Fluid limit-based tuning of some hybrid MCMC samplers

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We introduce

- a transformation of the Markov chain $\longrightarrow$ continuous time process
- such that the *stability* of this process, is related to the ergodicity of the Markov chain.

When applied to MCMC,

- the dynamic of this transformation depends upon the design parameters of the algorithm ;
- $\Rightarrow$ learn from the dynamic, how to tune the design parameters.

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$\hookrightarrow$ Outline of the talk

Fluid Limit : definition (I)

Let $\{\Phi_k, k \geq 0\}$ be a Markov chain, on X (X $= \mathbb{R}^d$).

$\hookrightarrow$ Family of rescaled process η_r, for $r > 0$

(i) in the initial point : $\eta_r(0; x) = \frac{1}{r}\Phi_0 = x, \qquad \Phi_0 = rx$

(ii) in time and space : $\eta_r(t; x) = \frac{1}{r}\Phi_{\lfloor tr \rfloor}$

i.e. $\eta_r(\cdot; x) = \dfrac{1}{r}\Phi_k$ on $\left[\dfrac{k}{r}; \dfrac{(k+1)}{r}\right)$.

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$$\text{i.e.} \quad \eta_r(\cdot; x) = \frac{1}{r}\Phi_k \qquad \text{on } \left[\frac{k}{r}; \frac{(k+1)}{r}\right).$$

$\hookrightarrow$ Distributions

- $\mathbb{P}_x$: distribution of $\{\Phi_k, k \geq 0\}$ with initial distribution δ_x.
- $\mathbb{Q}_{r;x}$: image prob. of $\mathbb{P}_{rx}$ by η_r,

  prob. on $\mathbb{D}(\mathbb{R}^+, \mathsf{X})$ the space of cad-lag functions $\mathbb{R}^+ \to \mathsf{X}$

Fluid Limit : definition (II)

$\hookrightarrow$ Definition $\mathbb{Q}_x$ probability on $\mathbb{D}(\mathbb{R}^+, \mathsf{X})$ - for $x \in \mathsf{X}$, is a fluid limit if there exist scaling factors $r_n \to +\infty$ such that

$$\mathbb{Q}_{r_n;x} \text{ converges weakly to } \mathbb{Q}_x.$$

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$\hookrightarrow$ Existence

$$\begin{aligned}
\Phi_{k+1} &= \Phi_k + \mathbb{E}\left[\Phi_{k+1}|\mathcal{F}_k\right] - \Phi_k + \Phi_{k+1} - \mathbb{E}\left[\Phi_{k+1}|\mathcal{F}_k\right] \\
&= \Phi_k + \underbrace{\mathbb{E}_x\left[\Phi_{k+1} - \Phi_k|\mathcal{F}_k\right]}_{\Delta(\Phi_k)} + \underbrace{\left(\Phi_{k+1} - \mathbb{E}_x\left[\Phi_{k+1}|\mathcal{F}_k\right]\right)}_{\epsilon_{k+1} \quad \text{martingale increment}}.
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▶ Result (Fort et al, 2007)

If

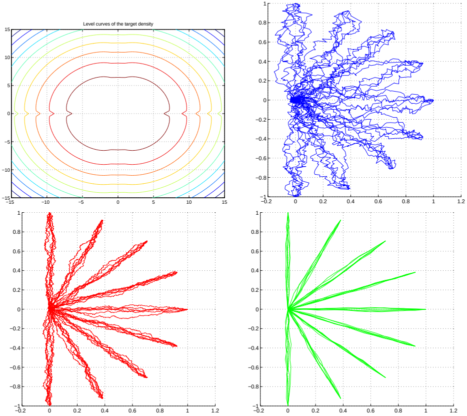
- $\exists p > 1, \quad \lim_{K\to+\infty} \quad \sup_{x\in\mathsf{X}} \mathbb{E}_x\left[|\epsilon_1|^p \mathbb{1}_{|\epsilon_1|>K}\right] \to 0.$
- $0 < \sup_{x\in\mathsf{X}} |\Delta(x)| < \infty.$

Then

- $\forall x, r_n \to +\infty$, $\exists$ subsequ. $\{r_{n_j}\}$ s.t. $\mathbb{Q}_{r_{n_j};x} \Rightarrow \mathbb{Q}_x$
- $\mathbb{Q}_x$ prob. on the space of continuous functions.

