Numerical Methods for Bayesian Inverse Problems

Lecture 3: Markov Chain Monte Carlo

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Autumn School – "Uncertainty Quantification for High-Dimensional Problems"
CWI Amsterdam, October 7-11, 2024

(Thanks to Björn Sprungk, TU Freiberg)

Bayesian Approach to Inverse Problems

Find parameter $u \in \mathcal{X}$ from noisy observations of the Bayesian statistical model

$$Y = \mathcal{G}(U) + \eta$$

- Y, U, η treated as random fields / variables
- Prior distribution $U \sim \pi_0$, Gaussian noise $\eta \sim \mathrm{N}(0, \Sigma)$
- Conditioning the prior on data $Y = y$ yields as the solution the posterior π^y.

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- point estimates for u (related to Tikhonov-regularized solution);
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But how to actually compute point estimates and quantify uncertainty?

Numerical Methods

Task

Generate (approximate) samples of $u \in \mathcal{X}$ according to the posterior measure

$$\pi_{u|y}(\mathrm{d}u) = \frac{1}{Z} \exp(-\Phi(u;y))\, \pi_0(\mathrm{d}u),$$

where $\mathcal{X}$ is high- or infinite-dimensional and the potential $\Phi(u;y)$ involves solving a complex infinite-dimensional physical (e.g., PDE) model.

Compute posterior expectations for quantities of interest $f : \mathcal{X} \to \mathcal{Z}$

$$\mathbb{E}_{\pi_{u|y}}[f] := \int_{\mathcal{X}} f(u)\, \pi_{u|y}(\mathrm{d}u),$$

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Numerical Challenges:

1. Error due to num. approximation of Φ.
2. Error due to discretisation of $u \in \mathcal{X}$.
3. High-dimensional numerical quadrature.
4. Normalizing constant Z inaccessible.
5. The more data, the more $\pi_{u|y}$ concentrates ('needle in a haystack')

Addressing the challenges

- The discretization error due to approximating $\mathcal{G}$ by $\mathcal{G}_h$ (e.g., via FEMs) can be addressed using the well-posedness result from the previous lecture for $\pi^h_{u|y}(\mathrm{d}u) \propto \exp(-\Phi_h(u))\,\pi_0(\mathrm{d}u)$

$$\|\mathbb{E}_{\pi^h_{u|y}}[f] - \mathbb{E}_{\pi_{u|y}}[f]\| \leq c\|\mathcal{G} - \mathcal{G}_h\|_{L^2_{\pi_0}} \leq Ch^p.$$

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- Similar result can be shown for the discretization error due to approximating the posterior $\pi_{u|y}$ on the infinite-dimensional parameter domain $\mathcal{X}$ via a posterior $\pi^s_{u|y}$ on an s-dimensional one $\mathcal{X}_s$ (e.g., truncated Karhunen-Loève) [Hoang, Schwab, Stuart, 2013]:

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Central Goal

Keeping those two errors small leads to **high cost per sample** (small FE mesh size h) and **high dimensional quadrature**! Thus, we need efficient (sampling-based) numerical integration methods that can deal with **high-dimensional, unnormalized densities** that **concentrate** in parts of the parameter domain.

Standard Monte Carlo Method

- Given a sequence $\{U_k\}$ of i.i.d. copies of a given random variable $U \sim \pi$, standard Monte Carlo simulation uses the estimator

$$\mathbb{E}_\pi[U] := \int_X u\,\pi(\mathrm{d}u) \approx \frac{S_M}{M}, \qquad S_M = U_1 + \cdots + U_M.$$

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- *Central Limit Theorem*: If $\mathbb{E}_\pi[U] = \mu$ and $\mathbb{V}_\pi[U] := \mathbb{E}_\pi\left[(U-\mu)^2\right] = \sigma^2$, then

$$\mathbb{E}_\pi[S_M] = M\mu, \;\; \mathbb{V}_\pi[S_M] = M\sigma^2 \text{ and } S_M^* = \frac{S_M - M\mu}{\sqrt{M}\sigma} \xrightarrow[M\to\infty]{\text{D}} \mathsf{N}(0,1)$$

i.e. the estimate is unbiased, its variance is σ^2/M and the distribution of the normalised RV S_M^* becomes Gaussian as $M \to \infty$.

Monte Carlo Convergence Statements

- Mean square convergence:

$$\mathbb{E}_\pi\left[\left(\frac{S_M}{M}-\mu\right)^2\right]=\mathbb{V}_\pi\left[\frac{S_M}{M}\right]=\frac{\sigma^2}{M}\xrightarrow[M\to\infty]{\text{a.s.}}0.$$

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$$\mathbb{P}\left(\left|\frac{S_M}{M}-\mu\right|>M^{-1/2+\epsilon}\right)\leq\frac{\sigma^2}{M^{2\epsilon}},$$

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- If $\rho:=\mathbb{E}\left[|U-\mu|^3\right]<\infty$, then the *Berry-Esseen Inequality* gives

$$\left|\mathbb{P}(S_M^*\leq x)-\Phi(x)\right|\leq\frac{\rho}{2\sigma^3\sqrt{M}},$$

where Φ denotes *cumulative density function (CDF)* of $\mathsf{N}(0,1)$.

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- Using Berry-Esseen, the asymptotic 95% confidence interval for S_M/M is

$$0.95-\frac{\rho}{\sigma^3\sqrt{M}}\leq\mathbb{P}\left(\mu\in\left[\frac{S_M}{M}-\frac{1.96\sigma}{\sqrt{M}},\frac{S_M}{M}+\frac{1.96\sigma}{\sqrt{M}}\right]\right)\leq 0.95+\frac{\rho}{\sigma^3\sqrt{M}}$$

Problems with plain Monte Carlo

Target measure

$$\pi(\mathrm{d}u) = \frac{1}{Z}\exp(-\Phi(\mathrm{d}u))\,\pi_0(\mathrm{d}u), \qquad \Phi(u) = \tfrac{1}{2}|y - \mathcal{G}(u)|^2_{\Sigma^{-1}}$$

- **Almost never possible** to draw samples u_i directly according to $\pi_{u|y}$ (particularly since normalizing constant Z is usually not known).

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- Rejection sampling
- Importance sampling and Quasi-Monte Carlo
- Markov chain Monte Carlo (MCMC) and multilevel variants
- Ensemble methods (Ensemble Kalman filter, sequential Monte Caro, ...)
- Simple approximations, surrogates, variational approaches, ...

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All have in common that they need a **good approximation** to $\pi_{u|y}$ as proposal, importance density, surrogate, ... (e.g., reduced order model, lower-dim. approx., ...)

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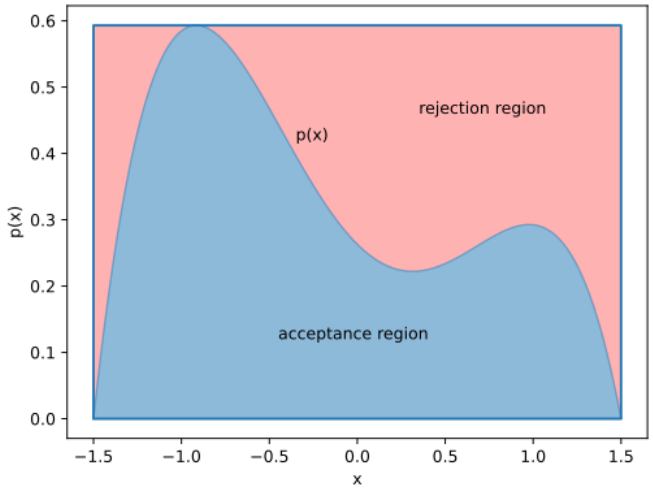

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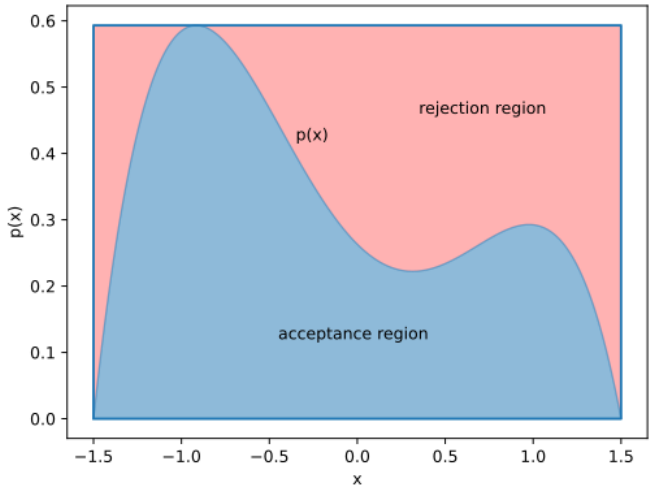

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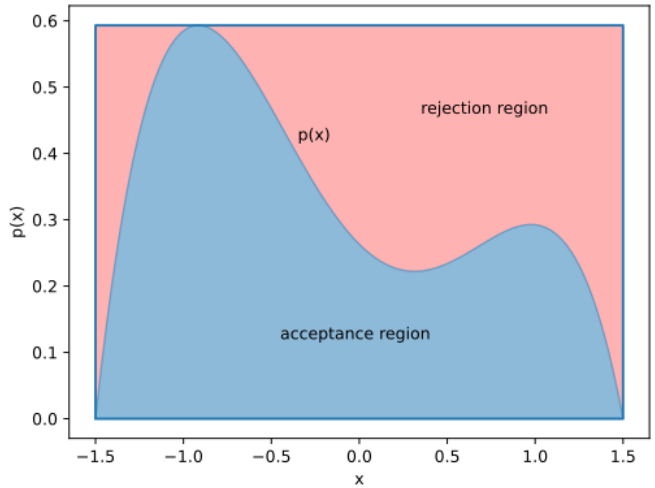

The accepted samples then follow target π, **but**

$$\mathbb{E}\left[\#\mathsf{Tries}\right] = \tfrac{1}{Z} \quad (Z \text{ is a measure of how much } \pi_{u|y} \text{ concentrates.})$$

Importance sampling

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Prior-based selfnormalizing importance sampling

Given i.i.d. samples $U_i \sim \pi_0$

$$\mathbb{E}_\pi[f] \approx IS_M := \frac{\sum_{i=1}^M f(U_i)\,\exp(-\Phi(U_i))}{\sum_{i=1}^M \exp(-\Phi(U_i))}.$$

Efficiency of importance sampling

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Again, this variance **grows very fast** when the **posterior concentrates!**

Efficiency of importance sampling (beyond prior-based)

- When posterior concentrates, prior π_0 not a good importance distribution. A better choice for μ is the Laplace approximation.
  (computable via numerical optimization if $\nabla^2\Phi$ is accessible).
- In that case, concentration even helps: Variance $\sigma^2_{f,p}$ of the selfnormalizing ratio estimator even reduces with $m \to \infty$ with a rate arbitrarily close to $1/2$ [Schillings, Sprungk, Wacker, 2020].

