

Adaptive Restore algorithm & Importance Monte Carlo

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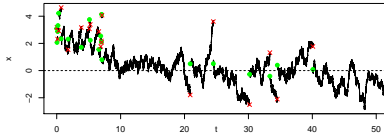
ERCall for applications

Ongoing 2023-2030 ERC funding for PhD and postdoctoral collaborations with

- ▶ Michael Jordan (Berkeley)
- ▶ Eric Moulines (Paris)
- ▶ Gareth O Roberts (Warwick)
- ▶ myself (Paris)



Part I: Adaptive Restore algorithm



Joint work with H McKimm, A Wang, M Pollock,
and GO Roberts
arXiv:2210.09901 – Bernoulli

MCMC regeneration

Reversibility attached with (sub-efficient) random walk behaviour

Recent achievements in **non-reversible MCMC with PDMPs**

[Bouchard-Côté et al., 2018; Bierkens et al., 2019]

Link with regeneration

[Nummelin, 1978; Mykland et al., X, 1995]

At **regeneration times**, Markov chain starts again: future independent of past

Scales poorly: regenerations recede exponentially with dimension

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PDMP: Marketing arguments

Current (?) default workhorse: reversible MCMC methods
(incl. NUTS)

[Hoffman & Gelman, 2014]

Non-reversible MCMC algorithms based on piecewise
deterministic Markov processes (aka PDMP) perform well
empirically

PDMP: Marketing arguments

Non-reversible MCMC algorithms based on piecewise deterministic Markov processes (aka PDMP) perform well empirically

Quantitative convergence rates and variance now available

- ▶ Physics origins

[Peters & De With, 2012; Krauth et al., 2009, 15, 16]

- ▶ geometric ergodicity for exponentially decaying tail target

[Mesquita & Hespanha, 2010]

- ▶ ergodicity targets on the real line

[Bierkens et al., 2016a,b]

Piecewise deterministic Markov process

PDMP sampler is a continuous-time, non-reversible, MCMC, method based on auxiliary variables

1. empirically state-of-the-art performances

[Bouchard et al., 2017]

2. exact subsampling for big data

[Bierkens et al., 2017]

3. geometric ergodicity for large class of distribution

[Deligiannidis et al., 2017]

4. Ability to deal with intractable potential

$$\log \pi(\mathbf{x}) = \int \mathbf{U}_\omega(\mathbf{x}) \mu(d\omega)$$

[Pakman et al., 2016]

Piecewise deterministic Markov process

Piecewise deterministic Markov process $\{z_t \in \mathcal{Z}\}_{t \in [0, \infty)}$, with three ingredients,

1. **Deterministic dynamics:** between events, deterministic evolution based on ODE

$$dz_t/dt = \Phi(z_t)$$

2. **Event occurrence rate:** $\lambda(t) = \lambda(z_t)$
3. **Transition dynamics:** At event time, τ , state prior to τ denoted by $z_{\tau-}$, and new state generated by $z_\tau \sim Q(\cdot | z_{\tau-})$.

[Davis, 1984, 1993]

Implementation hardships

Main difficulties of implementing PDMP come from

1. Computing the ODE flow Ψ : linear dynamic, quadratic dynamic
2. Simulating the inter-event time η_k : many techniques of superposition and thinning for Poisson processes

[Devroye, 1986]

Simulation by superposition plus thinning

Most implementations thru discrete-time schemes by sampling Bernoulli $B(\alpha(z))$

For

$$\Phi(z) = (x + v\varepsilon, v) \quad \text{and} \quad \alpha(z) = 1 \wedge \pi(x + v\varepsilon)/\pi(x)$$

sampling inter-event time for strictly convex $U(\cdot)$ obtained by solving

$$t^* = \arg \min_t U(x + vt)$$

and additional randomization

- ▶ **thinning**: if there exists $\bar{\alpha}$ such that $\alpha(\Phi(z)) \geq \bar{\alpha}(x, k)$, accept-reject
- ▶ **superposition and thinning**: when $\alpha(z) = 1 \wedge \rho(\Phi(z))/\rho(z)$ and $\rho(\cdot) = \prod_i \rho_i(\cdot)$ then $\bar{\alpha}(z, k) = \prod_i \bar{\alpha}_i(z, k)$

[Bouchard et al., 2017]

