Piecewise-Deterministic MCMC

P. Vanetti, A. Bouchard-Côté, G. Deligiannidis & A. Doucet

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- Consider a probability distribution on $\mathbb{R}^d$ of density

$$\pi(x) = \frac{\exp(-U(x))}{Z},$$

where the potential U can be evaluated pointwise but $Z = \int_{\mathbb{R}^d} \exp(-U(x))dx$ cannot.

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- MCMC are the tools of choice in statistics/physics/chemistry/CS.

Examples

- Bayesian inference for high-dimensional graphical models

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- Bayesian inference for intractable likelihood

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  - Exactness under subsampling (Bierkens et al. 2016, Bouchard-Côté et al. 2016; Kapfer & Krauth, 2016).
  - Ability to deal with intractable potential $U(x) = \int U_\omega(x)\,\mu(d\omega)$ (Pakman et al. 2016).

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- All MCMC schemes presented here target an extended distribution on $\mathcal{Z} = \mathbb{R}^d \times \mathbb{R}^d$

$$\rho(z) = \pi(x)\psi(v) = \exp(-H(z))$$

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- Sampling from ρ provides samples from π.

Continuous-time PDMP

- *Deterministic dynamics*: An ordinary differential of drift ϕ

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- Requires being able to simulate from Q.

PDMP for Sampling

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$$
\begin{aligned}
\mathcal{L}f(z) &= \lim_{\epsilon \to 0} \frac{\mathbb{E}\left[f(z_{t+\epsilon}) \,|z_t = z\right] - f(z)}{\epsilon} \\
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  - **C2** - For the flip operator $\mathcal{S}(z) = (x, -v)$, Q satisfies

$$\int \rho(dz)\,\lambda(z)\,Q\left(z, dz'\right) = \rho\left(\mathcal{S}\left(dz'\right)\right)\lambda\left(\mathcal{S}\left(z'\right)\right).$$

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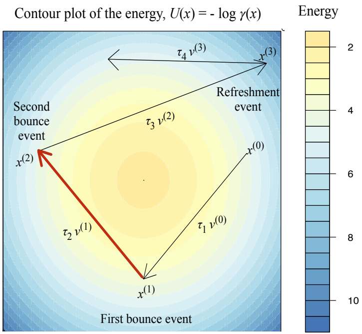
$$Q(z, dz') = \frac{\lambda_{\text{ref}}}{\lambda(z)} \delta_x(dx') \psi(dv') + \frac{\langle \nabla U(x), v \rangle_+}{\lambda(z)} \delta_x(dx') \delta_{R_{\nabla U(x)} v}(dv'),$$

where

$$R_{\nabla U}(x) v := v - 2 \frac{\langle \nabla U(x), v \rangle}{|\nabla U(x)|^2} \nabla U(x)$$

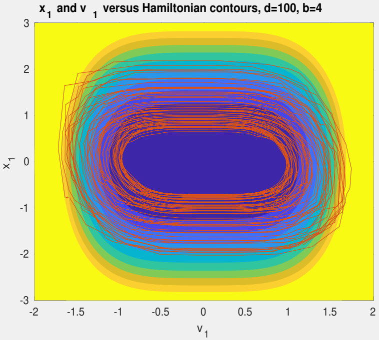
corresponds to a reflection on the hyperplane tangential to ∇U.

Bouncy Particle Sampler Path



A trajectory of BPS on a 2d isotropic normal

Bouncy Particle Sampler Path in High Dimensions



In high-dimensions, BPS converges towards randomized HMC (Deligiannidis et al., 2018).

Local Bouncy Particle Sampler: Graphical Models

- Graphical models: $U(x) = \sum_{i=1}^{n} U_i(x)$ where $U_i(x) = U_i(x_{S_i})$ depends only subset x_{S_i} of components of $x = (x_1, ..., x_d)$.

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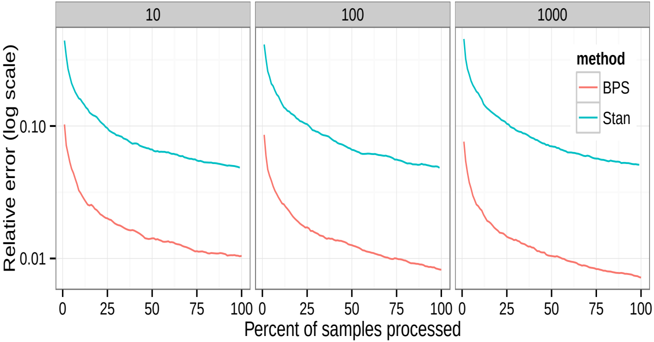
- Efficient implementation via alias method (Bouchard-Côté et al. 2016; Kapfer & Krauth, 2016).

Experimental Results on Poisson-Gaussian Random Fields



Relative error for BPS vs HMC for $d = 10$ (left), $d = 100$ (middle) and $d = 1000$ (right) at fixed computational budget

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- Is it possible to obtain discrete-time schemes enjoying similar features as continuous-time schemes?

