The Cut-off phenomenon for Monte Carlo Markov Chains

IRTG Stochastic Models of Complex Processes

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If π satisfies (1), known as *detailed balance equations*, then it is a stationary distribution for our chain *P*:

$$\pi P = \pi$$
.

Theorem (Ergodic theorem)

Let (X_t) be an irreducible and aperiodic Markov chain with transition matrix P. Then there exists a unique stationary distribution π for the chain. Moreover,

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Problem of the approach to the equilibrium: how *fast* is this convergence?

We have first to define a notion of *distance*.

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Then we can define the distance of a Markov Chain P from its stationary distribution π at step t as

$$d(t) := \max_{x \in \Omega} \|P^t(x, \cdot) - \pi\|_{TV}.$$
 (2)

It is easy to show that this is a decreasing function of t.

(3)

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Mixing time

The ε -mixing time of a Markov Chain is

 $t_{mix}(\varepsilon) := \min\{t : d(t) \le \varepsilon\}.$

We also set for simplicity $t_{mix} := t_{mix}(1/4)$.

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One possible approach to the study of the mixing time is the study of the eigenvalues of P. Let's label them in decreasing order:

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- *P* is irreducible $\implies \lambda_2 < 1;$
- P is lazy $\implies \lambda_i \ge 0, \forall i$.

Let $gap := 1 - \lambda_2$ be the spectral gap of the chain and call its inverse $t_{rel} := \frac{1}{gap}$ the relaxation time of the chain. Then

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Proposition

$$(t_{rel}-1)\log\left(\frac{1}{2\varepsilon}
ight) \leq t_{mix}(\varepsilon) \leq \log\left(\frac{1}{\varepsilon\pi_{min}}
ight)t_{rel}.$$
 (4)

Cut-off

Definition

Let $(X_t^{(n)})$ be a sequence of Markov Chains on state spaces $\Omega^{(n)}$, with transition matrices $P^{(n)}$, stationary distributions $\pi^{(n)}$ and ε -mixing times $t_{mix}^{(n)}(\varepsilon)$. We say that this sequence exhibits Cut-off if

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$$\lim_{n \to \infty} \frac{t_{mix}^{(n)}(\varepsilon)}{t_{mix}^{(n)}(1-\varepsilon)} = 1, \qquad \forall 0 \le \varepsilon \le \frac{1}{2}.$$
 (5)



Figure: For a sequence of chains with Cut-off, the graph of $d_n(t)$, zoomed on a time-scale of $t_{mix}^{(n)}$, approaches a step function as $n \to \infty$.

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• $\lim_{\alpha \to \infty} \liminf_{n \to \infty} d_n(t_{mix}^{(n)} - \alpha \omega_n) = 1,$
• $\lim_{\alpha \to \infty} \limsup_{n \to \infty} d_n(t_{mix}^{(n)} + \alpha \omega_n) = 0.$



Figure: In a small time-interval around $t_{mix}^{(n)}$, the distance falls from near 1 to almost 0.

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$$H(\sigma) := -\frac{1}{n} \sum_{\substack{\mathbf{v}, \mathbf{w} \in \mathbf{V} \\ \mathbf{v} \sim \mathbf{w}}} \sigma(\mathbf{v}) \sigma(\mathbf{w}).$$

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Then we can define the Gibbs measure on Ω given by

$$\mu(\sigma) := \frac{e^{-\beta H(\sigma)}}{Z(\beta)},$$

where $Z(\beta)$ is the partition function and the parameter β can be interpreted as the inverse of the temperature.

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The heat-bath Glauber dynamics on this model is the following:

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ullet replace it with a brand new spin generated according to $\mu.$

That is, if we choose vertex $w \in V$ to be updated in a configuration $\sigma \in \Omega$, the probability of putting a spin $x \in \pm 1$ in w is

$$p(\sigma, x) = \frac{e^{\beta S(\sigma, x)}}{e^{\beta S(\sigma, x)} + e^{-\beta S(\sigma, x)}},$$
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where $S(\sigma, x) := \sum_{v \sim w} \sigma(v).$

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where $S(\sigma, x) := \sum_{v \sim w} \sigma(v)$. This dynamics is reversible with respect to measure μ .