Restore process

Take $\{Y_t\}_{t \geq 0}$ diffusion / jump process on \mathbb{R}^d with infinitesimal generator \bar{L}_Y and $Y_0 \sim \mu$

Regeneration rate κ with associated tour length

$$\tau = \inf \left\{ t \geq 0 : \int_0^t \kappa(Y_s) ds \geq \xi \right\} \text{ with } \xi \sim \text{Exp}(1)$$

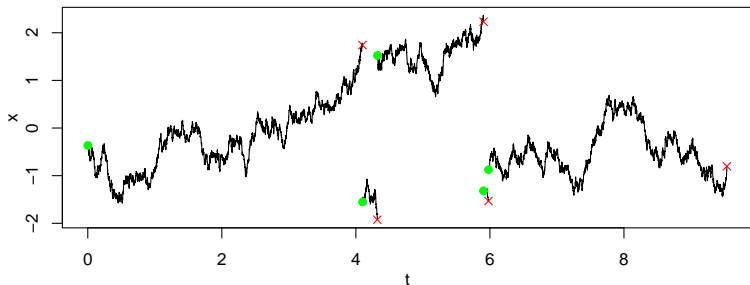
$(\{Y_t^{(i)}\}_{t \geq 0}, \tau^{(i)})_{i=0}^{\infty}$ iid realisations inducing regeneration times

$$T_j = \sum_{i=0}^{j-1} \tau^{(i)}$$

Restore process $\{X_t\}_{t \geq 0}$ given by:

$$X_t = \sum_{i=0}^{\infty} \mathbb{I}_{[T_i, T_{i+1})}(t) Y_{t-T_i}^{(i)}$$

Restore process



Path of five tours of Brownian Restore with $\pi \equiv \mathcal{N}(0, 1^2)$, $\mu \equiv \mathcal{N}(0, 2^2)$ and C such that $\min_{x \in \mathbb{R}} \kappa(x) = 0$, with $\mathcal{K} = 200$ and $\Lambda_0 = 1000$. First and last output states shown by green dots and red crosses

Stationarity of Restore

Infinitesimal generator of $\{X_t\}_{t \geq 0}$

$$L_X f(x) = L_Y f(x) + \kappa(x) \int [f(y) - f(x)] \mu(y) dy$$

with adjoint L_Y^\dagger

Regeneration rate κ chosen as

$$\kappa(x) = L_Y^\dagger \pi(x) / \pi(x) + C \mu(x) / \pi(x)$$

Implies $\{X_t\}_{t \geq 0}$ is π -invariant

$$\int_{\mathbb{R}^d} L_X f(x) \pi(x) dx = 0$$

Restore sampler

Rewrite

$$\kappa(\mathbf{x}) = \frac{L_Y^\dagger \pi(\mathbf{x})}{\pi(\mathbf{x})} + C \frac{\mu(\mathbf{x})}{\pi(\mathbf{x})} = \tilde{\kappa}(\mathbf{x}) + C \frac{\mu(\mathbf{x})}{\pi(\mathbf{x})}$$

with

- ▶ $\tilde{\kappa}$ partial regeneration rate
- ▶ $C > 0$ regeneration constant and
- ▶ $C\mu$ regeneration measure, large enough for $\kappa(\cdot) > 0$

Resulting Monte Carlo method called **Restore Sampler**

[Wang et al., 2021]

Restore sampler convergence

Given π -invariance of $\{X_t\}_{t \geq 0}$, Monte Carlo validation follows:

$$\mathbb{E}_\pi[f] = \mathbb{E}_{X_0 \sim \mu} \left[\int_0^{\tau^{(0)}} f(X_s) dx \right] / \mathbb{E}_{X_0 \sim \mu}[\tau^{(0)}] \quad (1)$$

and a.s. convergence of ergodic averages:

$$\frac{1}{t} \int_0^t f(X_s) ds \rightarrow \mathbb{E}_\pi[f] \quad (2)$$

For iid $Z_i := \int_{T_i}^{T_{i+1}} f(X_s) ds$, CLT

$$\sqrt{n} \left(\int_0^{T_n} f(X_s) dx / T_n - \mathbb{E}_\pi[f] \right) \rightarrow \mathcal{N}(0, \sigma_f^2) \quad (3)$$

where

$$\sigma_f^2 := \mathbb{E}_{X_0 \sim \mu} \left[\left(Z_0 - \tau^{(0)} \mathbb{E}_\pi[f] \right)^2 \right] / \left(\mathbb{E}_{X_0 \sim \mu}[\tau^{(0)}] \right)^2$$