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- The optimal importance density is in fact $p_{\text{opt}} \propto |f|\,\pi_{u|y}$. The DIRT sampler can in fact even obtain arbitrarily accurate approximations of p_{opt} at very low cost and in high dimensions [Cui, Dolgov, **RS**, 2024].

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  (computable via numerical optimization if $\nabla^2\Phi$ is accessible).
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- In principle, any approximation to the (unnormalized) $\pi_{u|y}$ can be used, e.g., surrrogates based on low-rank tensor approximation, such as the TT-CD [Dolgov, Anaya-Izquierdo, Fox, **RS**, 2020] or DIRT sampler [Cui, Dolgov, 2022].
- The optimal importance density is in fact $p_{\text{opt}} \propto |f|\,\pi_{u|y}$. The DIRT sampler can in fact even obtain arbitrarily accurate approximations of p_{opt} at very low cost and in high dimensions [Cui, Dolgov, **RS**, 2024].
- Crucial advantage of importance sampling, compared to MCMC (see below): Other quadrature rules with faster asymptotic convergence can be used, such as **quasi-Monte Carlo** [**RS**, Stuart, Teckentrup, 2017], ...
  (i.e., $\mathcal{O}(M)$ w.r.t. number of samples M instead of $\mathcal{O}(M^{1/2})$ for MC)

Markov chain Monte Carlo

Markov chain Monte Carlo (MCMC)

- Rejection sampling generates i.i.d. samples $U_i \sim \pi$, but very inefficient, particularly in high dimensions $\mathcal{X} = \mathbb{R}^n$, $n \gg 1$, and for concentrated π.

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- **Main tool:** Generate a Markov chain $(U_i)_{i \in \mathbb{N}}$ in $\mathcal{X}$ with π as its stationary or limit distribution

- Resulting Markov chain Monte Carlo estimator $\frac{1}{M} \sum_{i=1}^{M} f(U_i)$ for $\mathbb{E}_\pi[f]$ has, in general, a (mildly) dimension-dependent efficiency but also dimension independent MCMC possible.

Markov chain Basics

A sequence of random variables $(U_i)_{i \in \mathbb{N}_0}$ is a (time-homogeneous) **Markov chain** if there exists a stochastic kernel K such that for each $i \in \mathbb{N}$ and $A \subseteq \mathcal{X}$

$$\mathbb{P}(U_{i+1} \in A \mid U_i = u_i, \ldots, U_0 = u_0) \;=\; K(u_i, A)$$

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Given an initial distribution ν for U_0 we have $U_i \sim \nu K^i$ where

$$\nu K^i(A) := \int_{\mathcal{X}} K^i(u, A)\, \nu(\mathrm{d}u), \qquad K^i(u, A) := \int_{\mathcal{X}} K(v, A)\, K^{i-1}(u, \mathrm{d}v),$$

i.e., $K^i(u, A) = \mathbb{P}(U_{k+i} \in A \mid U_k = u, U_{k-1} = u_{k-1}, \ldots, U_0 = u_0)$ denotes the i-step transition kernel.

Invariance and Reversibility

Definition. A probability measure $\pi \in \mathcal{P}(\mathcal{X})$ is an **invariant measure** of a Markov chain with transition kernel K, if $\pi = \pi K$.

Invariant measure means: $U_i \sim \pi \;\Rightarrow U_{i+1} \sim \pi$

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Proposition. Reversibility of K w.r.t. π implies invariance of π.

Proof. $\pi(A) = \int_A K(u, \mathcal{X})\, \pi(\mathrm{d}u) = \int_{\mathcal{X}} K(u, A)\, \pi(\mathrm{d}u) = \pi K(A)$

Ergodicity

Definition. A Markov chain with transition kernel K and invariant measure π is called **ergodic**, if

$$\lim_{i \to \infty} d_{\mathsf{TV}}(K^i(x, \cdot), \pi) = 0 \qquad \forall x \in \mathcal{X}.$$

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Definition. A transition kernel K is π-**irreducible** if for any $A \subset \mathcal{X}$ with $\pi(A) > 0$ and any $x \in \mathcal{X}$ there exists an $i \in \mathbb{N}$ such that $K^i(x, A) > 0$

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Definition. A transition kernel K is p-**periodic** if there exists $A_1, \ldots, A_p \subset \mathcal{X}$ such that for $j = 1, \ldots, p$

$$K(u, A_{j+1}) = 1 \qquad \forall u \in A_j$$

where $A_{p+1} := A_1$. If K is not p-periodic for any $p \in \mathbb{N}$, then K is **aperiodic**.

$\Rightarrow$ Markov chain does not "oscillate".

Theorem

Let the transition kernel K have invariant measure π and let $(U_i)_{i \in \mathbb{N}_0}$ be a Markov chain starting at $U_0 = u$ with transition kernel K.

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1. If K is irreducible, then for π-almost all $u \in \mathcal{X}$ we have a Strong Law of Large Numbers:

$$\frac{1}{M}\sum_{i=1}^{M} f(U_i) \xrightarrow[M\to\infty]{\text{a.s.}} \int_{\mathcal{X}} f(u)\,\pi(\mathrm{d}u), \qquad f \in L^1_\pi(\mathcal{X}).$$

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2. If K is aperiodic and irreducible, then for π-almost all $u \in \mathcal{X}$ we have

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3. If K is irreducible and for each $u \in \mathcal{X}$ und $A \subseteq \mathcal{X}$ with $\pi(A) > 0$

$$\mathbb{P}\left(U_i \in A \text{ infinitely often} \mid U_0 = u\right) = 1, \qquad \text{('Harris recurrence')}$$

then the above statements hold for each $u \in \mathcal{X}$.

Efficiency of MCMC

- Consider $f : \mathcal{X} \to \mathbb{R}$ and a stationary, reversible Markov chain $(U_i)_{i \in \mathbb{N}_0}$ with $U_0 \sim \pi$
- For the L^2-error of the Monte Carlo estimator $S_M = \frac{1}{M} \sum_{i=1}^{M} f(U_i)$ we have

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$$\begin{aligned}
\mathbb{E}\left[|S_M - \mathbb{E}_\pi[f]|^2 \right] &= \mathbb{E}\left[\left(\frac{1}{M} \sum_{i=1}^{M} (f(U_i) - \mathbb{E}[f(U_i)]) \right)^2 \right] \\
&= \frac{1}{M^2} \sum_{i,j=1}^{M} \mathbb{C}\mathrm{ov}\, f(U_i) f(U_j) \\
&= \frac{1}{M} \mathrm{Var}_\pi f + \frac{2}{M^2} \sum_{i<j \leq M} \mathbb{C}\mathrm{ov}\, f(U_i) f(U_j)
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\end{aligned}$$

- Thus, we get as asymptotic error (if finite)

$$\lim_{M\to\infty} M\mathbb{E}\left[\left| S_M - \mathbb{E}_\pi\left[f\right] \right|^2 \right] = \mathrm{Var}_\pi(f) \underbrace{\left[1 + 2 \sum_{j=0}^{\infty} \mathrm{Corr}\left(f(U_1), f(U_{1+j}) \right) \right]}_{\text{integrated autocorrelation time } \mathrm{IACT}_f}$$

Markov Chain Central Limit Theorem

For a reversible, stationary Markov chain $(U_i)_{i\in\mathbb{N}_0}$ with invariant measure π and an $f \in L^2_\pi(\mathcal{X})$ with finite

$$\mathrm{IACT}_f = 1 + 2\sum_{j=0}^{\infty} \mathrm{Corr}\left(f(U_1), f(U_{1+j})\right) < \infty$$

we have $$\sqrt{M}\Big(S_M - \mathbb{E}_\pi\left[f\right]\Big) \xrightarrow[M\to\infty]{\mathcal{D}} \mathrm{N}\Big(0, \mathrm{Var}_\pi(f)\,\mathrm{IACT}_f\Big)$$

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- Intrinsic accuracy estimate and allows for confidence intervals for $\mathbb{E}_\pi\left[f\right]$
- In practice, given a finite path $(u_i)_{i=1,\ldots,M}$ of the Markov chain, we estimate the autocorrelation empirically

$$\mathrm{Corr}\left(f(U_1), f(U_{1+j})\right) \approx \frac{\frac{1}{M-j}\sum_{i=1}^{M-j}\left(f(u_i) - s_M\right)\,\left(f(u_{i+j}) - s_M\right)}{\frac{1}{M-1}\sum_{i=1}^{M}\left(f(u_i) - s_M\right)^2}$$

and truncate the series above after sufficiently many terms[1]

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Geometric ergodicity

Definition. A Markov chain with transition kernel K and invariant measure π is **geometrically ergodic** if there exists a $C\colon \mathcal{X} \to [0,\infty)$ and $\beta < 1$ such that

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Theorem

If $(U_i)_{i\in\mathbb{N}_0}$ is a reversible and geometrically ergodic Markov chain with invariant measure π, then for any $f \in L^2_\pi(\mathcal{X})$ we have $\mathrm{IACT}_f < \infty$ and thus for any initial distribution $U_0 \sim \nu$ there holds

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Geometric ergodicity is equivalent to a functional analytic property of transition kernels and their related transition operators.

Spectral gaps

Definition. Given a π-invariant transition kernel K on $\mathcal{X}$ the associated **transition operator** $\mathrm{K}\colon L^2_\pi \to L^2_\pi$ is defined by

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Theorem. If $\gamma(K) > 0$, then

$$\mathrm{IACT}_f \leq \frac{2}{\gamma(K)} \quad \text{and} \quad d_{\mathrm{TV}}\left(K^i(u,\cdot), \pi\right) \leq C(1-\gamma(K))^i.$$

Metropolis-Hastings Algorithm

The Metropolis–Hastings (MH) algorithm[2,3]

Let $\pi \in \mathcal{P}(\mathbb{R}^n)$ have unnormalized density $\pi : \mathbb{R}^n \to [0, \infty)$.

