad. Sci. USA 93 (4) (1996) 1659–1664.
[11] S. Martínez, B. Ycart, Decay rates and cutoff for convergence and hitting times of Markov chains with countably infinite state space, Adv. Appl. Probab. 33 (1) (2001) 188–205.
[12] E. Olivieri, E. Scoppola, Markov chains with exponentially small transition probabilities: first exit problem from a general domain. I. The reversible case, J. Statist. Phys. 79 (3–4) (1995) 613–647.
[13] E. Olivieri, E. Scoppola, Markov chains with exponentially small transition probabilities: first exit problem from a general domain. II. The general case, J. Statist. Phys. 84 (5–6) (1996) 987–1041.
[14] E. Olivieri, M.E. Vares, Large Deviations and Metastability, Encyclopedia of Mathematics and its Applications, vol. 100, Cambridge University Press, Cambridge, 2005.
[15] L. Saloff-Coste, Lectures on finite Markov chains, in: Lectures on Probability Theory and Statistics, Saint-Flour, 1996, in: Lecture Notes in Math., vol. 1665, Springer, Berlin, 1997, pp. 301–413.
[16] L. Saloff-Coste, Random walks on finite groups, in: Probability on Discrete Structures, in: Encyclopaedia Math. Sci., vol. 110, Springer, Berlin, 2004, pp. 263–346.
[17] R.H. Schonmann, The pattern of escape from metastability of a stochastic Ising model, Commun. Math. Phys. 147 (2) (1992) 231–240.
[18] E. Scoppola, Metastability for Markov chains: a general procedure based on renormalization group ideas, in: Probability and Phase Transition, Cambridge, 1993, in: NATO Adv. Sci. Inst. Ser. C Math. Phys. Sci., vol. 420, Kluwer Acad. Publ., Dordrecht, 1994, pp. 303–322.
[19] B. Ycart, Cutoff for Markov chains: some examples and applications, in: Complex Systems, Santiago, 1998, in: Nonlinear Phenom. Complex Systems, vol. 6, Kluwer Acad. Publ., Dordrecht, 2001, pp. 261–300.
[20] B. Ycart, Modèles et algorithmes markoviens, Mathématiques & Applications (Berlin) (Mathematics & Applications), vol. 39, Springer-Verlag, Berlin, 2002.