Discrete-time PDMP

- *Deterministic dynamics*: a diffeomorphism $\Phi : \mathcal{Z} \to \mathcal{Z}$ and define $\Phi^0(z) = z$ and $\Phi^{r+1}(z) = \Phi^r \circ \Phi(z)$ for $r \in \mathbb{N}$.

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- (Φ, α, Q) defines a Markov transition kernel

$$K(z, dz') = \alpha(z)\, \delta_{\Phi(z)}(dz') + (1 - \alpha(z))\, Q(z, dz').$$

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$$\mathbb{P}(\tau_k = j) = \left\{1 - \alpha\left(\Phi^j\left(z_{t_{k-1}}\right)\right)\right\} \prod_{i=0}^{j-1} \alpha\left(\Phi^i\left(z_{t_{k-1}}\right)\right).$$

  - If $\tau_k \geq 1$ then for $r \in \{1, ..., \tau_k\}$, set

$$z_{t_{k-1}+r} \leftarrow \Phi^r(z_{t_{k-1}}).$$

  - Set $t_k \leftarrow t_{k-1} + \tau_k + 1$ and sample

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- For $M(z, dz') = \delta_{\Psi(z)}(dz')$, this kernel is well-defined if Ψ admits an inverse $\Psi^{-1} = \mathcal{S} \circ \Psi \circ \mathcal{S}$ and $\beta(z, z') = \beta(z) = \min\left(1, \frac{\nu(\mathcal{S} \circ \Psi(dz))}{\nu(dz)}\right)$.

Existing PD-MCMC algorithms and Extensions

- *Guided random walk* (Gustfason 1998): $\Phi(z) = (x + \epsilon v, v)$,
  $\alpha(z) = \min\{1, \rho(\Phi(z)) / \rho(z)\} = \min\{1, \pi(x + v\epsilon) / \pi(x)\}$,
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- Randomized bounces & gradient-free algorithms can be derived (Sherlock & Thiery, 2017, Vanetti et al., 2017).

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  - "Superposition then thinning": If $\alpha(z) = \min\{1, \rho(\Phi(z))/\rho(z)\}$ for $\rho(z) = \prod_{i=1}^n \rho_i(z)$ then $\bar{\alpha}(z,k) = \prod_{i=1}^n \min\left\{1, \rho_i\left(\Phi^{k+1}(z)\right)/\rho_i\left(\Phi^k(z)\right)\right\}$ is a lower bound.

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- *Markov kernel*: conditional upon B, where $|B| \geq 1$, sample $Z' \sim Q_B(Z, \cdot)$ so

$$Q(z, dz') = \sum_{b \in \mathcal{B}} \mathbb{P}(B = b | z, |B| \geq 1) Q_b(z, dz'),$$

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Sufficient conditions for invariance

- **C1** - For mappings such that $|\nabla\Phi| = 1$, the acceptance probabilities α_i satisfy for all $i \in [n]$

$$\{-\log \alpha_i\left(\mathcal{S}\circ\Phi\left(z\right)\right)\} - \{-\log \alpha_i\left(z\right)\} = -\left\{H_i\left(\Phi\left(z\right)\right) - H_i\left(z\right)\right\}.$$

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- Condition **C2** is satisfied if Q_b satisfies a skewed detailed balance w.r.t. $\rho(dz)(1-\alpha(z))\mathbb{Q}_{|B|\geq 1}(b|z)$.

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- Same idea provides a discrete-time version of multidimensional Zig-Zag (Bierkens et al. 2016).

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  output $z' = (x, v^*)$, otherwise output $z' = (x, v^*)$.

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Discrete-time local BPS

- For $i \in [n]$, sample $B_i \sim \mathrm{Ber}\left\{\left[\pi_i\left(x\right) - \pi_i\left(x + v\epsilon\right)\right]_+ / \pi_i\left(x\right)\right\}$.
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  - Optional: For $i \in I \setminus \mathcal{A}$, set $X_i \leftarrow 0$.

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- For logistic regression, sufficient conditions for geometric ergodicity presented in (Cornish et al., 2018).

Discrete-time local BPS via Priority Queue

- Initialization: For $i \in [n]$, sample inter-event times τ_i with distribution

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- *Markov kernel:* Conditional on P, with $|P| \geq 1$, sample $Z' \sim Q_P(Z,\cdot)$ so that

$$Q(z, dz') = \int_{\mathcal{P}} \mathbb{P}(dP|z, |P| \geq 1)\, Q_P(z, dz')$$

  where $\mathbb{P}(dP|z, |P| \geq 1)$ is the law of P conditioned upon $|P| \geq 1$

$$\mathbb{P}(dP|z, |P| \geq 1) = \frac{\mathbb{I}(|P| \geq 1)}{1-\alpha(z)}\mathbb{P}(dP|z).$$

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