Restore sampler convergence

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and a.s. convergence of ergodic averages:

$$\frac{1}{t} \int_0^t f(X_s) ds \rightarrow \mathbb{E}_\pi[f] \quad (2)$$

Estimator variance depends on expected tour length: prefer μ favouring long tours

[Wang et al., 2020]

Minimal regeneration

Minimal regeneration measure, $C^+ \mu^+$ corresponding to smallest possible rate

$$\kappa^+(x) := \tilde{\kappa}(x) \vee 0 = \tilde{\kappa}(x) + C^+ \mu^+(x) / \pi(x)$$

leading to

$$\mu^+(x) = \frac{1}{C^+} [0 \vee -\tilde{\kappa}(x)] \pi(x)$$

Frequent regeneration not necessarily detrimental, except when when μ is not well-aligned to π , leading to wasted computation

"Minimal Restore" maximizes expected tour length / minimizes asymptotic variance

[Wang et al., 2021]

Constant approximation

When target π lacks its normalizing constant Z

$$\pi(\mathbf{x}) = \tilde{\pi}(\mathbf{x})/Z,$$

take **energy** $\mathbf{U}(\mathbf{x}) := -\log \pi(\mathbf{x}) = \log Z - \log \tilde{\pi}(\mathbf{x})$

E.g., when $\{Y_t\}_{t \geq 0}$ Brownian, $\tilde{\kappa}$ function of $\nabla \mathbf{U}(\mathbf{x})$ and $\Delta \mathbf{U}(\mathbf{x})$

$$\tilde{\kappa}(\mathbf{x}) := \frac{1}{2} \left(\|\nabla \mathbf{U}(\mathbf{x})\|^2 - \Delta \mathbf{U}(\mathbf{x}) \right)$$

Constant approximation

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In regeneration rate, Z absorbed into C

$$\kappa(\mathbf{x}) = \tilde{\kappa}(\mathbf{x}) + C \frac{\mu(\mathbf{x})}{(\tilde{\pi}(\mathbf{x})/Z)} = \tilde{\kappa}(\mathbf{x}) + CZ \frac{\mu(\mathbf{x})}{\tilde{\pi}(\mathbf{x})} = \tilde{\kappa}(\mathbf{x}) + \tilde{C} \frac{\mu(\mathbf{x})}{\tilde{\pi}(\mathbf{x})}$$

where $\tilde{C} = CZ$ **set by user**. Since

$$C = 1/\mathbb{E}_{\mu}[\tau],$$

using n tours with simulation time T ,

$$Z \approx \tilde{C}T/n$$

Adapting Restore

Adaptive Restore process defined by enriching underlying continuous-time Markov process with regenerations at rate κ^+ from distribution μ_t at time t

Convergence of (μ_t, π_t) to (μ^+, π) : a.s. convergence of stochastic approximation algorithms for discrete-time processes on compact spaces

[Benaïm et al., 2018; McKimm et al., 2024]

Adapting Restore

Initial regeneration distribution μ_0 and updates by addition of point masses

$$\mu_t(x) = \begin{cases} \mu_0(x), & \text{if } N(t) = 0, \\ \frac{t}{a+t} \frac{1}{N(t)} \sum_{i=1}^{N(t)} \delta_{X_{\zeta_i}}(x) + \frac{a}{a+t} \mu_0(x), & \text{if } N(t) > 0, \end{cases}$$

where $a > 0$ constant and ζ_i arrival times of inhomogeneous Poisson process $(N(t) : t \geq 0)$ with rate $\kappa^-(X_t)$

$$\kappa^-(x) := [0 \vee -\tilde{\kappa}(x)]$$

Poisson process simulated by Poisson thinning, under (strong) assumption

$$K^- := \sup_{x \in \mathcal{X}} \kappa^-(x) > 0$$

Adaptive Brownian Restore Algorithm

$t \leftarrow 0, E \leftarrow \emptyset, i \leftarrow 0, X \sim \mu_0.$

while $i < n$ **do**

$\tilde{\tau} \sim \text{Exp}(K^+), s \sim \text{Exp}(\Lambda_0), \tilde{\zeta} \sim \text{Exp}(K^-).$

