Asymptotically exponential hitting times and metastability: a pathwise approach without reversibility

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(in progress)

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Plan of the talk

-1- Metastability and first hitting

-2- Known results and tools

-3- The non reversible case [FMNS]

-4- Recurrence as a robust tool

-1- Metastability and first hitting

Physical systems near a phase transition (e.g. ferromagnet or saturated gas)

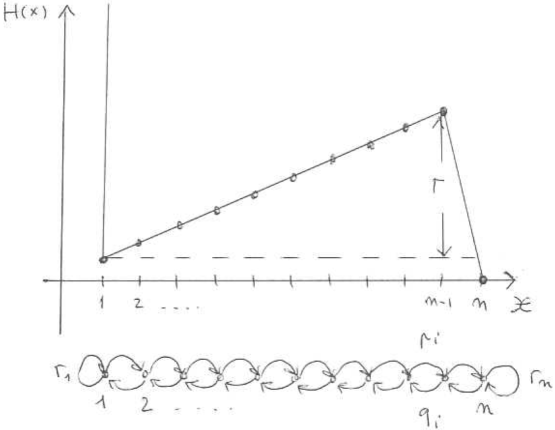
- trapped for an abnormal long time in a state —the metastable phase— different from the eventual equilibrium state consistent with the thermodynamical potentials;
- subsequently, undergoing a *sudden* transition at a *random time* from the metastable to the stable state.

Statistical mechanics model:

- space state $\mathcal{X}$, e.g. $\mathcal{X} = \{-1, +1\}^{\Lambda}$; interaction, e.g. Ising hamiltonian;
- evolution: Markov chain on $\mathcal{X}$, reversible w.r.t. Gibbs measure $\frac{e^{-\beta H}}{Z}$;
- decay of the metastable state: convergence to equilibrium of the chain, (equilibrium state), e.g. configuration of minimal energy in the limit of small temperature $\beta \to \infty$.

An example to introduce the problem

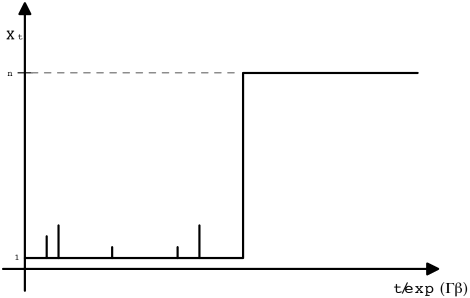
Random walk on $\mathcal{X} = \{1, ..., n\}$ reversible w.r.t. the following hamiltonians, i.e., with stationary measure $\pi(x) = \frac{e^{-\beta H(x)}}{Z}$:



Let $\delta = H(x) - H(x-1)$ for $x = 2, ..., n-1$ and define

$$p_x := P(x, x+1) = \frac{e^{-\delta\beta}}{1 + e^{-\delta\beta}}, \quad x = 1, .., n-1, \quad r_1 := P(1, 1) = 1-p_1,$$

$$q_x := P(x, x-1) = 1-p_x,\ x = 2, .., n-1, \quad q_n = \frac{e^{-\beta[H(n-1)-H(n)]}}{1 + e^{\delta\beta}},\ r_n = 1-q_n$$



For large β (similarly large n [Barrera,Bertoncini,Fernandez]): after many unsuccessful attempts there is a fast transition to n.

Metastability is characterized by:

- Exit from a well (valley) of H with a motion against the drift: large deviation regime.
- Many visits to the metastable state (bottom of the well, point 1 in the ex.) before the transition to the stable one (n), large tunneling time with exponential distribution if properly rescaled.
- The existence of critical configurations separating the metastable state from the stable one, ($n - 1$), first hitting to rare events.

Our goal

Metastability / first hitting to rare events is usually studied in the literature for reversible Markov chain.

Our goal: prove asymptotic exponential behavior in a non reversible context, when $|\mathcal{X}| \to \infty$.

Example:
deck of n cards, $|\mathcal{X}| = n!$
Markov chain: top-in-at-random shuffling
invariant maesure = uniform distribution
first hitting to a particular configuration G.

