Genuinely unbiased Metropolis schemes for Langevin-like dynamics

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CECAM Mixed-gen Season 2 - Session 7: Simulating non-equilibrium phenomena and rare events

Diffusion dependent Overdamped Langevin dynamics

- **Aim**: **Unbiased** estimation of $\mathbb{E}_\pi[f] = \int_{\mathcal{X}} f(q)\pi(q)\mathrm{d}q, \quad \pi \propto \mathrm{e}^{-\beta V}$

with the estimator

$$\hat{I}_N := \frac{1}{N}\sum_{i=1}^{N} f(q^i), \qquad q^i \sim \pi$$

- **Difficulty**: explore **anisotropic** potentials with **multiple minima**

- **Solution**: Position dependent positive definite symmetric matrix D[1]

$$\mathrm{d}q_t = \left(-D(q_t)\nabla V(q_t) + \beta^{-1}\mathrm{div}\ D(q_t)\right)\ \mathrm{d}t + \sqrt{2\beta^{-1}D(q_t)}\ \mathrm{d}W_t$$
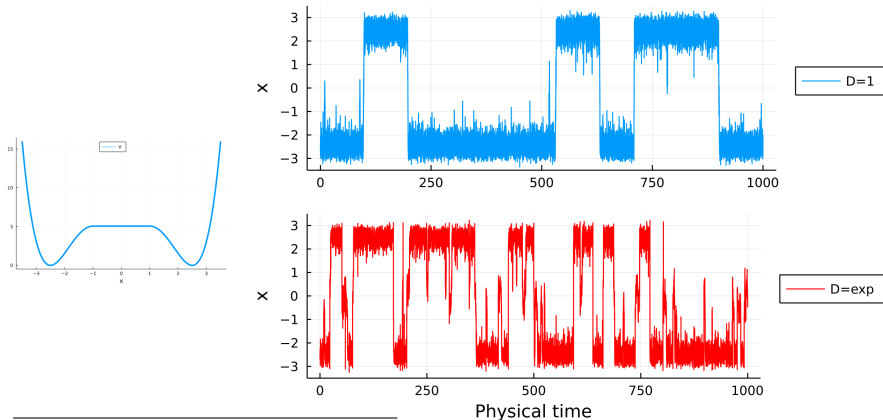
- **Challenge**: Efficient unbiased numerical integration

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[1]Bou-Rabee/Donev/Vanden-Eijnden (2014)

Which diffusion coefficient? Metastable case

- Approach mainly used in Bayesian Inference[2]: $D \equiv (\nabla^2 V)^{-1}$
- Various works[3] suggest $D \propto e^{\beta V} I_d$

$\Rightarrow$ Helps to **cross energy barriers**: if $V \uparrow$, then $D \uparrow$

[2] Girolami/Calderhead (2011)
[3] Roberts/Stramer (2002), Lelièvre/Pavliotis/Robin/Stoltz (In prep.)

Which diffusion coefficient? Anisotropic case

- Isotropic diffusion coefficient $D_{\mathsf{One}} \equiv (1 + \varepsilon)I_2,\ \varepsilon = 0.1$
- Anisotropic diffusion coefficient $D_{\mathsf{Tan}}(q) = \varepsilon I_2 + \tilde{q}\tilde{q}^{\mathsf{T}}/\|q\|^2,\ \tilde{q} = (-y\ x)^{\mathsf{T}}$