Theorem (Levin, Luczak, Peres, 2007)

Let $(X_t^{(n)})$ be the Glauber dynamics for the Ising model on the n-complete graph. If $\beta < 1$, there is a Cut-off at time $t_n := \frac{n \log n}{2(1-\beta)}$ with window $\omega_n = O(n)$.

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exponential behaviour, and in both case there is no Cut-off.

Main idea:

• The big symmetry of the model allows us to deal just with a simpler process, namely the magnetization chain:

$$M_t^{(n)} := \frac{1}{n} \sum_{v=1}^n X_t^{(n)}(v),$$

with state space $\Omega_M^{(n)} := \{-1, -1 + \frac{2}{n}, ..., 1\}$ (B&D chain).

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• We use a coupling of the original dynamics to make the magnetization of the two copies of the chain merge in t_n steps (in particular the most of the work is to make them differ for less than $\frac{cost.}{\sqrt{n}}$, which is achieved via the monotone coupling strategy).

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- We use a coupling of the original dynamics to make the magnetization of the two copies of the chain merge in t_n steps (in particular the most of the work is to make them differ for less than $\frac{cost.}{\sqrt{n}}$, which is achieved via the monotone coupling strategy).
- Once the magnetizations have met, we need only other O(n) steps to make the two copies coincide.

Theorem (Lubetzky, Sly, 2009)

Let $(X_t^{(n)})$ be the continuous-time Glauber dynamics for the Ising model on the lattice $\left(\frac{\mathbb{Z}}{n\mathbb{Z}}\right)^2$ with periodic boundary conditions. Let $\beta_c = \frac{1}{2}\log(1+\sqrt{2})$ be the critical inverse-temperature.

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The Theorem can be extended to the case of the $\left(\frac{\mathbb{Z}}{n\mathbb{Z}}\right)^d$, with $d \in \mathbb{N}$, whenever β and h (the external field) are such that the strong spatial mixing property holds.

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- This set is shown to be sparse with high probability, that is, concentrated in small islands far enough from each other to be considered almost independent.
- Studying the *L*²-mixing of these smaller lattices is enough to control the mixing of the whole dynamics.

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$$\operatorname{gap}^{(n)} \cdot t_{\operatorname{mix}}^{(n)} \xrightarrow{n \to \infty} \infty.$$

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This was shown not to be always true, but is still believed to hold for many 'natural' classes of Markov Chains (e.g. proved for B&D Markov Chains in 2008);

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Bibliography

Aldous D. and Diaconis P. (1986) Shuffling cards and stopping times, Amer. Math. Monthly 93, 333-348.

 $\label{eq:loss_loss} Aldous \ D. \ and \ Fill \ J. \ (1999) \ Reversible \ Markov \ chains \ and \ random \ walks \ on \ graphs, \ in \ progress. \ Manuscript \ available \ at \ http://www.stat.berkeley.edu/~aldous/RWG/book.html.$

Chen G.-Y. and Saloff-Coste L. (2008) The cutoff phenomenon for ergodic Markov processes. Electronic Journal of Probability, Vol. 13, paper no. 3, 26-78, http://www.math.washington.edu/~ejpecp.

Ding J., Lubetzky E. and Peres Y. (2008) The mixing time evolution of Glauber dynamics for the mean-field Ising model, arXiv:0806.1906v2.

Ding J., Lubetzky E. and Peres Y. (2008) Total variation cutoff in birth and death chains, arXiv:0801.2625v4.

Levin D. A., Malwina L. J. and Peres Y. (2007) Glauber dynamics for the mean-field Ising model: cut-off, critical power law, and metastability, arXiv:0712.0790v2.

Levin D. A., Peres Y. and Wilmer E. L. (2009) Markov Chains and Mixing Times, American Mathematical Society.

Lubetzky E. and Sly A. (2009) Cutoff for the Ising model on the lattice, arXiv:0909.4320v1.

Saloff-Coste L. (1997) Lectures on finite Markov chains, Lectures On Probability Theory and Statistics, École d'Ete de Probabilites de Saint-Flour XXVI, 301-413.

Thank you!

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