- non reversible case
- entropic barrier

People:

The *"first hitting"* community:

[K]	Keilson (1979) *(FM)*
[AB], [B]	Aldous, Brown (1982-92)...
	Day (1983), Galves, Schmitt (1990),
[IMcD]	Iscoe, McDonald (1994),
	Asselah, Dai Pra (1997), Abadi, Galves (2001)...
[FL]	Fill, Lyzinski (2012)
...	

The *"metastable"* community:

[LP]	Lebowitz, Penrose (1966) *(FM)*
[FW]	Freidlin, Wentzell (1984) *(FM)*
[CGOV]	Cassandro, Galves, Olivieri, Vares (1984)
[it]	Martinelli, Olivieri, S. (1989)...
[fr]	Catoni, Cerf (1995)...
[B.et al]	Bovier, Eckhoff, Gayrard, Klein (2001)...
[BL]	Bertrand, Landim (2011/12)
[BG]	Bianchi, Gaudillière (2012)
...	

(FM) = founding member

-2- Known results and tools: first hitting community

The model: $X_t;\ t \geq 0$ irreducible, finite-state, reversible Markov chain in continuous time, with transition rate matrix Q and stationary distribution π, so that $\pi Q = 0$ and

$$DBC : \pi_i Q_{ij} = \pi_j Q_{ji}$$

$$P = \mathbb{1} + Q$$

$0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq ...$ real eigenvalues of the matrix $-Q$,
$R = 1/\lambda_1$: relaxation time of the chain.
If the set A is such that $R/\mathbb{E}_\pi \tau_A$ is small then is possible [AB] to obtain estimate like :

$$|\mathbb{P}_\pi(\tau_A/\mathbb{E}_\pi \tau_A > t) - e^{-t}| \leq \frac{R/\mathbb{E}_\pi \tau_A}{1 + R/\mathbb{E}_\pi \tau_A} \qquad \forall t > 0 \tag{1}$$

$$\mathbb{P}_\pi(\tau_A > t) \geq (1 - \frac{R}{\mathbb{E}_\alpha \tau_A}) \exp\{-\frac{t}{\mathbb{E}_\alpha \tau_A}\} \tag{2}$$

Moreover in the regime $R \ll t \ll \mathbb{E}_\pi \tau_A$ bounds on the density function are given [AB] in order to obtain a control on the distribution of τ_A also on scale smaller than $\mathbb{E}_\pi \tau_A$.

Results by metastability community

$(\mathcal{X}^{(n)},\ n \geq 1)$ sequence of finite state spaces, with $|\mathcal{X}^{(n)}| = n$
$\left(X_t^{(n)}\right)_{t\in\mathbb{R}}$ sequence of continuous time, irreducible, reversible Markov chains on $\mathcal{X}^{(n)}$
$Q^{(n)}$ transition rate matrix generating the chain $X_t^{(n)}$
$(\pi^{(n)},\ n \geq 1)$ invariant measures
asymptotics $n \to \infty$.
starting at $x \in \mathcal{X}^{(n)}$, and the hitting time to a set $G^{(n)} \subset \mathcal{X}^{(n)}$:

$$\tau_{G^{(n)}}^{(n),x} = \inf\left\{t \geq 0 :\ X_t^{(n),x} \in G^{(n)}\right\} \tag{3}$$

$x_0^{(n)} \in \mathcal{X}^{(n)}$ = metastable state
$G^{(n)} \subset \mathcal{X}^{(n)}$ = critical configurations (or stable state)

$$\frac{\tau_{G^{(n)}}^{x_0^{(n)}}}{\mathbb{E}\tau_{G^{(n)}}^{x_0^{(n)}}} \xrightarrow[n\to\infty]{(d)} Y \sim Exp(1)$$

Hypotheses for metastability

i) pathwise approach: ([CGOV], [it], [fr])

recurrence to $x_0^{(n)}$ in a time $R_n \ll \mathbb{E}\tau_{G^{(n)}}^{(n),x_0^{(n)}}$ with large probability.