Computing: after fixed number of iterations, distance to the invariant measure of the angle distribution (uniform on $[0, 2\pi]$)
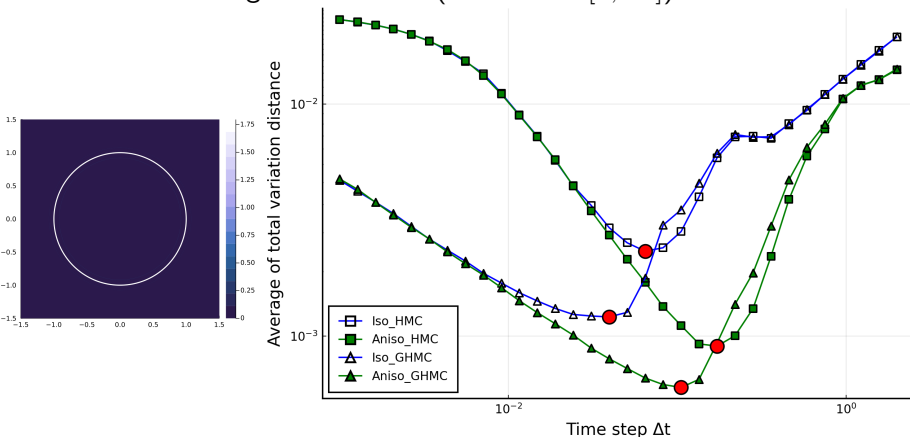
$\Rightarrow$ Compromise: small/large time steps (exploration vs rejection)

Unbiased sampling with Metropolis schemes

- **Metropolis-Hastings**: accept/reject with proba $\min\left(1, \dfrac{\pi(q')T(q',\mathrm{d}q)}{\pi(q)T(q,\mathrm{d}q')}\right)$

- Natural candidate: **Large** rejection rates[4] $\mathcal{O}\left(\Delta t^{1/2}\right)$

$$q' = q + \left(-D(q)\nabla V(q) + \beta^{-1}\mathrm{div}\ D(q)\right)\Delta t + \sqrt{2\Delta t\beta^{-1}D(q)}G$$

- **Better choice**: (Generalized) Hamiltonian Monte Carlo[5] based on

$$\begin{cases} \mathrm{d}q_t = \nabla_p H(q_t, p_t)\ \mathrm{d}t \\ \mathrm{d}p_t = -\nabla_q H(q_t, p_t)\ \mathrm{d}t - \gamma\nabla_p H(q_t, p_t)\ \mathrm{d}t + \sqrt{2\gamma\beta^{-1}}\ \mathrm{d}W_t \end{cases}$$

with

$$H(q, p) = V(q) - \frac{1}{2}\ln\left(\det D(q)\right) + \frac{1}{2}p^{\mathsf{T}}D(q)p$$

- Marginal in position of $\mathrm{e}^{-\beta H}$ is π

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[4]Rossky/Doll/Friedman (1978), Fathi/Stoltz (2017)
[5]Duane/Kennedy/Pendleton/Roweth (1987), Neal (1993)

Riemann Manifold HMC[7]

i) Sample momenta (Ornstein-Ulhenbeck or direct sampling)

ii) Integrate Hamiltonian dynamics
$\Rightarrow$ Generalized Störmer–Verlet[6] (time-reversible, symplectic but implicit)

$$\begin{cases} p^{n+1/2} = p^n - \dfrac{\Delta t}{2} \nabla_q H(q^n, p^{n+1/2}) \\[2mm] q^{n+1} = q^n + \dfrac{\Delta t}{2} \left(\nabla_p H(q^n, p^{n+1/2}) + \nabla_p H(q^{n+1}, p^{n+1/2}) \right) \\[2mm] p^{n+1} = p^{n+1/2} - \dfrac{\Delta t}{2} \nabla_q H(q^{n+1}, p^{n+1/2}) \end{cases}$$
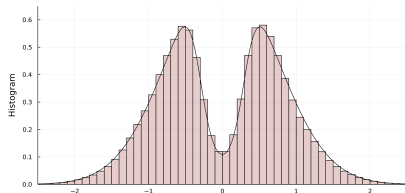
iii) Apply M–H procedure

• (Effective) Rejection rates scale as $\mathcal{O}(\Delta t^{3/2})$

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[6]Hairer/Lubich/Wanner (2006)
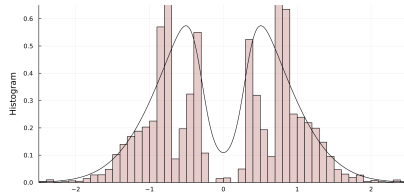[7]Girolami/Calderhead (2011)