Ex. : Plot of $\eta_r(\cdot, x)$ on $[0, T]$, for diff. x on the unit sphere

- Random Walk Hastings-Metropolis on $\mathbb{R}^2$
- Target distribution $\pi(x_1, x_2) \propto (1 + x_1^2 + x_2^2 + x_1^8 x_2^2) \exp(-(x_1^2 + x_2^2))$
- Gaussian proposal : $q \sim \mathcal{N}_2(0, 4\mathbb{I})$



Level curves of π and r=100, r=1000, r=5000

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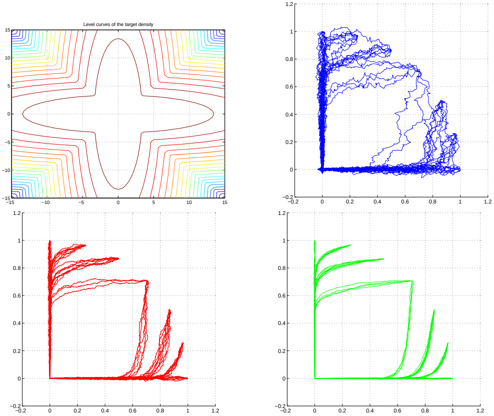
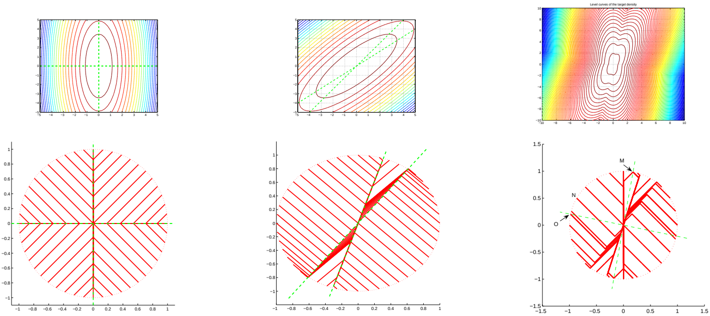


Level curves of π and r=100, r=1000, r=5000

Ex. : Draws from $\mathbb{Q}_x$ for diff. x on the unit sphere

- Metropolis within Gibbs on $\mathbb{R}^2$
- Target distribution $\pi =$ (mixture of) $\mathcal{N}_2$
- Gaussian proposal : $q_i \sim \mathcal{N}(0, c)$ and $\omega_i = 0.5$.



Level curves of π and realizations of the fluid limit

Existence (I)

$$\Phi_{k+1} = \Phi_k + \mathbb{E}[\Phi_{k+1} - \Phi_k | \mathcal{F}_k] + \epsilon_{k+1} = \Phi_k + \Delta(\Phi_k) + \epsilon_{k+1}.$$

$\hookrightarrow$ Sufficient conditions :

- $\exists p > 1, \qquad \lim_{K \to +\infty} \quad \sup_{x \in \mathsf{X}} \mathbb{E}_x \left[|\epsilon_1|^p \mathbb{1}_{|\epsilon_1| > K} \right] \to 0.$
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↪ Extension :

- $\exists \beta \in [0, 1 \wedge (p-1)[, \quad 0 < \sup_{x \in \mathsf{X}} |x|^\beta \; |\Delta(x)| < \infty.$

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↪ Extension :

- $\exists \beta \in [0, 1 \wedge (p-1)[, \qquad 0 < \sup_{x \in \mathsf{X}} |x|^\beta \; |\Delta(x)| < \infty.$

In that case, change the definition of the re-scaled process :

$$\eta_{r,\beta}(t;x) = \frac{\Phi_{\lfloor t r^{1+\beta} \rfloor}}{r} \qquad \eta_{r,\beta}(0;x) = x.$$

$\hookrightarrow$ Example : RWHM chains

$$\Phi_{k+1} = \Phi_k + \mathbb{E}[\Phi_{k+1} - \Phi_k | \mathcal{F}_k] + \epsilon_{k+1} = \Phi_k + \Delta(\Phi_k) + \epsilon_{k+1}.$$

- $\mathbb{E}\left[|\epsilon_{k+1}|^p\right] \longleftrightarrow \mathbb{E}\left[|\Phi_{k+1} - \Phi_k|^p\right]$:
  p-moment of the proposal distribution q.

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- Since

$$\Delta(x) = \int_{\{y, \pi(x+y) < \pi(x)\}} y \left(\frac{\pi(x+y)}{\pi(x)} - 1 \right) q(y) dy,$$

$\beta = 0$, and p-moment of the proposal distribution q.