ii) potential theoretical approach: ([B. et al], [BL])

$$Hp.A: \qquad \lim_{n\to\infty} n\rho_A(n) = 0 \tag{4}$$

$$Hp.B: \qquad \lim_{n\to\infty} \rho_B(n) = 0 \tag{5}$$

$$\rho_A(n) := \sup_{z\in\mathcal{X}^{(n)}\setminus\{x_0^{(n)},G^{(n)}\}} \frac{\mathbb{P}\left(\widetilde{\tau}_{G^{(n)}}^{(n),x_0^{(n)}} < \widetilde{\tau}_{x_0^{(n)}}^{(n),x_0^{(n)}}\right)}{\mathbb{P}\left(\widetilde{\tau}_{\{x_0^{(n)},G^{(n)}\}}^{(n),z} < \widetilde{\tau}_z^{(n),z}\right)}$$

$$\rho_B(n) := \sup_{z\in\mathcal{X}^{(n)}\setminus\{x_0^{(n)},G^{(n)}\}} \frac{\mathbb{E}\tau_{\{x_0^{(n)},G^{(n)}\}}^{(n),z}}{\mathbb{E}\tau_{G^{(n)}}^{(n),x_0^{(n)}}}\,.$$

$$\widetilde{\tau}_A^{(n),x} := \min\left\{t > 0 : X_t^{(n),x} \in A\right\}$$

Some tools (fh)

- collapsed chain technique: hitting to a single state $A \equiv j$ ([K], [AB])
- For reversible chains for each j, by using spectral representation and Laplace transform, τ_j^π is a geometric convolution of suitable i.i.d.r.v. W_i:

$$\tau_j^\pi = \sum_{i=1}^{N} W_i \tag{6}$$

with N a geometric random variable of parameter π_j, approximately exponential in the sup norm [B] when $\pi(j)$ is small.
- [FL] generalize (6) to non reversible chains under additional hypotheses.
- τ_j^π is completely monotone [K]:

$$\mathbb{P}_\pi(\tau_j > t) = \sum_{l=1}^{m} p_i \exp\{-\gamma_i t\} \tag{7}$$

with $p_i \geq 0$ and $0 < \gamma_1 < \gamma_2 < ... < \gamma_m$ the distinct eigenvalues of $-Q_j$. Complete monotonicity is a powerful tool and exponential behavior follows from it [AB].

- interlacing between eigenvalues of $-Q_j$ and $-Q$

$$0 = \lambda_0 < \gamma_1 \leq \lambda_1 \leq \gamma_2 \leq \lambda_2 \leq \dots$$

Canceling out common pairs of eigenvalues from the two spectra and renumbering them we obtain

$$0 = \lambda_0 < \gamma_1 < \lambda_1 < \gamma_2 < \lambda_2 < \dots < \gamma_m < \lambda_m$$

again by Laplace transform [B]

$$\tau_j^\pi \sim \sum_{i-1}^{m} Y_i$$

with

$$\mathbb{P}(Y_i > t) = \left(1 - \frac{\gamma_i}{\lambda_i}\right) e^{-\gamma_i t}, \qquad t > 0, \ i = 1, \dots, m$$

Moreover

$$\left(1 - \frac{\gamma_1}{\lambda_1}\right) e^{-\gamma_1 t} \leq \mathbb{P}_\pi(\tau_j > t) \leq (1 - \pi(j)) e^{-\gamma_1 t}.$$

- [IMcD] exponential behavior in the non reversible case under additional implicit hypotheses (related to auxiliary processes involved in the proof) by studying the smallest real eigenvalue of a suitable Dirichlet problem.

Some tools (m)

i) Different strategies in different regimes.
Freidlin Wentzell techniques, cycle decomposition, cycle paths...
In FW theory reversibility is not required, cycles and cycle path are easily defined in the reversible case.

ii) Spectral characteristic of the generator, tools from potential theory, variational principles,...

$$c(i,j) = \frac{1}{r(i,j)} = \pi_i P_{ij}$$

$$r(i,j) = r(j,i) \iff DBC$$

Extension to non reversible chains by Eckhoff (not published) (??)
[BL] non reversible case under additional implicit hypotheses, which are not easy to verify in the non reversible case.