if $\tilde{\tau} < s$ **and** $\tilde{\tau} < \tilde{\zeta}$ **then**

$X \sim \mathcal{N}(X, \tilde{\tau}), t \leftarrow t + \tilde{\tau}, u \sim \mathcal{U}[0, 1].$

if $u < \kappa^+(X)/K^+$ **then**

if $|E| = 0$ **then**

$X \sim \mu_0.$

else

$X \sim \mathcal{U}(E)$ with probability $t/(a + t)$, **else** $X \sim \mu_0.$

end

$i \leftarrow i + 1.$

end

else if $s < \tilde{\tau}$ **and** $s < \tilde{\zeta}$ **then**

$X \sim \mathcal{N}(X, s), t \leftarrow t + s,$ record $X, t, i.$

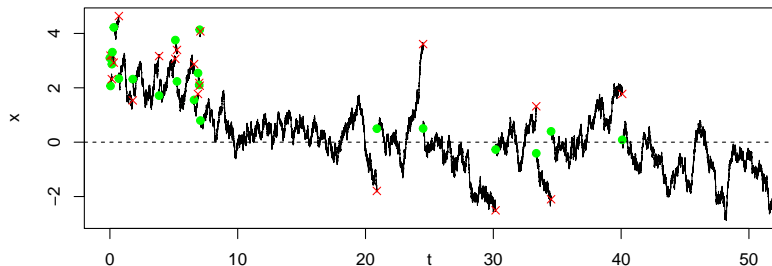
else

$X \sim \mathcal{N}(X, \tilde{\zeta}), t \leftarrow t + \tilde{\zeta}, u \sim \mathcal{U}[0, 1].$

If $u < \kappa^-(X)/K^-$ **then** $E \leftarrow E \cup \{X\}.$

end

end



Path of an Adaptive Brownian Restore process with $\pi \equiv \mathcal{N}(0, 1)$, $\mu_0 \equiv \mathcal{N}(2, 1)$, $\alpha = 10$. Green dots and red crosses as first and last output states of each tour.

Calibrating initial regeneration and parameters

- ▶ μ_0 as initial approximate of π , e.g., $\mu_0 \equiv \mathcal{N}_d(0, I)$ with π pre-transformed
- ▶ trade-off in choosing discrete measure dominance time: smaller choices of \mathbf{a} for faster convergence versus larger values of \mathbf{a} for more regenerations from μ_0 , hence better exploration (range of \mathbf{a} : between 10^3 and 10^4)
- ▶ \mathcal{K}^+ and \mathcal{K}^- based on quantiles of $\tilde{\kappa}$, from preliminary MCMC runs
- ▶ or, assuming π close to Gaussian, initial guess of \mathcal{K}^- is $d/2$ and initial estimate for \mathcal{K}^+ based on χ^2 approximation

Final remarks

- ▶ Adaptive Restore benefits from global moves, for targets hard to approximate with a parametric distribution, with large moves across the space
- ▶ Use of minimal regeneration rate makes simulation computationally feasible and more likely in areas where π has significant mass
- ▶ In comparison with wandom walk Metropolis, ABRA can be slow but with higher efficiency for targets π with skewed tails

Part II: Importance Monte Carlo

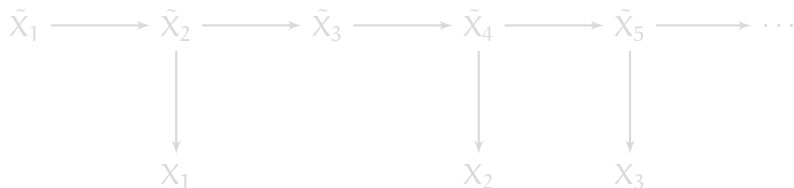


Joint work with C Andral, R Douc and H Marival
arXiv:2207.08271 – Stoch Proc & Appli

Rejection Markov chain

Mixing MCMC and rejection sampling :