Bias arising with standard RMHMC implementation

$\Delta t = 0.18$
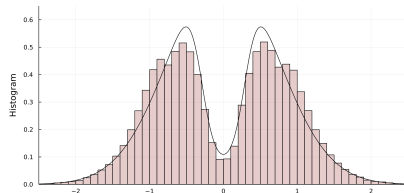
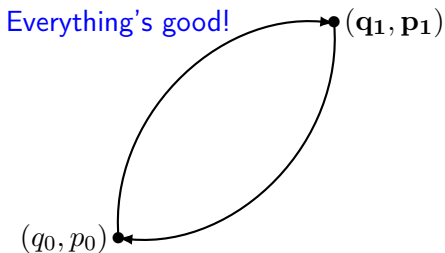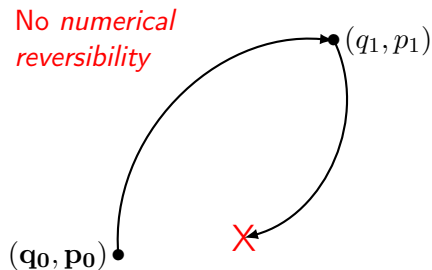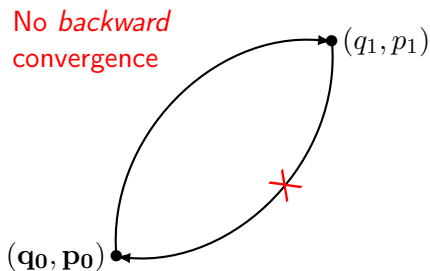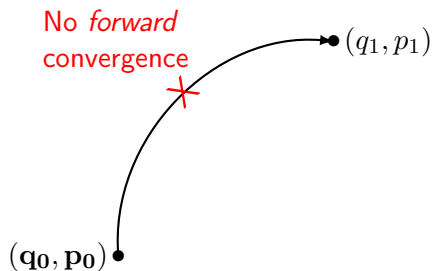$\Delta t = 0.69$
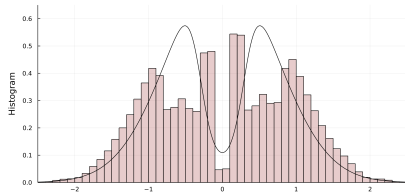
$\Delta t = 0.86$

$\Delta t = 1.68$

Implicit methods $\Rightarrow$ **convergence** and **numerical reversibility issues**[8]
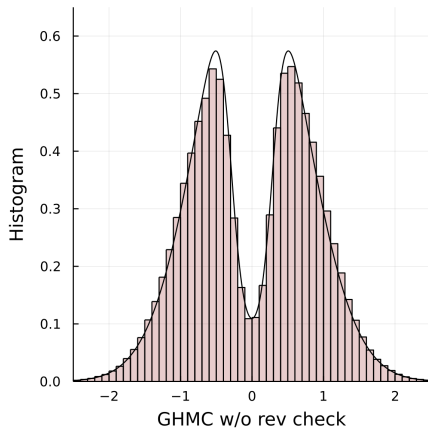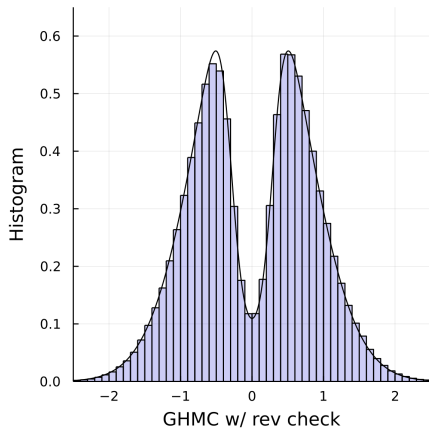
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[8]Brofos/Lederman (2021)

RMHMC with enforced numerical reversibility[9]

No *forward* convergence

(q_1, p_1)

$(\mathbf{q_0}, \mathbf{p_0})$

No *backward* convergence

(q_1, p_1)

$(\mathbf{q_0}, \mathbf{p_0})$

No *numerical* reversibility

(q_1, p_1)