-3-The non reversible case [FMNS1]

$(\mathcal{X}^{(n)}, n \geq 1)$ sequence of finite state spaces, with $|\mathcal{X}^{(n)}| = n$

$\left(X_t^{(n)}\right)_{t\in\mathbb{R}}$ continuous time, irreducible Markov chains on $\mathcal{X}^{(n)}$

$x_0^{(n)}$ = metastable state, $G^{(n)}$ = critical configurations (or stable state) in the following sense:

Hp.$G(T_n)$:

there exist sequences $r_n \to 0$ and $R_n \ll T_n$ such that

$$\sup_{x\in\mathcal{X}} \mathbb{P}\left(\tau^{(n),x}_{\{x_0^{(n)},G^{(n)}\}} > R_n\right) \leq r_n \, .$$

asymptotic results: the following are equivalent

$$\frac{\tau_{G^{(n)}}^{x_0^{(n)}}}{T_n} \xrightarrow[n\to\infty]{(d)} Y \sim Exp(1)$$

$$\exists\, \ell \geq 1, \xi < 1 \ : \ P\left(\tau_{G^{(n)}}^{(n),x_0^{(n)}} > \ell\, T_n\right) \leq \xi \text{ uniformly in } n$$

quantitative results:

$$|\mathbb{P}_x(\tau_G/\mathbb{E}_{x_0}\tau_G > t) - e^{-t}| \leq f\left(\frac{R}{E_{x_0}\tau_G}, r\right)$$

Comparison of hypotheses

[FMNS]

$$T_n^{LT} =$$

mean local time spent in $x_0^{(n)}$ before reaching $G^{(n)}$ starting from $x_0^{(n)}$

$$T_n^{Q^\xi} := \inf\left\{ t : \ \mathbb{P}\left(\tau_{G^{(n)}}^{(n),x_0^{(n)}} > t \right) \leq \xi \right\}$$

$$T_n^{E} = \mathbb{E}\left(\tau_{G^{(n)}}^{(n),x_0^{(n)}} \right)$$

The following implications hold:

$$Hp.A \implies Hp.G(T_n^{LT}) \implies Hp.G(T_n^{E}) \iff Hp.(T_n^{Q^\xi}) \iff Hp.B$$

for any $\xi < 1$. Furthermore, the missing implications are false.

-4-Recurrence as a robust tool

a) Factorization property:

If $S > R$ with

$$\sup_{x\in\mathcal{X}} \mathbb{P}\left(\tau^{x}_{\{x_0,G\}} > R\right) \;\leq\; r\;.$$

then for any $t, s > \frac{R}{S}$

$$\mathbb{P}\left(\tau^{x_0}_G > (t+s)S\right) \begin{array}{l} \geq \left[\mathbb{P}\left(\tau^{x_0}_G > tS + R\right) - r\right] \mathbb{P}\left(\tau^{x_0}_G > sS\right) \\ \leq \left[\mathbb{P}\left(\tau^{x_0}_G > tS - R\right) + r\right] \mathbb{P}\left(\tau^{x_0}_G > sS\right) \end{array}\;.$$

$$\tau(tS) = \inf\{T > tS;\; X_T \in \{x_0, G\}\}$$

$$\mathbb{P}(\tau(tS) - tS > R) \leq r$$

b) Control on $\mathbb{P}(\tau_G^{x_0} \leq tS \pm R)$

Let $S > R$ with

$$\sup_{x \in \mathcal{X}} \mathbb{P}\left(\tau^{x}_{\{x_0, G\}} > R\right) \leq r\,.$$

then

$$\mathbb{P}(\tau_G^{x_0} \leq S) \leq \mathbb{P}(\tau_G^{x_0} \leq S + R) \leq \mathbb{P}(\tau_G^{x_0} \leq S)\,[1 + a] \quad (8)$$

$$\mathbb{P}(\tau_G^{x_0} \leq S) \geq \mathbb{P}(\tau_G^{x_0} \leq S - R) \geq \mathbb{P}(\tau_G^{x_0} \leq S)\,[1 - a] \quad (9)$$

with

$$a = \frac{\mathbb{P}(\tau_G^{x_0} \leq 2R)}{\mathbb{P}(\tau_G^{x_0} \leq S)} + \frac{r}{\mathbb{P}(\tau_G^{x_0} \leq S)}\,. \quad (10)$$