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Given current state $U_i = u$, generate the next state as follows

1. Draw v according to chosen proposal kernel $P(u,\cdot)$ where P admits density p such that

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2. Draw a according to $\mathrm{U}[0,1]$
3. If
$$a \leq \alpha(u,v) := \min\left\{1, \frac{\pi(v)\ p(v,u)}{\pi(u)\ p(u,v)}\right\}$$
then set $U_{i+1} = v$ (accept) otherwise set $U_{i+1} = u$ (reject).

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- MH algorithm basically implements a Markov chain rejection sampling and corrects "wrong" proposal chain with kernel P to achieve π-invariance.
- Efficiency of the MH algorithm depends on good choice of proposal kernel P.

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- By construction MH algorithm generates paths of a π-reversible Markov chain.
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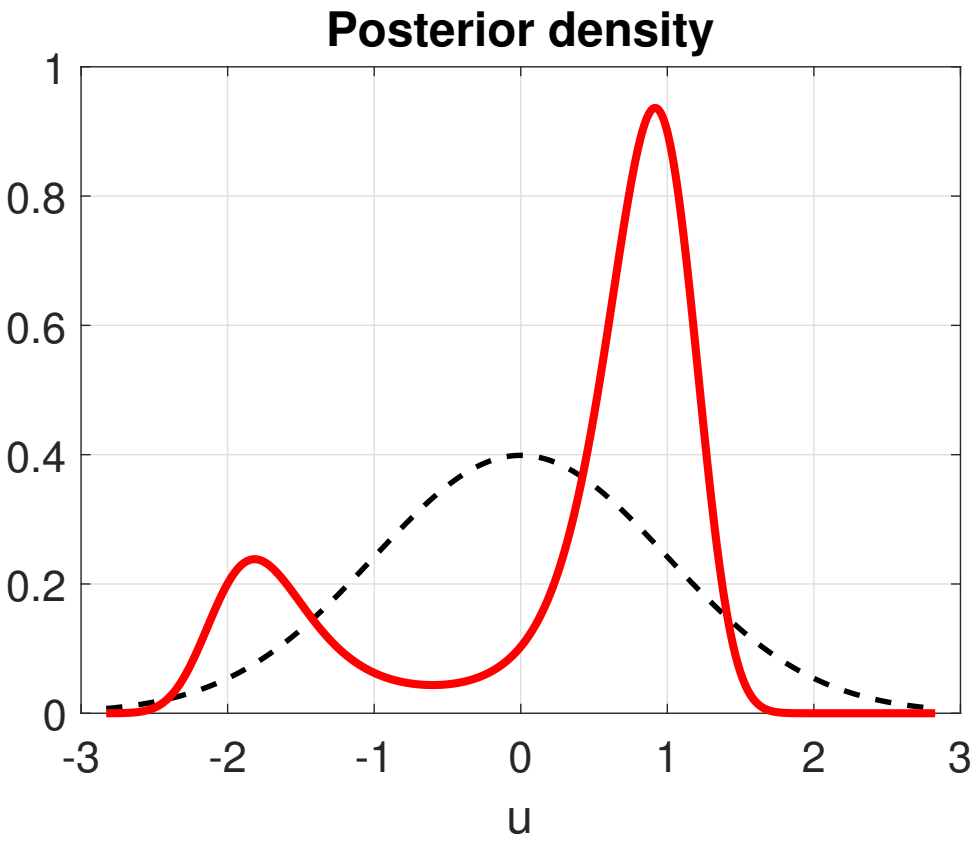

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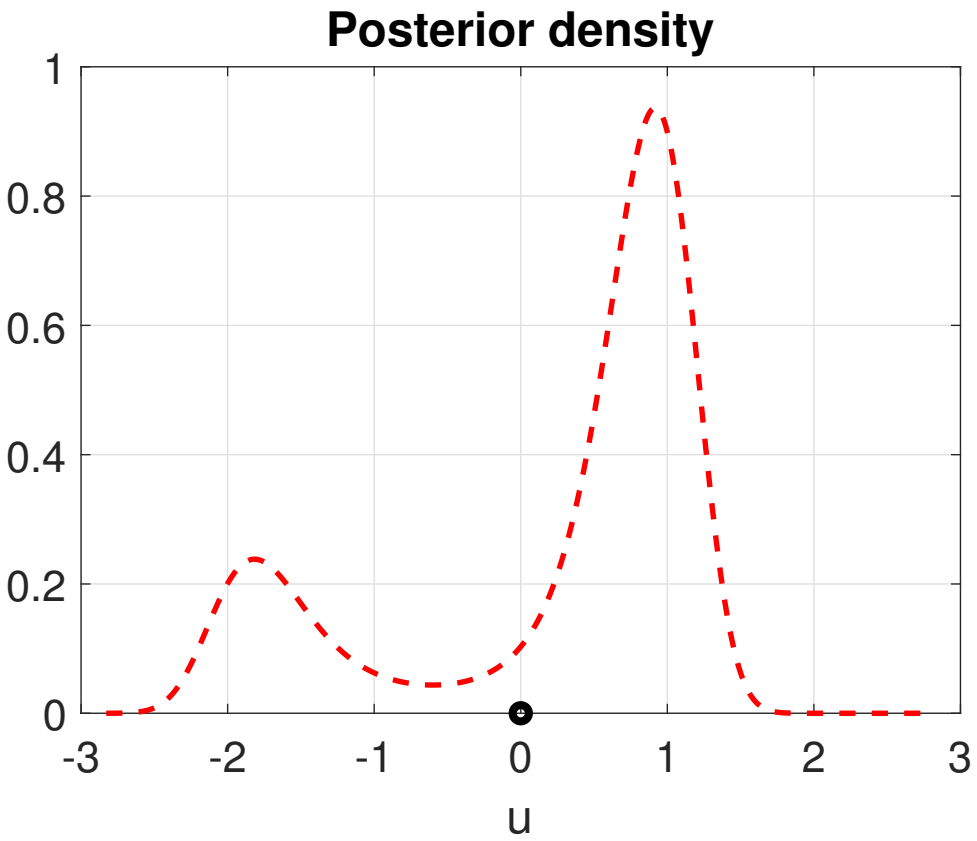

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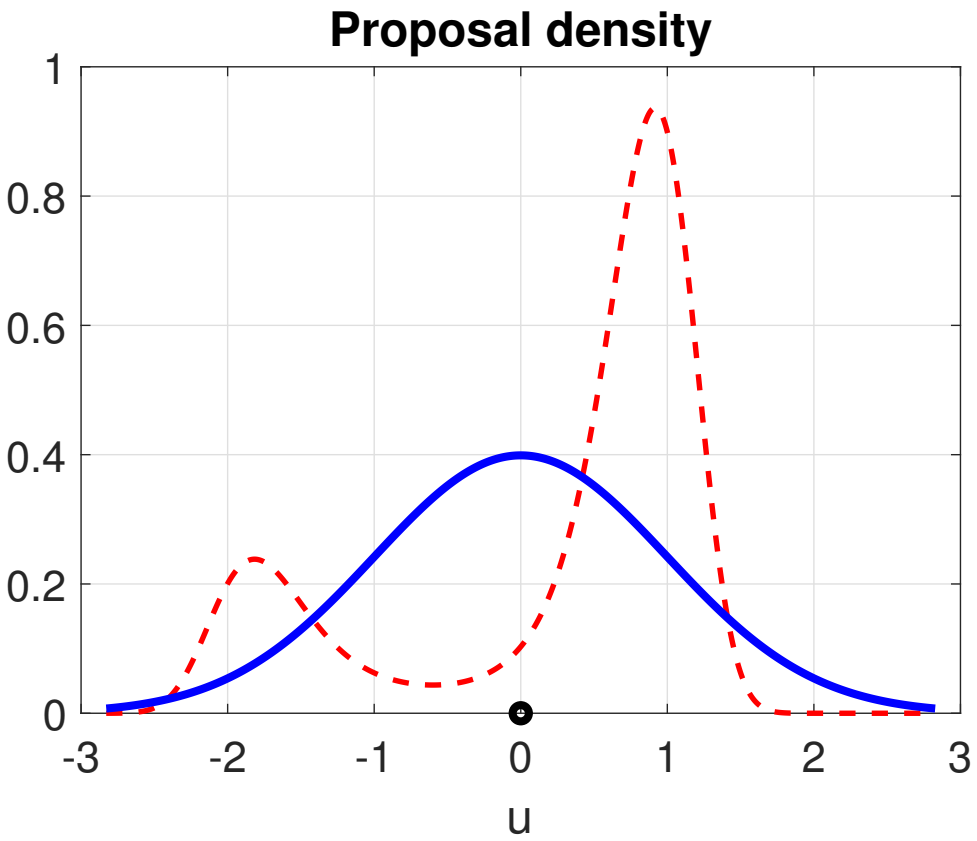

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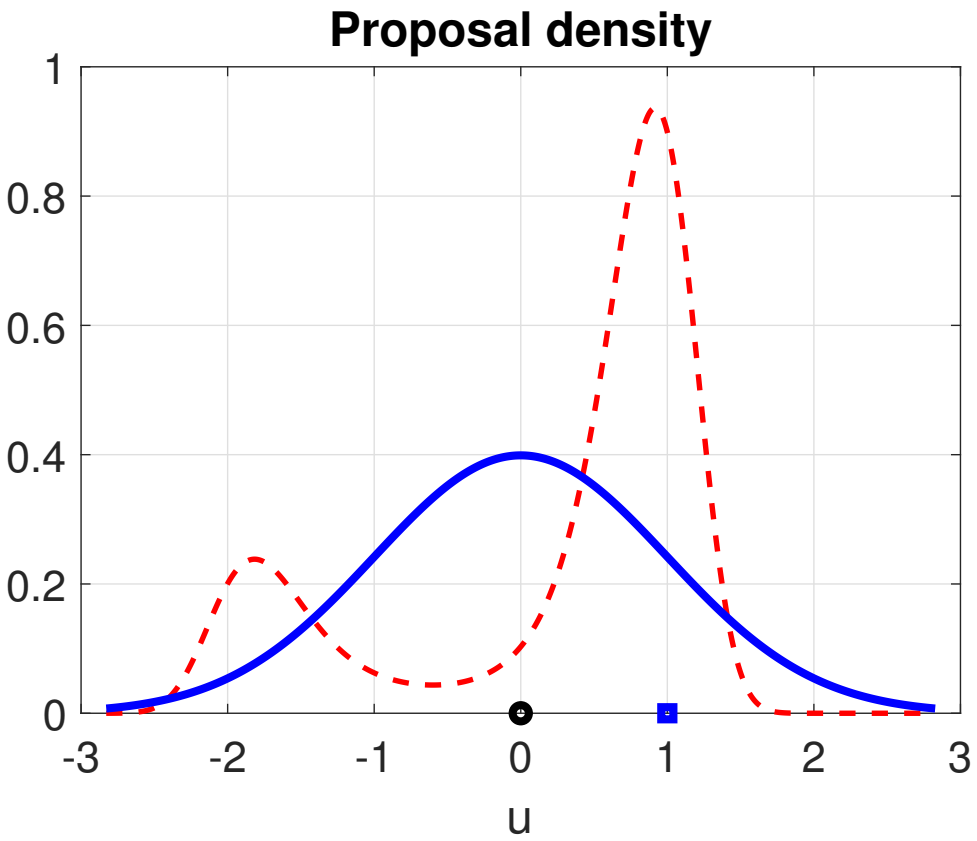