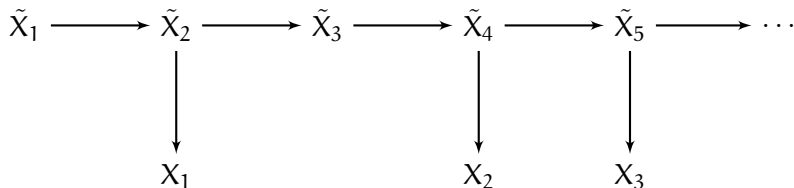
1. **Draw** Markov chain $(\tilde{X}_i)_{1 \leq i \leq m}$ from kernel Q targeting $\tilde{\pi}$
2. With probability $\rho(\tilde{X}_i) \in (0, 1)$ (e.g. $\rho = \pi/(M\tilde{\pi})$), **accept** proposal
3. Resulting in new Markov chain $(X_i)_{1 \leq i \leq n}$, ($n \leq m$)



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Rejection Markov Chain (cont'd)

Corresponding to kernel S for (X_i)

$$Sh(x) = \sum_{k=1}^{\infty} \mathbb{E}_x^Q \left[\rho(X_k) h(X_k) \left(\prod_{i=1}^{k-1} (1 - \rho(X_i)) \right) \right]$$

Nice (recursive) equation

$$Sh(x) = Q(\rho h)(x) + Q((1 - \rho)Sh)(x)$$

Rejection Markov Chain (cont'd)

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Invariant measure for S

If $\tilde{\pi}Q = \tilde{\pi}$, then S is $\rho \cdot \tilde{\pi}$ invariant

$$\int \rho(x) \tilde{\pi}(dx) S(x, dy) = \rho(y) \tilde{\pi}(dy)$$

Direct consequence : if $\rho = \frac{\pi}{M\tilde{\pi}}$, S is π -invariant

Invariant measure for S

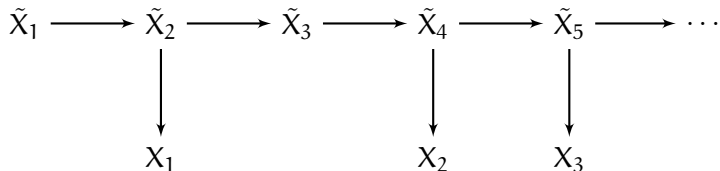
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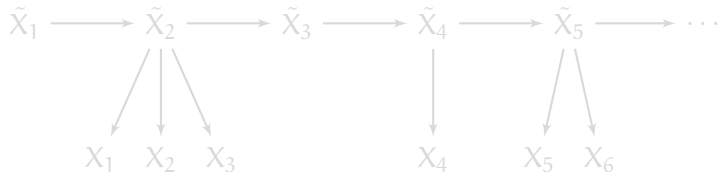
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From rejection to importance

From

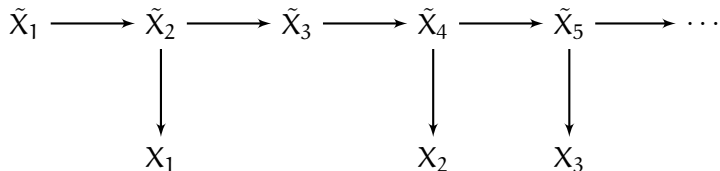


to

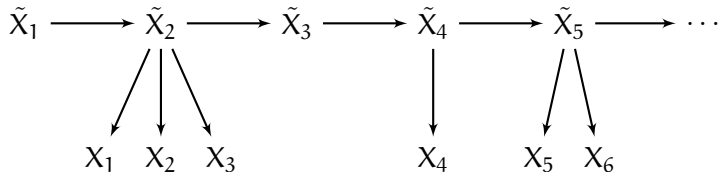


From rejection to importance

From



to



Importance Markov chain

- ▶ Case when ρ may take values above 1
- ▶ Define $\rho_\kappa(\mathbf{x}) := \kappa \frac{\pi(\mathbf{x})}{\tilde{\pi}(\mathbf{x})}$ for free parameter κ
- ▶ Allow to **repeat** elements of the chain
- ▶ Accept $\tilde{N}_i \sim \tilde{R}(\tilde{X}_i, \cdot)$ copies of \tilde{X}_i , with \tilde{R}_i kernel in \mathbb{N} s.t. $\mathbb{E}[\tilde{N}_i | \tilde{X}_i] = \rho_\kappa(\tilde{X}_i)$, e.g.