$(\mathbf{q_0}, \mathbf{p_0})$

Everything's good!
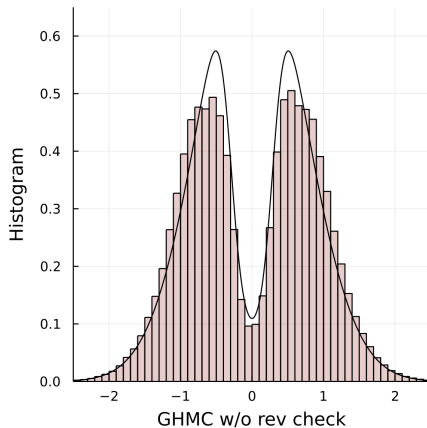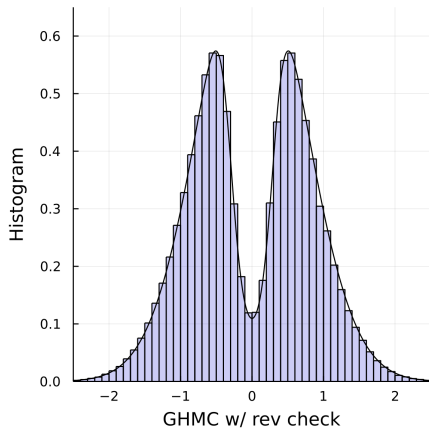
$(\mathbf{q_1}, \mathbf{p_1})$

(q_0, p_0)

[9]Zappa/Holmes-Cerfon/Goodman (2018)
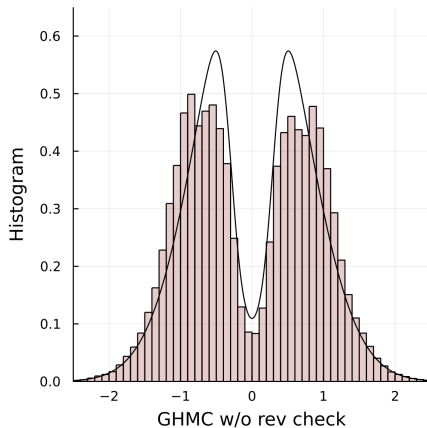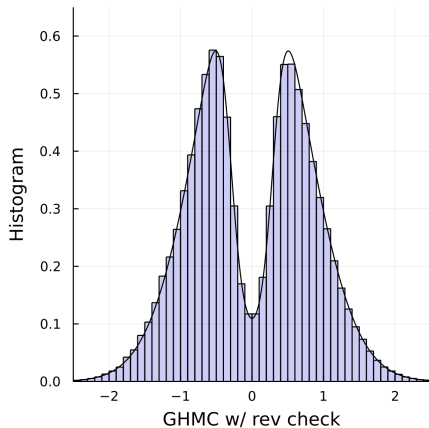
Unbiased sampling with corrected RMHMC

Sampling results with $\Delta t = 0.28$. Left histogram: reversibility checks.

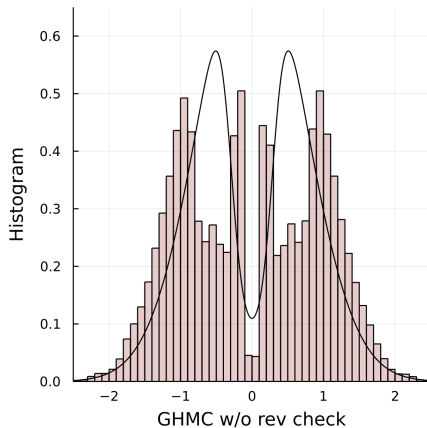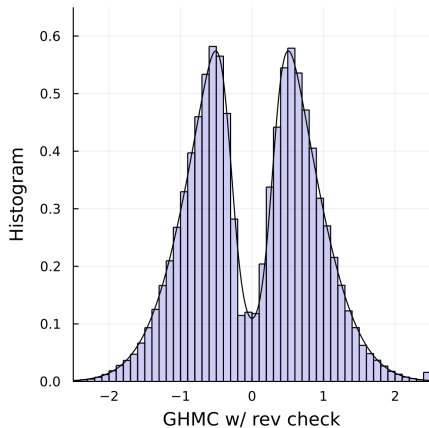# Unbiased sampling with corrected RMHMC

Sampling results with $\Delta t = 0.44$.