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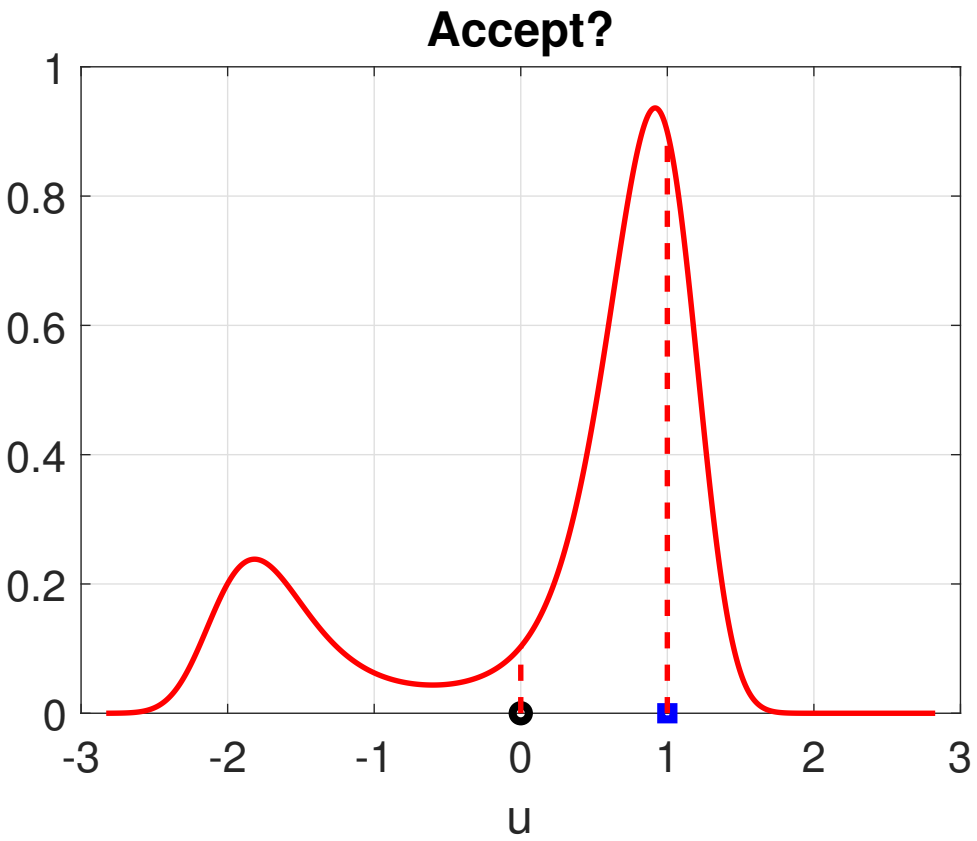

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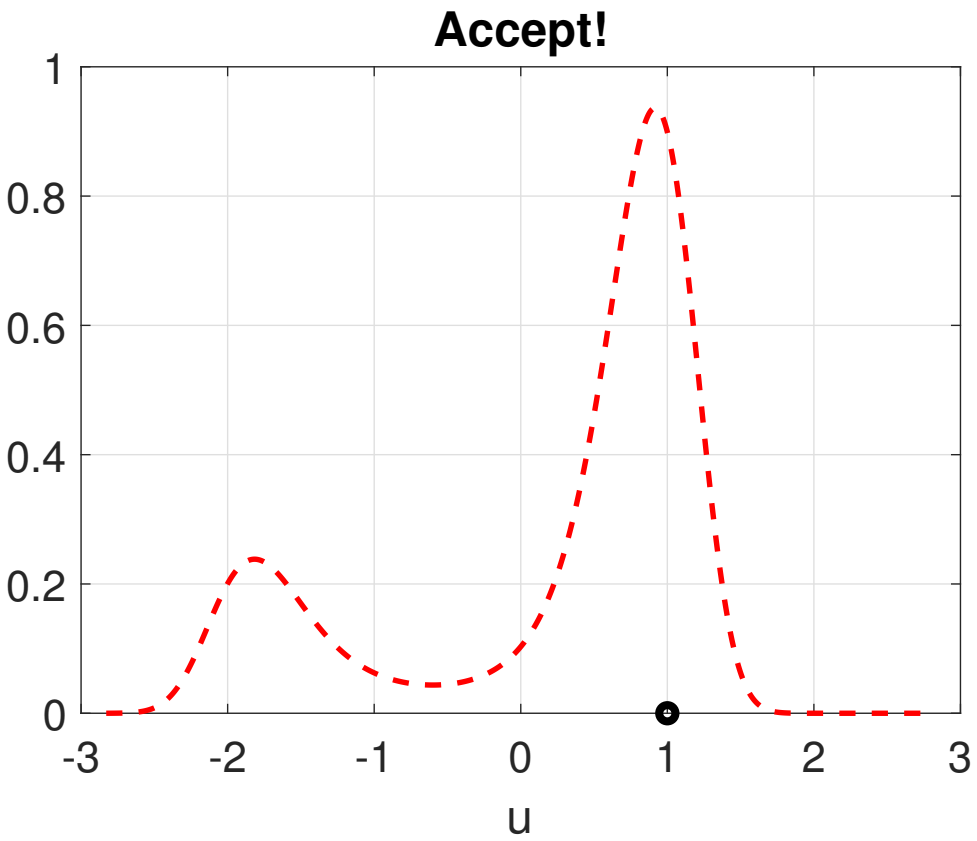

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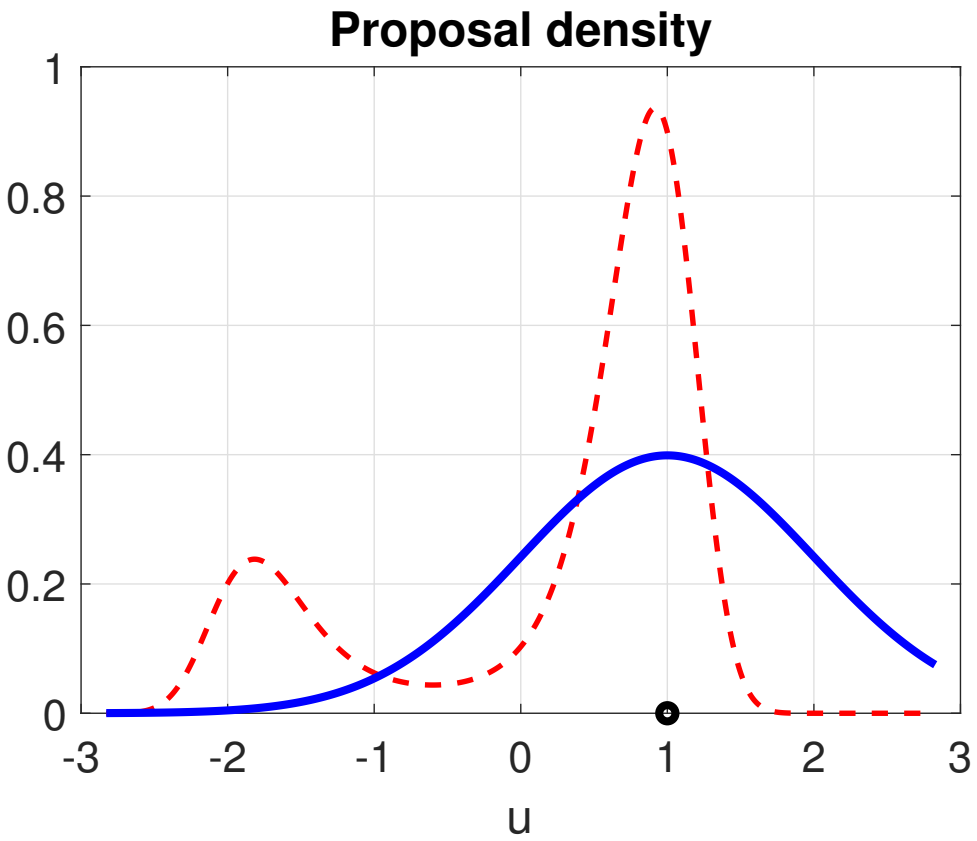