This result is useful when $\mathbb{P}(\tau_G^{x_0} \leq 2R)$ and r are small w.r.t. $\mathbb{P}(\tau_G^{x_0} \leq S)$. In this case we can conclude that a is small and so we get a multiplicative error estimate.

c) Exponentian behavior

By iterating a) and b) we get the exponential law on a suitable time scale in the interval $(R, \mathbb{E}\tau_G^{x_0})$.
Let $T := \mathbb{E}\tau_G^{x_0}$ and $\varepsilon := \frac{R}{T}$

$$b \;=\; \mathbb{P}(\tau_G^{x_0} \leq 2R) + 2r. \tag{11}$$

If $\varepsilon + r < \frac{1}{4}$ and $S < T\Big(1 - 4(\varepsilon + r)\Big)$. Then $\mathbb{P}(\tau_G^{x_0} > S) > b$ and for each positive integer k

$$\mathbb{P}(\tau_G^{x_0} > kS) \begin{array}{l} \leq \left[\mathbb{P}(\tau_G^{x_0} > S) + b\right]^k \\ \geq \left[\mathbb{P}(\tau_G^{x_0} > S) - b\right]^k \end{array}$$

d) Generic starting point

By recurrence to $\{x_0, G\}$ we have for all $x \in B(x_0)$

$$\tau_G^x \sim \tau_G^{x_0}$$

Improvement of recurrence

These result are relevant only if r is small. It is possible to decrease exponentially r by increasing linearly $\varepsilon := \frac{R}{T}$ with $T = \mathbb{E}\tau_G^{x_0}$.
Let R be such that

$$\sup_{x \in \mathcal{X}} \mathbb{P}\left(\tau_{\{x_0,G\}}^{x} > R\right) \ \leq \ r \ .$$

and suppose $\varepsilon = \frac{R}{T}$ small.
We can chose another return time $R^+ \in (R, T)$ with $\Gamma := \frac{R^+}{R} < \frac{1}{\varepsilon}$.
Define $\varepsilon^+ := \frac{R^+}{T} = \varepsilon\Gamma < 1$. The recurrerce property in time R^+ is immediately estimate by the following

$$\sup_{x \in \mathcal{X}} \mathbb{P}(\tau_{\{x_0,G\}}^{x} > R^+) \leq r^{\frac{R^+}{R}} = r^{\Gamma} =: r^+ \qquad (12)$$

This meas that with this new recurrence time R^+ we have $\varepsilon^+ = \varepsilon\Gamma$ and $r^+ = r^{\Gamma}$.
From this we get a control on exponential behavior on small time scales

Time scale for exponential behavior

With this improvement of recurrence, if

$$\lim_{n\to\infty} \frac{(r_n)^{\frac{R_n^+}{R_n}}}{p_n} = 0 \,.$$

with

$$p_n := \mathbb{P}\left(\tau_{G^{(n)}}^{(n),x_0^{(n)}} < 3R_n^+\right) \to 0$$

and if S_n is such that $R_n^+ < S_n \leq T_n$, then $\tau_{G^{(n)}}^{(n),x_0^{(n)}}$ has asymptotic exponential behaviour at scale S_n i.e., for every integer k

$$\lim_{n\to\infty} \frac{\mathbb{P}\big(\tau_{G^{(n)}}^{(n),x_0^{(n)}} \in (kS_n, (k+1)S_n]\big)}{\mathbb{P}(\tau_{G^{(n)}}^{(n),x_0^{(n)}} > S_n)^k \; \mathbb{P}(\tau_{G^{(n)}}^{(n),x_0^{(n)}} \leq S_n)} = 1$$

Recurrence on a set instead of on a single state x_0 [FMNS2]

Work in progress.

Back to the example: deck of n cards, top-in-at-random. First hitting to a particular configuration G.

- mixing time of order $T_{mix} = n \log n \Longrightarrow$ recurrence with large probability to a suitable set B of configurations such that:
  - B is "large" : $\pi(B) > 1 - o_n(1)$;
  - τ_G^x is controlled uniformely in B:

$$\sup_{x \in B} \mathbb{P}(\tau_G^x < T_{mix}) \leq f_n \to 0.$$

- recurrence in $B \Longrightarrow$ asymptotic exponential behavior.