Stability

$\hookrightarrow$ Stable fluid limit model : if there exist $T > 0$ and $\rho < 1$ s.t. for any x on the unit sphere,

$$\mathbb{Q}_x \left(\eta \in \mathbb{D}(\mathbb{R}^+, \mathsf{X}), \inf_{[0,T]} |\eta(t)| \leq \rho \right) = 1.$$

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▶ Result (Fort et al, 2007)

If

- $\{\Phi_k, k \geq 0\}$ is phi-ireducible and aperiodic ; and compact sets are petite.
- fluid limit model exists and is stable,

Then the Markov chain is (f, r)-ergodic

$$(n+1)^{q-1} \sup_{\{f, |f| \leq 1 + |x|^{p-q}\}} |\mathbb{E}_x[f(\Phi_n)] - \pi(f)| \longrightarrow_{n \to +\infty} 0, \qquad 1 \leq q \leq p.$$

Characterisation : case 1

- If
  - $\exists \;\; h$ continuous s.t. for any compact set H of X $\setminus \{0\}$,
    $$\lim_{r \to +\infty} \sup_{x \in \mathsf{H}} |\Delta(rx) - h(x)| = 0.$$
  - the ODE $\dot{\mu} = h(\mu)$ is stable.

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- Example : RWHM

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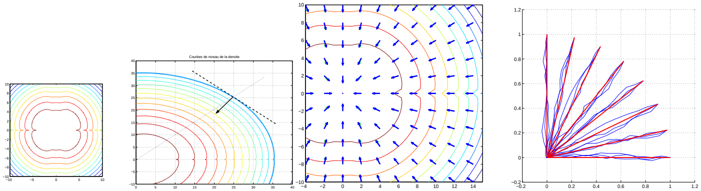

Level curves of π and Rejection area and the fields Δ, h and realizations of the fluid limit

Characterisation : case 2a

- If
  - $\exists\ h$ continuous s.t. for any compact set H of cone of X $\setminus \{0\}$,
$$\lim_{r \to +\infty} \sup_{x \in \mathsf{H}} |\Delta(rx) - h(x)| = 0.$$
  - the ODE $\dot{\mu} = h(\mu)$ started in the cone is stable.
  - the cone is " attractive".

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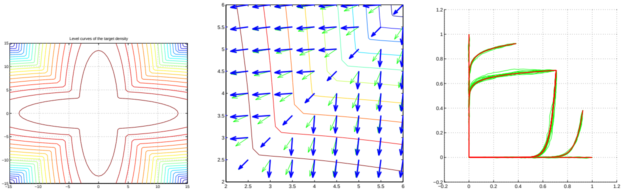
- Example : RWHM



Level curves of π and the fields Δ, h and realizations of the fluid limit

Characterisation : case 2b $(\mathsf{X} = \mathbb{R}^2)$

-
  - $\mathsf{X} = \bigcup_{\alpha=1}^{a} \mathsf{O}_\alpha \cup \bigcup_{\beta=1}^{b} \{x, f'_\beta x = 0\}$.
  - $\exists \ \Sigma_\alpha$ s.t. for any compact set H of O_α,

$$\lim_{r \to +\infty} \sup_{x \in \mathsf{H}} |\Delta(rx) - \Sigma_\alpha| = 0.$$

  - "attractive" hyperplanes.

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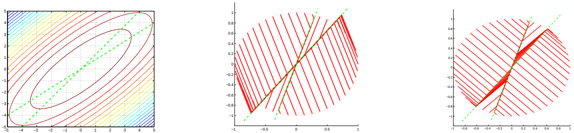
- Example : RW Metropolis within Gibbs



Level curves of π and fluid limits when $\omega_1 = 0.25$ and fluid limits when $\omega_1 = 0.5$

Characterisation : Conclusion / Perspectives

- Characterisation based on the radial behavior of $\Delta(x) = \mathbb{E}_x[\Phi_1 - \Phi_0]$,

$$\lim_{r \to +\infty} \sup_{x \in \mathsf{H}} |\Delta(rx) - h(x)| = 0,$$

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- Deterministic fluid limit more or less everywhere since

$$\eta_{r,\beta}(t;x) = \frac{\Phi_{\lfloor tr^{1+\beta} \rfloor}}{r} \qquad \eta_{r,\beta}(0;x) = x,$$

with $0 \leq \beta < 1$.

When $\beta = 1 \longrightarrow$ diffusion (work in progress, M. Bédart and E. Moulines).

The design parameters

$\hookrightarrow$ At each iteration,

- Choose a component $i \in \{1, \cdots, d\}$ with probability ω_i.
- Update the i-th component with a RW move, with distribution q_i.