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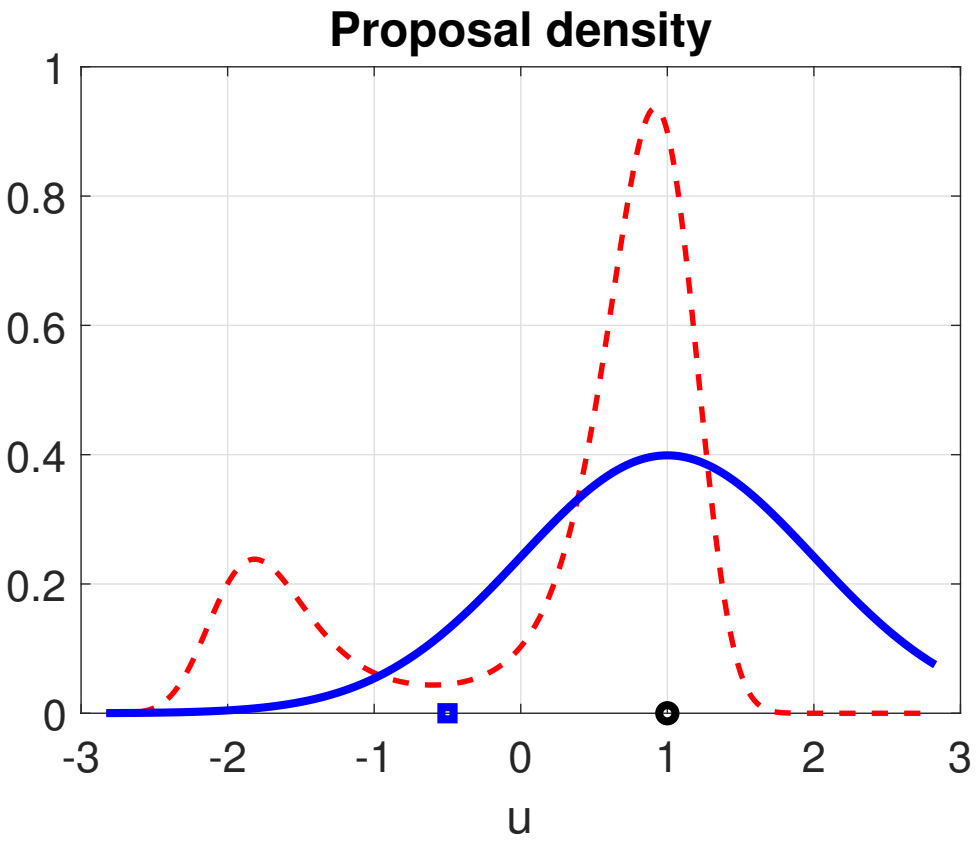

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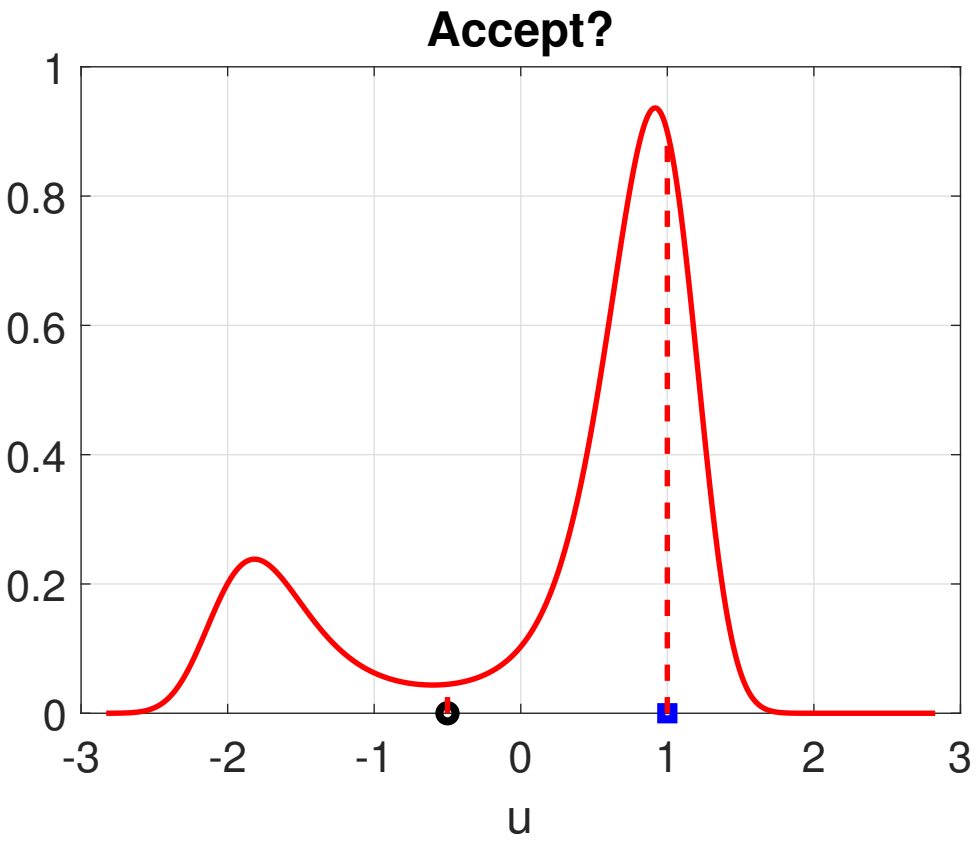

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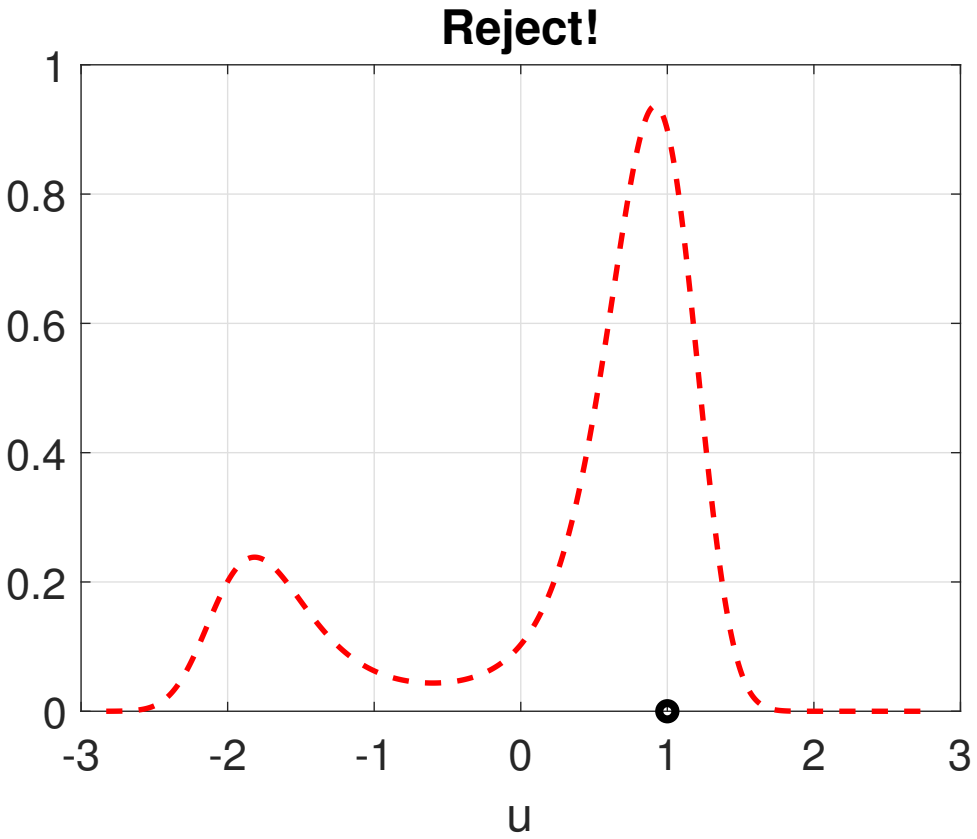

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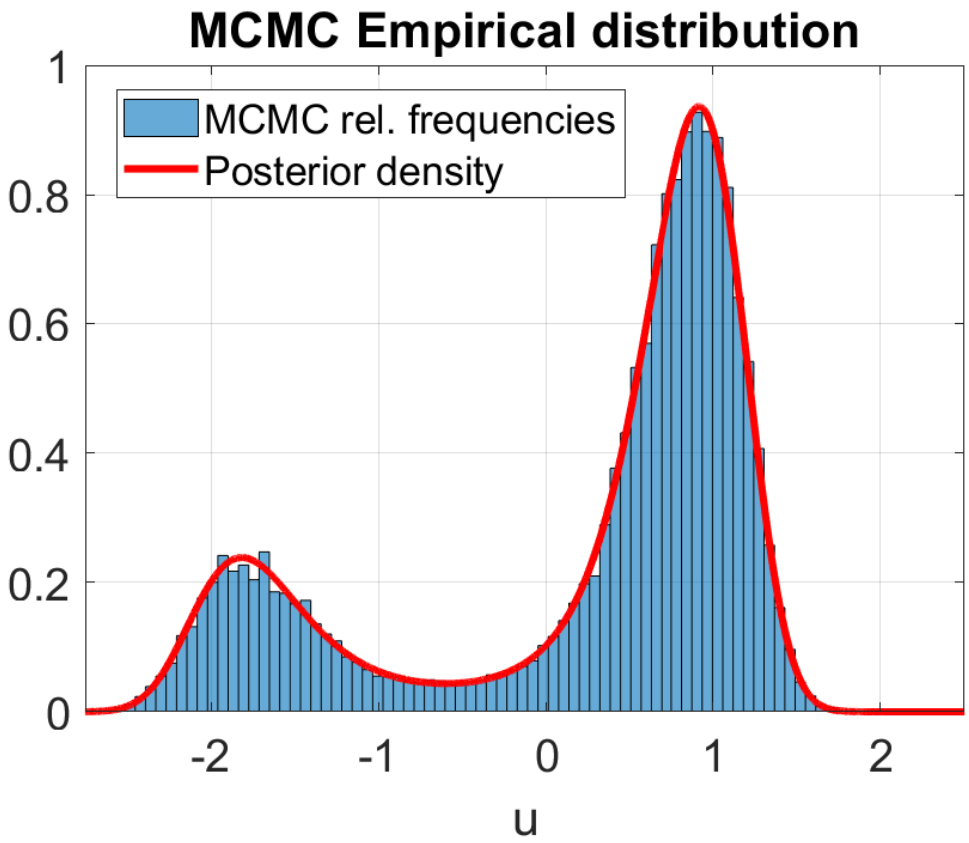