$$\tilde{N}_i = \lfloor \rho_\kappa(\tilde{X}_i) \rfloor + \mathcal{B}e(\{\rho_\kappa(\tilde{X}_i)\})$$

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$$\tilde{N}_i = \left\lfloor \rho_\kappa(\tilde{X}_i) \right\rfloor + \mathcal{B}e\left(\left\{\rho_\kappa(\tilde{X}_i)\right\}\right)$$

Related works

(i) Self-regenerative chain: independent draws ($Q(x, \cdot) = \tilde{\pi}$) and $N_i = V \cdot S$ copies where $S \sim \mathcal{Geo}(q)$, $V \sim \mathcal{Be}(p)$

[Sahu and Zhigljavsky 2003; Gåsemyr 2002]

(ii) Proposals in a semi-Markov approach

[Malefaki and Iliopoulos 2008]

(iii) Dynamic Weighting Monte Carlo and *correctly weighted* joint density:

$$\int w f(x, w) dw \propto \pi(x)$$

[Wong and Liang 1997; Liu, Liang, and Wong 2001]

IMC algorithm

Algorithm 1: Importance Markov chain (IMC)

$\ell \leftarrow 0$

Set an arbitrary \tilde{X}_0

for $k \leftarrow 1$ **to** n **do**

 Draw $\tilde{X}_k \sim Q(\tilde{X}_{k-1}, \cdot)$ and $\tilde{N}_k \sim \tilde{R}(\tilde{X}_k, \cdot)$

 Set $N_\ell = \tilde{N}_k$

while $N_\ell \geq 1$ **do**

 Set $(X_\ell, N_\ell) \leftarrow (\tilde{X}_k, N_\ell - 1)$

 Set $\ell \leftarrow \ell + 1$

end

end

Dynamics of the chain

If $N_k > 0$:

$$X_k \longrightarrow X_{k+1} = X_k$$

$$N_k \neq 0 \longrightarrow N_{k+1} = N_k - 1$$

If $N_k = 0$:

$$X_k \longrightarrow X_{k+1} \sim Q(X_k, \cdot)$$



$$N_k = 0 \quad N_{k+1} \sim R(X_{k+1}, \cdot)$$

Formalisation of IMC

Define an **extended Markov chain** (X_i, N_i) where X_i and \tilde{X}_i in same space, and $N_i \in \mathbb{N}$ (counting number of repetitions)

Associated kernel

$$\begin{aligned} P_h(x, n) &= \mathbb{I}_{\{n \geq 1\}} h(x, n-1) \\ &+ \mathbb{I}_{\{n=0\}} \sum_{n'=0}^{\infty} \int_{\mathcal{X}} S(x, dx') R(x', n') h(x', n') \end{aligned}$$

where

$$\begin{aligned} \rho_{\tilde{R}}(x) &= \tilde{R}(x, [1, \infty)) \in [0, 1] \\ R(x, n) &:= \tilde{R}(x, n+1) / \rho_{\tilde{R}}(x) \end{aligned}$$

Formalisation of IMC

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Invariant for P

Measure $\bar{\pi}$ on $\mathbf{X} \times \mathbb{N}$:

$$\bar{\pi}(\mathbf{h}) = \kappa^{-1} \sum_{n=1}^{\infty} \int_{\mathbf{X}} \tilde{\pi}(d\mathbf{x}) \tilde{\mathbf{R}}(\mathbf{x}, n) \sum_{k=0}^{n-1} h(\mathbf{x}, k)$$

such that

1. If $\sum_{n=0}^{\infty} \tilde{\mathbf{R}}(\mathbf{x}, n) n = \rho_{\kappa}(\mathbf{x})$, **marginal** of $\bar{\pi}$ on the first component equal to π
2. if $\tilde{\pi}Q = \tilde{\pi}$, Markov kernel **$\bar{\pi}$ -invariant**

Invariant for P

Measure $\bar{\pi}$ on $X \times \mathbb{N}$:

$$\bar{\pi}(h) = \kappa^{-1} \sum_{n=1}^{\infty} \int_X \tilde{\pi}(dx) \tilde{R}(x, n) \sum_{k=0}^{n-1} h(x, k)$$