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$\hookrightarrow$ Design parameters when Gaussian proposal

- Selection weights : $\omega_1, \cdots, \omega_d$.
- Variances of the Gaussian proposals : $\sigma_1^2, \cdots, \sigma_d^2$.

Radial behavior of Δ (I)

$$\Delta_i(x) = \omega_i \int_{\{y \in \mathbb{R}, \pi(x+ye_i)<\pi(x)\}} y \left(\frac{\pi(x+ye_i)}{\pi(x)} - 1 \right) q_i(y)\, dy.$$

$\hookrightarrow$ For the target densities π in the class

- $\lim_{r \to +\infty} |\nabla \ln \pi(rx)| = +\infty$.
- ℓ given by $\lim_{r \to +\infty} \frac{\nabla \ln \pi(rx)}{|\nabla \ln \pi(rx)|} = \ell(x)$ is continuous.

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$\hookrightarrow$ As $r \to +\infty$

$$\Delta_i(rx) \longrightarrow \text{sign}(\ell_i(x))\, \omega_i \int_{\mathbb{R}+} y q_i(y) dy = \text{sign}(\ell_i(x))\, \frac{\omega_i\ \sigma_i}{\sqrt{2\pi}}.$$

Radial behavior of Δ (II)

$$\Delta_i(rx) \longrightarrow \mathrm{sign}(\ell_i(x)) \, \frac{\omega_i \, \sigma_i}{\sqrt{2\pi}}.$$

$\hookrightarrow$ This implies

- The radial limit depends upon the design parameters through the product $\omega_i\sigma_i$.
- The radial limit is constant on the sets

$$\mathsf{O}_\alpha = \{x, \mathrm{sign}(\ell(x)) = \gamma_\alpha\}$$

where $\gamma_\alpha \in \{-1, 1\}^d$.

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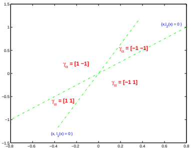
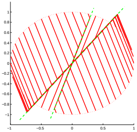
$\hookrightarrow$ Example : RW MwG, $\pi \sim \mathcal{N}_2(0, \Gamma)$ $\Longrightarrow \ell(x) = -\frac{\Gamma^{-1}x}{|\Gamma^{-1}x|}$.





Piecewise Linear Fluid limits

$\hookrightarrow$ Linear till the first time it reaches $\partial[\cup_{\alpha=1}^{a} \mathsf{O}_\alpha]$

- $\forall x \in \mathsf{O}_\alpha$,

$$\forall t \leq T(x) \qquad \eta(t) = x + t \;\; \gamma_\alpha \circ \omega \circ \sigma, \qquad \mathbb{Q}_x - \text{a.s.}$$

where $T(x)$: hitting-time of $\partial \mathsf{O}_\alpha$.

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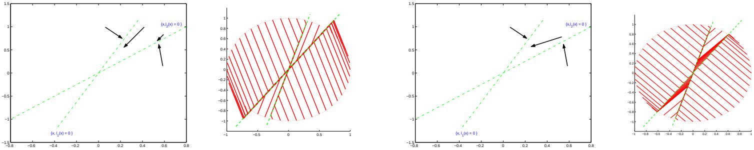
$\hookrightarrow$ Attractive boundaries (Results in the case : $d = 2$ and boundaries are hyperplanes)

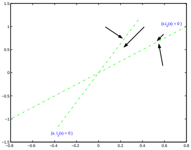
- If the reached boundary is "attractive", the fluid limit is trapped on the boundary.
- Example : RW MwG, $\pi \sim \mathcal{N}_2(0, \Gamma)$

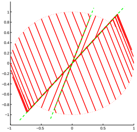


Stability of the fluid limit

$\hookrightarrow$ Stable attractive boundaries (Results in the case : $d = 2$ and boundaries are hyperplanes)

▶ The fields in the neighborhood of the boundaries, "point" towards the origin.





▶ Example : RW MwG, $\pi \sim \mathcal{N}_2(0, \Gamma)$.
Any attractive boundary is stable.

Adaptive strategies : state-dependent design parameters

Since the fluid limit depends upon the design parameters through $\omega_i \sigma_i$,

Strategy 1. Fix $\omega_i = 1/d$ and choose $\sigma_i(x)$.

Strategy 2. Fix $\sigma_i = c$ and choose $\omega_i(x)$.