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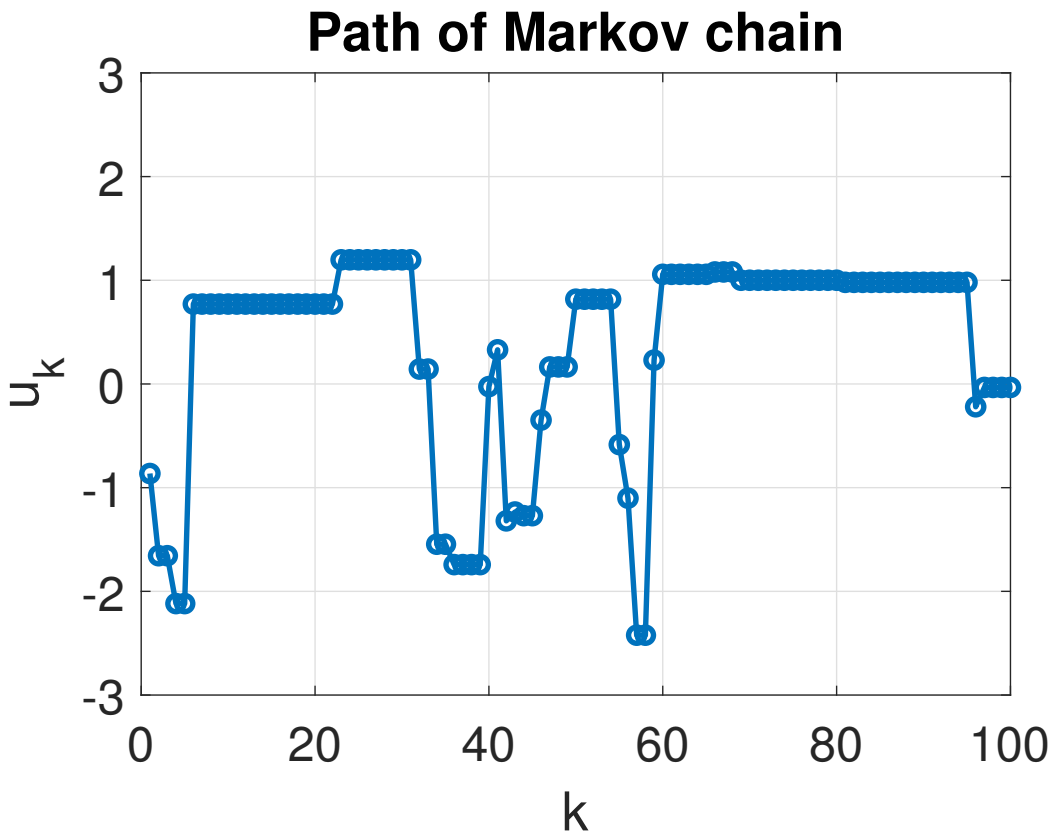

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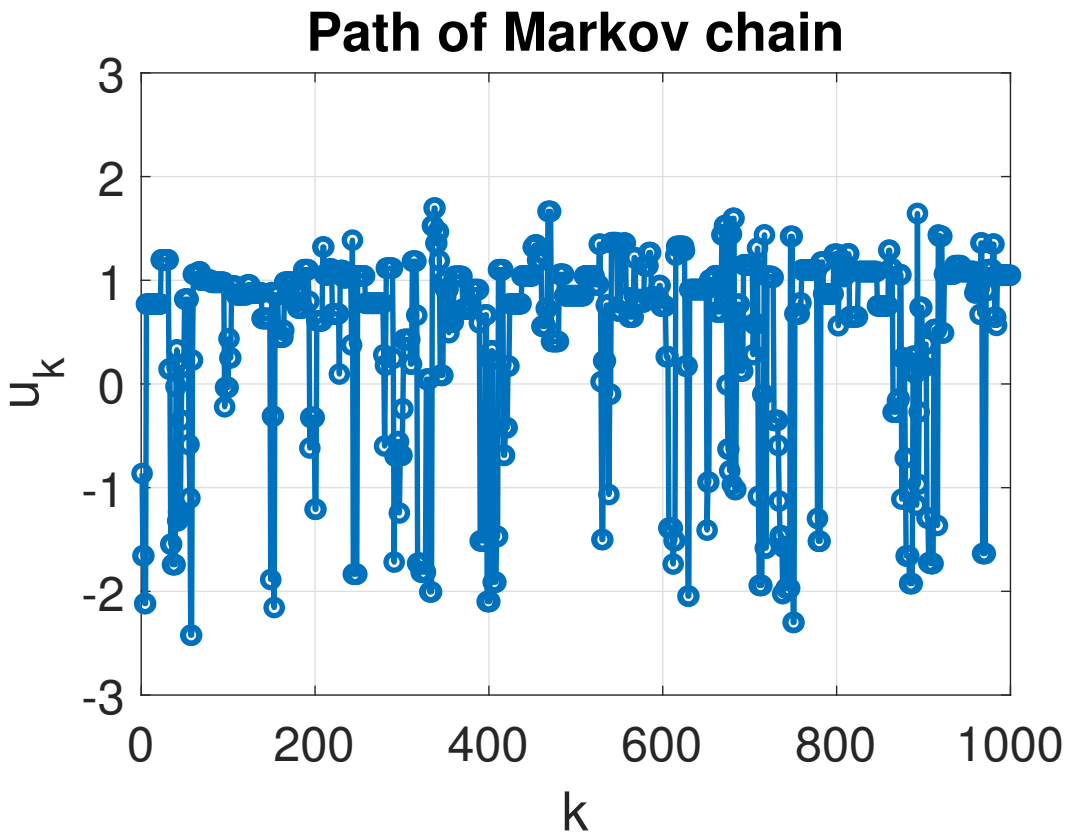

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- How to choose the stepsize s? Is it better to propose larger moves or samller and obtain high acceptance probability?

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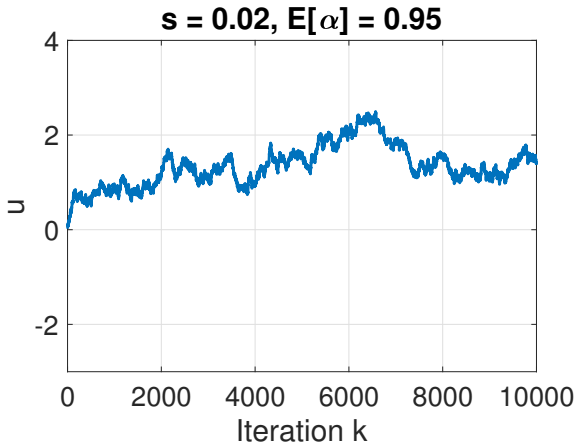

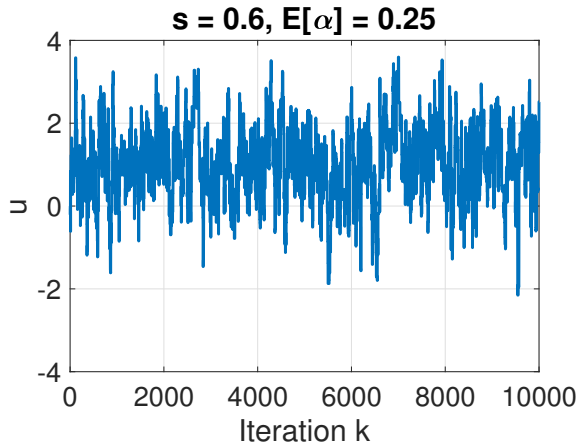

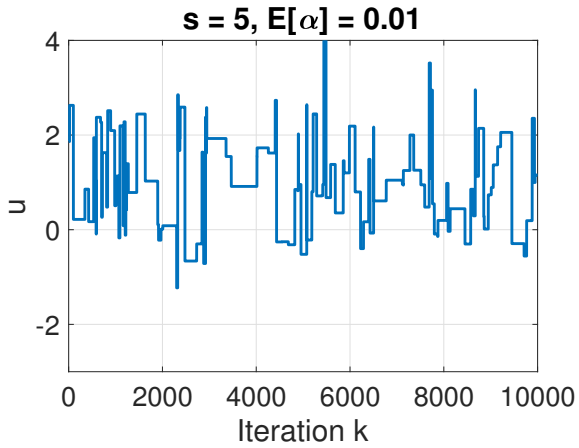

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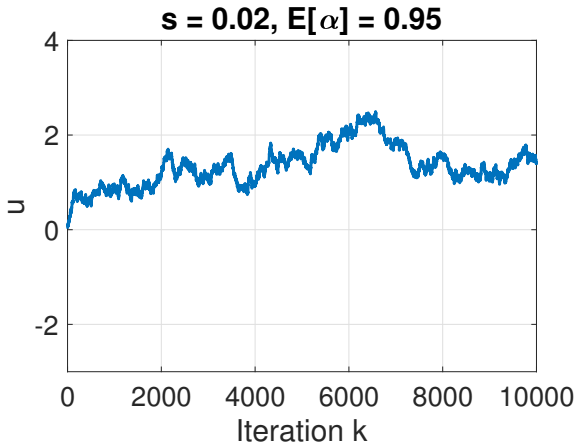

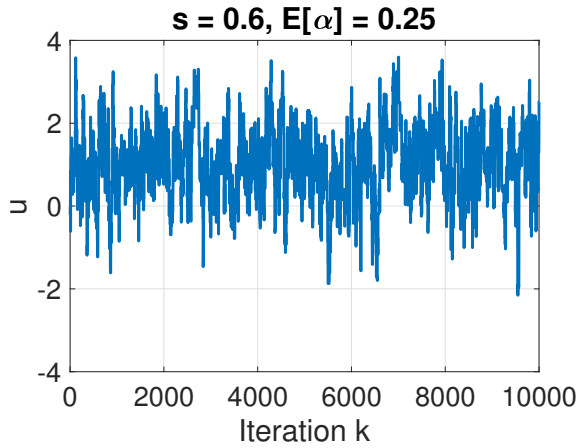

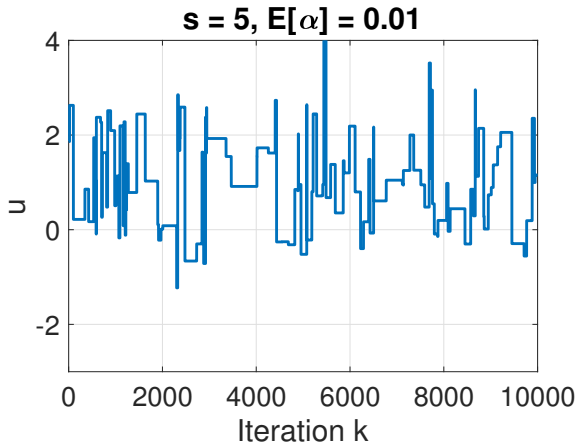

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Choose s such that $\mathbb{E}\left[\alpha(U, V)\right] = 0.234$