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1. If $\sum_{n=0}^{\infty} \tilde{R}(x, n) n = \rho_{\kappa}(x)$, **marginal** of $\bar{\pi}$ on the first component equal to π
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Strong Law of Large Numbers

Theorem 1

If for every $\xi \in M_1(X)$ and $\tilde{\pi}$ integrable function g ,

$$\lim_{n \rightarrow \infty} n^{-1} \sum_{k=0}^{n-1} g(\tilde{X}_k) = \tilde{\pi}(g), \quad \mathbb{P}_\xi^Q - \text{as}$$

then, for every $\bar{\pi}$ integrable function g ,

$$\lim_{n \rightarrow \infty} n^{-1} \sum_{k=0}^{K_n-1} g(X_k) N_k = \bar{\pi}(g), \quad \mathbb{P}_\xi^P - \text{as}$$

Central limit theorem

Theorem 2

Under conditions on Q , $\tilde{\pi}$, take $h : X \rightarrow \mathbb{R}$ as solution of a Poisson equation for Q , then

$$\frac{1}{\sqrt{n}} \sum_{i=1}^n (h(X_i) - \pi(h)) \stackrel{\mathbb{P}_X^P\text{-law}}{\rightsquigarrow} \mathcal{N}(0, \sigma^2(h)),$$

where

$$\sigma^2(h) = \kappa \tilde{\sigma}^2(\rho h_0) + \kappa^{-1} \hat{\sigma}^2(h_0, \kappa),$$

$\tilde{\sigma}^2(\rho h_0)$ is the variance obtained with Q ,

$$\hat{\sigma}^2(h_0, \kappa) := \int_X h_0^2(x) \text{Var}_x^{\tilde{R}}[N] \tilde{\pi}(dx),$$

$$\text{Var}_x^{\tilde{R}}[N] := \int_{\mathbb{N}} \tilde{R}(x, dn) n^2 - \left(\int_{\mathbb{N}} \tilde{R}(x, dn) n \right)^2.$$

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$$\frac{1}{\sqrt{n}} \sum_{i=1}^n (h(X_i) - \pi(h)) \stackrel{\mathbb{P}_X^{\text{P-law}}}{\rightsquigarrow} \mathcal{N}(0, \sigma^2(h)),$$

where

$$\sigma^2(h) = \kappa \tilde{\sigma}^2(\rho h_0) + \kappa^{-1} \hat{\sigma}^2(h_0, \kappa),$$

$\tilde{\sigma}^2(\rho h_0)$ variance coming from instrumental chain, $\hat{\sigma}^2(h_0, \kappa)$
variance from random number of repetitions

$\hat{\sigma}$ depends on the variance of \tilde{R}

$$\text{Var}_{\tilde{R}}[N] := \int_{\mathbb{N}} \tilde{R}(x, dn) n^2 - \left(\int_{\mathbb{N}} \tilde{R}(x, dn) n \right)^2$$

For N integer-value random variable such that $\mathbb{E}[N] = \rho < \infty$,

$$\text{Var}(N) \geq \{\rho\} (1 - \{\rho\})$$

LoBound met by $N = \lfloor \rho \rfloor + S$, where $S \sim \text{Ber}(\{\rho\})$ (used as “shifted Bernoulli” kernel default)

Theorem 3

Under assumptions on Q and \tilde{R} , P has *unique invariant probability measure* $\bar{\pi}$ and there exist constants $\delta, \beta_r > 1$, $\zeta < \infty$, such that for all $\xi \in \mathbf{M}_1(\mathbf{X} \times \mathbb{N})$,

$$\sum_{k=1}^{\infty} \delta^k d_{TV}(\xi P^k, \bar{\pi}) \leq \zeta \int_{\mathbf{X} \times \mathbb{N}} \beta_r^n V(x) \xi(dx dn).$$

Pseudo-marginal version

- ▶ Cases when the density π not available but replaced by (unbiased) estimate, leading to **pseudo-marginal** method.