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Choose

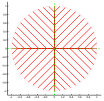
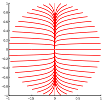
$$[\omega_i \sigma_i](x) = c\,|\ell_i(x)| \qquad \ell_i(x) = \lim_r \frac{\nabla_i \ln \pi(rx)}{|\nabla \ln \pi(rx)|}.$$

so that in both strategies, the fluid limit $\longleftrightarrow$ ODE $\dot{\mu} = h(\mu)$ with

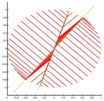
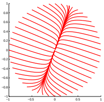
$$h(x) = \frac{c}{\sqrt{2\pi}}\,\ell(x) \qquad \ell_i(x) = \lim_r \frac{\nabla_i \ln \pi(rx)}{|\nabla \ln \pi(rx)|}.$$

Ex. : Fluid limits [left] non-adaptive [right] adaptive

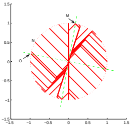
- When $\pi \sim \mathcal{N}_2(0, \Gamma_1)$ Γ_1 diagonal

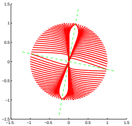



- When $\pi \sim \mathcal{N}_2(0, \Gamma_2)$ Γ_2 non-diagonal

- When $\pi \sim \mathcal{N}_2(0, \Gamma_1) + \mathcal{N}_2(0, \Gamma_2)$





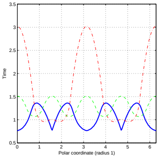
Assessing efficiency (I)

$\hookrightarrow$ Criterion 1 : Based on the Limit fluid and on the time the fluid limit started on the unit sphere, enters a ball of radius $\rho \in]0, 1[$.

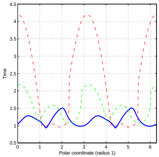
▶ Example

x-axes : polar coordinate of the initial value.
y-axes : hitting-time.

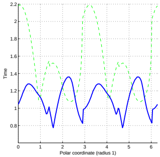
for the three algorithms Adaptive strategy Non-Adaptive, $\omega_1 = 0.25$ Non-Adaptive, $\omega_1 = 0.5$



$\pi \sim \mathcal{N}_2(0, \Gamma_1)$ Γ_1 diagonal



$\pi \sim \mathcal{N}_2(0, \Gamma_2)$ Γ_2 non diagonal



$\pi \sim \mathcal{N}_2(0, \Gamma_1) + \mathcal{N}_2(0, \Gamma_2)$

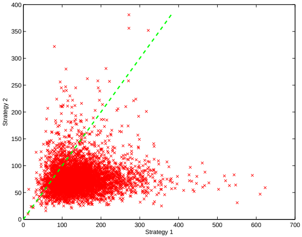
Assessing efficiency (II)

↪ Criterion 2 : Based on the Markov chain and the hitting-time of the "center of the space" when started "far" from the center.

▶ Example : $\pi \sim \mathcal{N}_8(0, \Gamma) \qquad d = 8$

Γ : diagonal, with entries $\Gamma_{i,i} \sim \mathcal{E}(1)$.
5000 adaptive chains, started from $x \in \{z'\Gamma^{-1}z = d\}$.

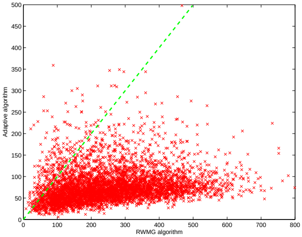
x-axes : hitting-time of the ball of radius $\sqrt{d}$ with the Strat 1 (adapt σ)
y-axes : hitting-time of the ball of radius $\sqrt{d}$ with the Strat 2 (adapt ω)



▶ Example : $\pi \sim \mathcal{N}_8(0, \Gamma)$ $d = 8$

Γ : diagonal, with entries $\Gamma_{i,i} \sim \mathcal{E}(1)$.
5000 adaptive chains, started from $x \in \{z'\Gamma^{-1}z = d\}$.

x-axes : hitting-time of the ball of radius $\sqrt{d}$ with the non-adaptive strategy
y-axes : hitting-time of the ball of radius $\sqrt{d}$ with the Strat 2 (adapt ω)



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3. Based on the fluid limit, modify the chain
   3.1 state-dependent procedures more efficient.
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Talk based on the papers

- G. Fort, S. Meyn, E. Moulines and P. Priouret. `The ODE method for the stability of skip-free Markov Chains with applications to MCMC`. To be published, Ann. Appl. Probab. (2007)
- G. Fort. `Fluid limit-based tuning of some hybrid MCMC samplers`. Submitted (2007).