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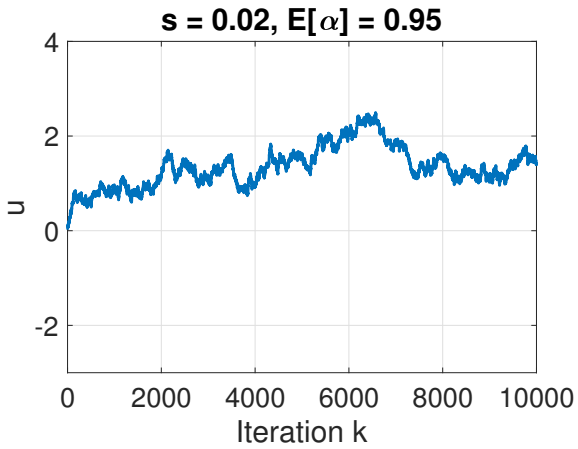

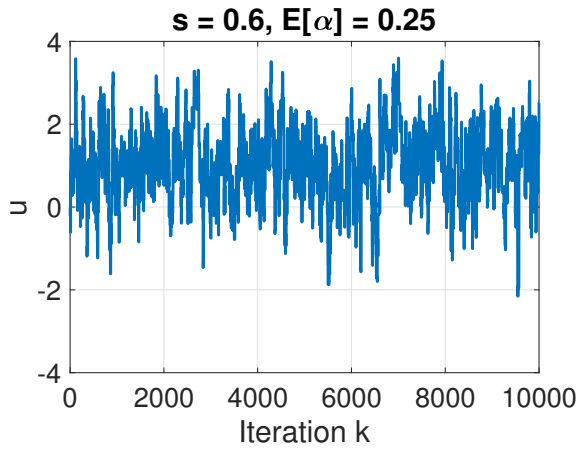

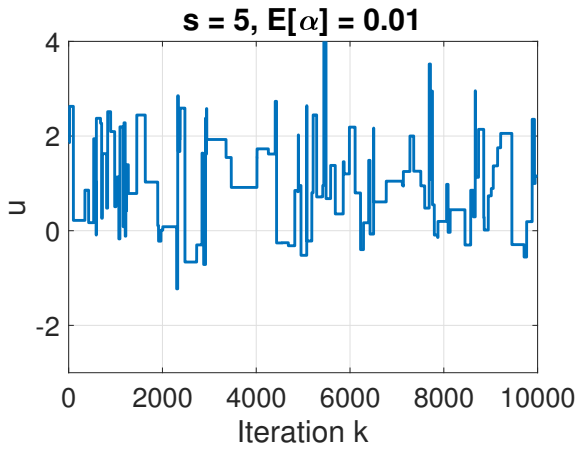

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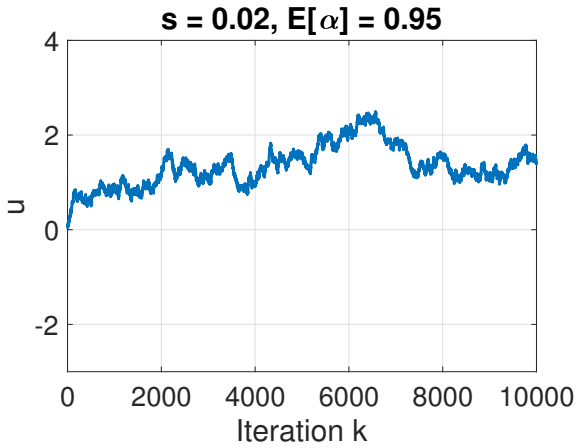

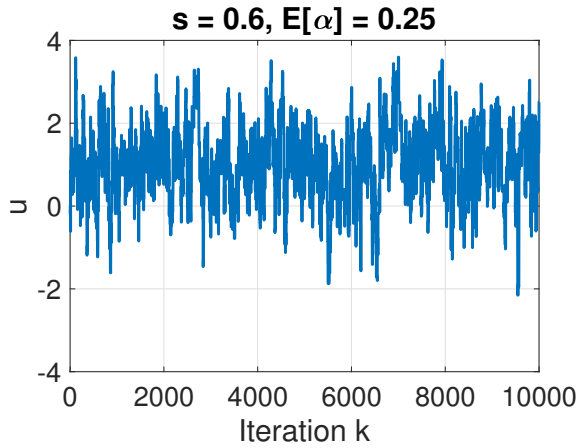

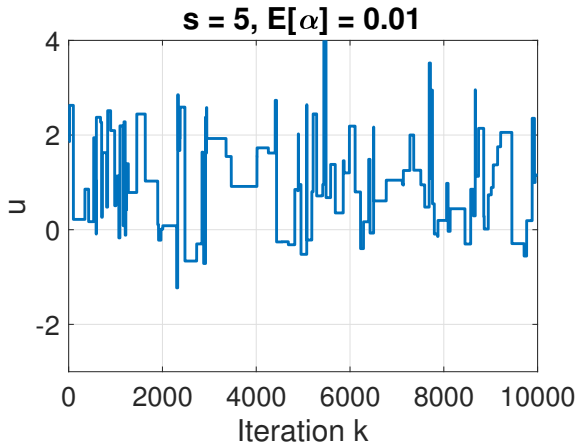

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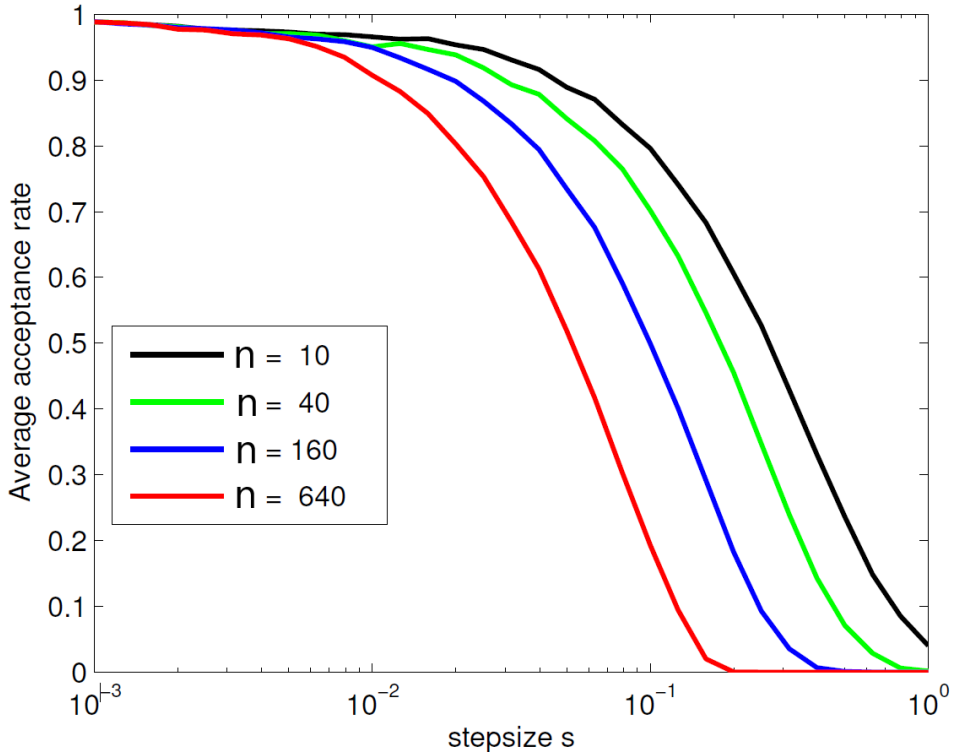
Random walk-proposal $P(u) = N(u, s^2 C)$



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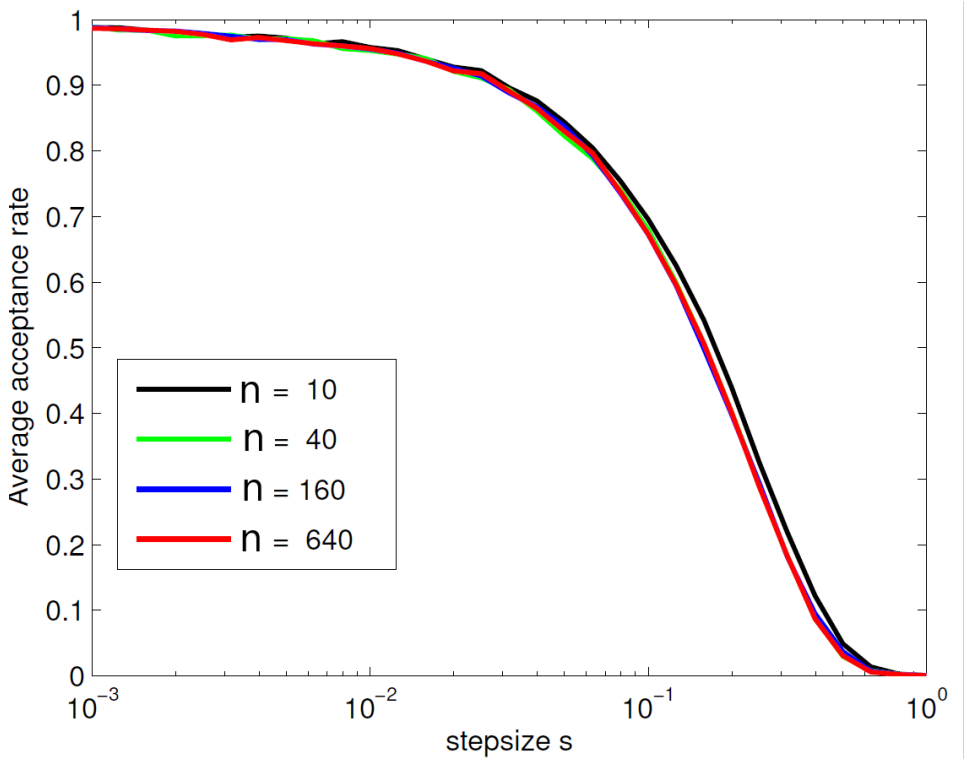

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This follows by Fubini and

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&= \min\left\{\frac{p(u,v)\ \pi(x)}{p(v,u)\ \pi(v)}, 1\right\} p(v,u)\ \pi(v) = \alpha(v,u)\ p(v,u)\ \pi(v).
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Corollary for Random Walk in $\mathcal{X} = \mathbb{R}^n$

Given target measure π with Lebesgue density $\pi(u) \propto \exp(-\Phi(u))\, \pi_0(u)$ the MH algorithm with proposal kernel $P(u) = \mathrm{N}(u, s^2 C)$ generates

1. an irreducible, aperiodic, Harris recurrent, and, thus, ergodic, Markov chain
2. which is, moreover, geometrically ergodic (under suitable conditions on π).