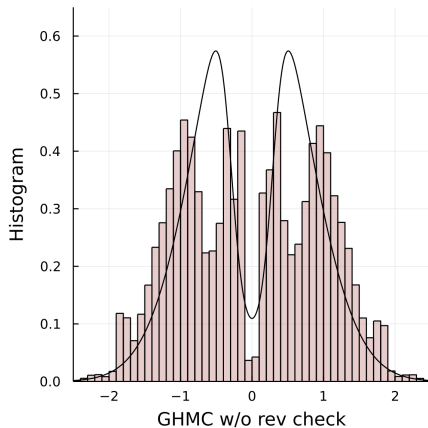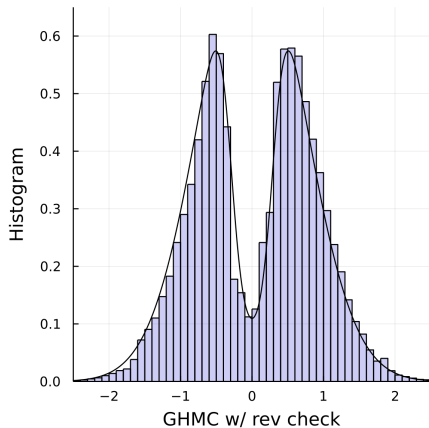# Unbiased sampling with corrected RMHMC

Sampling results with $\Delta t = 0.69$.

Unbiased sampling with corrected RMHMC

Sampling results with $\Delta t = 0.86$.

Unbiased sampling with corrected RMHMC

Sampling results with $\Delta t = 1.08$.

Conclusion and perspectives

Conclusions

• Overdamped Langevin with position dependent diffusion can dramatically **accelerate convergence**

• Care is required in numerical integration

Perspectives

• Higher dimension case: **use free energy F**, coordinate reaction ξ

$$D(q) \propto e^{\beta F(\xi(q))}$$

• Extension to **non-equilibrium** systems, F non-gradient force

$$dq_t^\eta = \left(D(q_t)\left[-\nabla V(q_t^\eta) + \eta F(q_t^\eta)\right] + \beta^{-1}\mathrm{div}D(q_t^\eta)\right) dt + \sqrt{2\beta^{-1}D(q_t^\eta)}\, dW_t$$

Thank you !

HMC: canonical measure preservation

Theorem

HMC algorithm preserves the probability measure

$$\mu = \exp\left(-H(q,p)\right)/Z_\mu \, \mathrm{d}q \, \mathrm{d}p$$

Proof

$T_{\Delta t}((q,p), \mathrm{d}q' \, \mathrm{d}p') = r_{\Delta t} \delta_{\varphi_{\Delta t}(q,p)}(\mathrm{d}q' \, \mathrm{d}p') + (1 - r_{\Delta t}(q,p))\delta_{(q,p)}(\mathrm{d}q' \, \mathrm{d}p')$

If $f \colon \mathbb{R}^d \to \mathbb{R}^d \to \mathbb{R}$ measurable & bounded, [x=(q,p), S(q,p)=(q,-p)]

$$\int r_{\Delta t}(x) f(\varphi_{\Delta t}(x)) \mu(\mathrm{d}x) \quad = \int r_{\Delta t}(\varphi_{\Delta t}^{-1}(y)) f(y) \frac{\mathrm{e}^{-\beta\left[H \circ \varphi_{\Delta t}^{-1}\right](y)}}{Z_\mu} \mathrm{d}y$$

$$[|\nabla \varphi_{\Delta t}| = 1] \quad = \int r_{\Delta t}((S \circ \varphi_{\Delta t})(z)) f(z) \frac{\mathrm{e}^{-\beta[H \circ S \circ \varphi_{\Delta t}](z)}}{Z_\mu} \mathrm{d}z$$

$$\left[S \circ \varphi_{\Delta t} \circ S = \varphi_{\Delta t}^{-1}\right] \quad = \int r_{\Delta t}(z) f(z) \mu(\mathrm{d}z)$$