[Andrieu and Roberts 2009]

- ▶ **Extension:** Importance Markov chain “pseudo-marginal compatible” when unbiased estimate available draw $\hat{\pi}(X_i)$ (with expectation $\pi(x)$) and

$$N_i \sim \lfloor \hat{\pi}/\tilde{\pi}(X_i) \rfloor + \mathcal{B}e(\{\hat{\pi}/\tilde{\pi}(X_i)\})$$

by enlarging the chain structure

- ▶ ... and even with unbiased estimate of $\tilde{\pi}$
- ▶ resulting in higher variance

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Several factors to choose :

- ▶ auxiliary distribution $\tilde{\pi}$
- ▶ kernel Q
- ▶ value of κ

Several things to note

- ▶ κ is arbitrary if π and $\tilde{\pi}$ are unnormalized.
- ▶ the length of the final chain (X_i) grows linearly in κ for a fixed length n chain (\tilde{X}_i)
- ▶ hence, automatic tuning κ achieved by setting length of chain
- ▶ For $ESS_{\kappa} := (\sum_{i=1}^n \tilde{N}_i)^2 / \sum_{i=1}^n \tilde{N}_i^2$ and usual IS ESS:
 $ESS_{IS} := (\sum_{i=1}^n \rho(\tilde{X}_i))^2 / \sum_{i=1}^n \rho(\tilde{X}_i)^2$

$$ESS_{\kappa} \xrightarrow{\kappa \rightarrow \infty} ESS_{IS}$$

Warning: notion of ESS not accounting for convergence of Markov chain

About κ

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- ▶ κ is arbitrary if π and $\tilde{\pi}$ are unnormalized.
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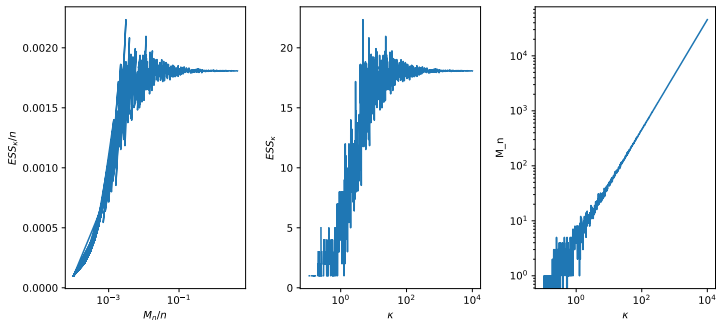
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Impact of κ

Dimension = 5, mixture of 6 gaussians



Impact of κ on ESS and Markov chain length

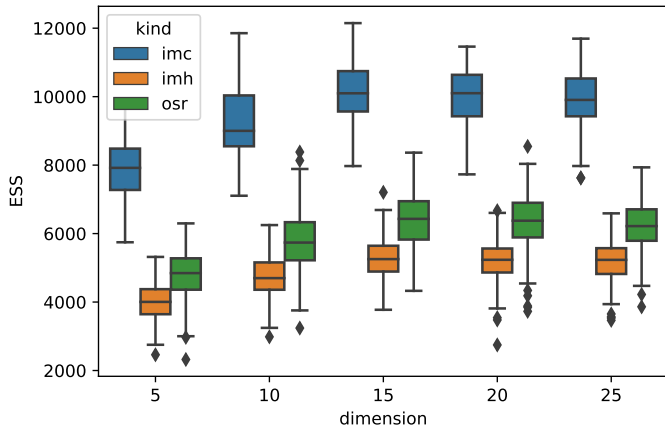
Independent IMC and normalizing flows

- ▶ Target: π a d -dimensional distribution, with 2^d modes, concentrated around the sphere

$$\pi(\mathbf{x}) \propto \exp \left(-\frac{1}{2} \left(\frac{\|\mathbf{x}\| - 2}{0.1} \right)^2 - \sum_{i=1}^d \log \left(e^{-\frac{1}{2} \left(\frac{x_i + 3}{0.6} \right)^2} + e^{-\frac{1}{2} \left(\frac{x_i - 3}{0.6} \right)^2} \right) \right)$$

- ▶ Instrumental density and kernel: a normalizing flow T is trained to approximate π : $Q(\mathbf{x}, \cdot) = \tilde{\pi}(\cdot) = T_{\#} \mathcal{N}(0, 1)$
- ▶ Comparison with Metropolis–Hastings and Self Regenerative MCMC







[Sahu and Zhigljavsky 2003; Gabrié et al 2022]



Conclusion

- ▶ Versatile framework that applies to many different kernels Q and auxiliary distributions $\tilde{\pi}$
- ▶ Extensions: adaptive version – multiple auxiliary chains – delayed acceptance

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