Metropolis–Hastings in Hilbert spaces

- Now $\pi \in \mathcal{P}(\mathcal{X})$ and $\mathcal{X}$ is a separable Hilbert space.
- Then, the MH algorithm targeting π and using "any" proposal kernel $P\colon \mathcal{X} \times \mathcal{B}(\mathcal{X}) \to [0,1]$ is **not always well-defined**.

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- The slightly modified pCN-proposal kernel $P = \mathrm{N}(\sqrt{1-s^2}u, s^2 C)$ on the other hand is π_0-reversible and yields a **well-defined MH algorithm on infinite-dimensional Hilbert spaces**.

Remarks

- pCN stands for "preconditioned Crank-Nicolson"

[4] A. Beskos, G. Roberts, A. Stuart, J. Voss. MCMC Methods for diffusion bridges. *Stoch. Dynam.* 8, 2008.

[5] R. M. Neal. Regression and Classification using Gaussian Process Priors. In: *Bayesian Statistics* 6, 1999.

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- In practice, also require 'burn-in' to overcome pre-asymptotic phase for $U_0 \not\sim \pi$

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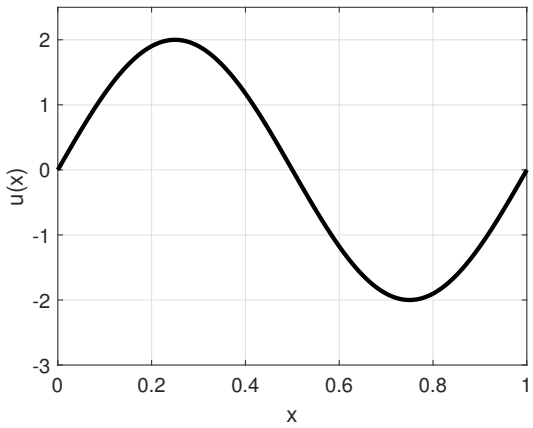
Numerical Experiment

Task: Infer unknown $u\colon [0,1] \to \mathbb{R}$ based on 4 noisy observations of p

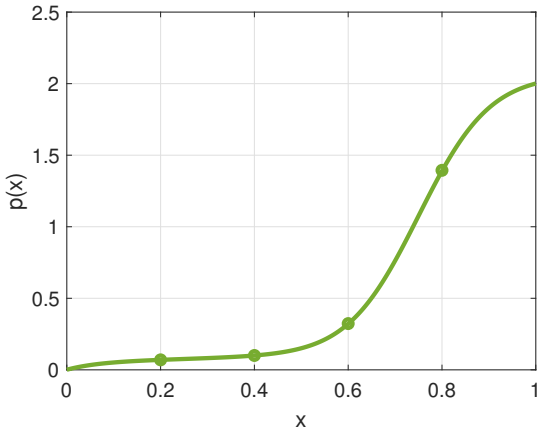
$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\mathrm{e}^{u(x)}\frac{\mathrm{d}p}{\mathrm{d}x}(x)\right) = 0, \qquad p(0) = 0,\ p(1) = 2.$$

Prior: $u \sim \pi_0 = \mathrm{N}(0, (-\Delta)^{-1})$ **Noise:** $\eta \sim \mathrm{N}(0, \sigma^2 I_4)$

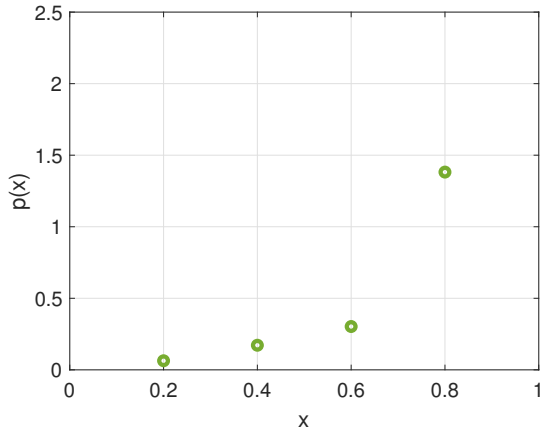
True u



True p



Noisy data $\boldsymbol{\delta}$



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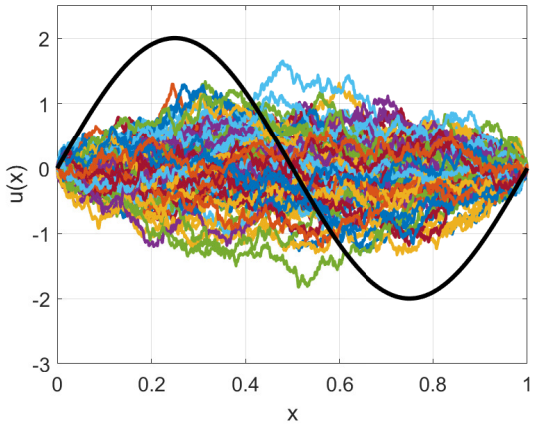
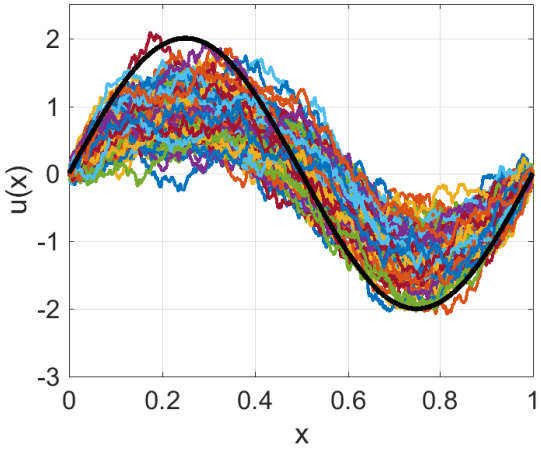
Prior π_0



π^y for $\sigma^2 = 0.01$



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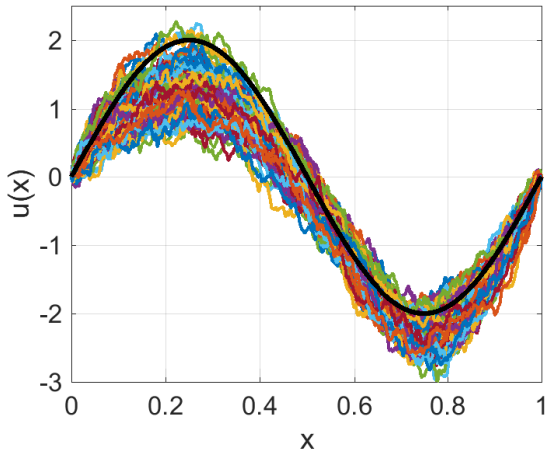

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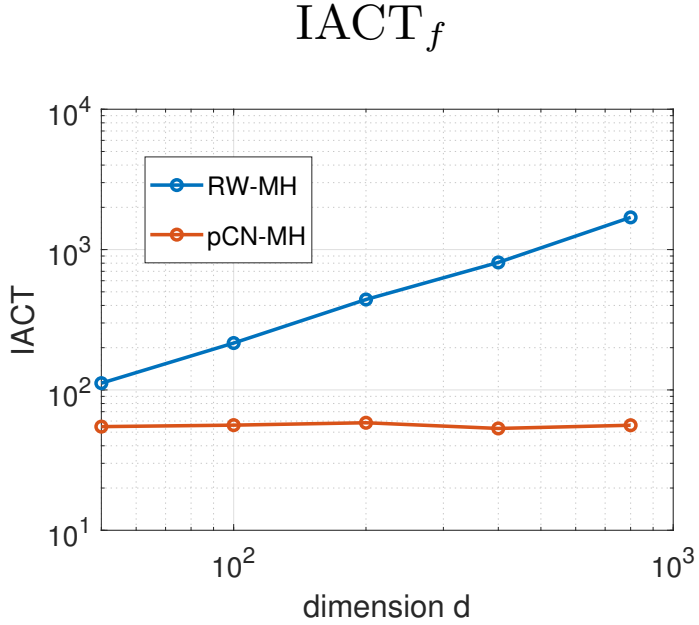
Performance:

RW $P(u) = \mathrm{N}(u, s^2(-\Delta)^{-1})$

pCN $P(u) = \mathrm{N}(\sqrt{1-s^2}u, s^2(-\Delta)^{-1})$

for increasing dimension, i.e., truncation length in KL expansion for u.



$\Longrightarrow$ **Dimension-independent efficiency of pCN-MH algorithm for sampling posterior in Bayesian inverse problem**

Summary – Part I

- Several Monte Carlo methods available to sample or integrate (approximately) w.r.t. posterior measure $\pi_{u|y}$.
- Markov chain Monte Carlo yields correlated samples U_i that are asymptotically distributed according to $\pi_{u|y}$ as $i \to \infty$
- Nonetheless preferable due to mild dimension-(in)dependence and usually robust performance
- Broad class of Metropolis–Hastings algorithms easy to implement
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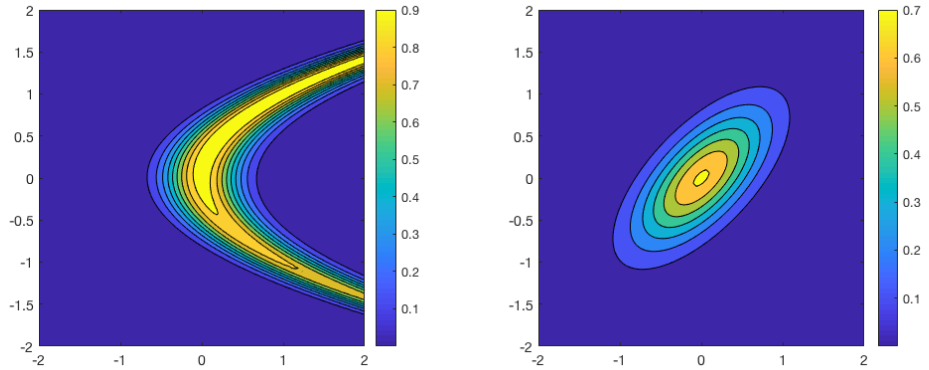
However, for concentrating posteriors in high dimensions the spectral gap of the pCN-Metropolis algorithm is very close to 1 and it **converges very slowly!**

(like Jacobi method for linear systems)

Better Proposals

How to incorporate gradient information?

- The proposals we have seen so far are agnostic about which parts of state space are more probable.
- Ideally we would like proposals that take this into account ($\Rightarrow$ make it more probable to move to areas where π is large).



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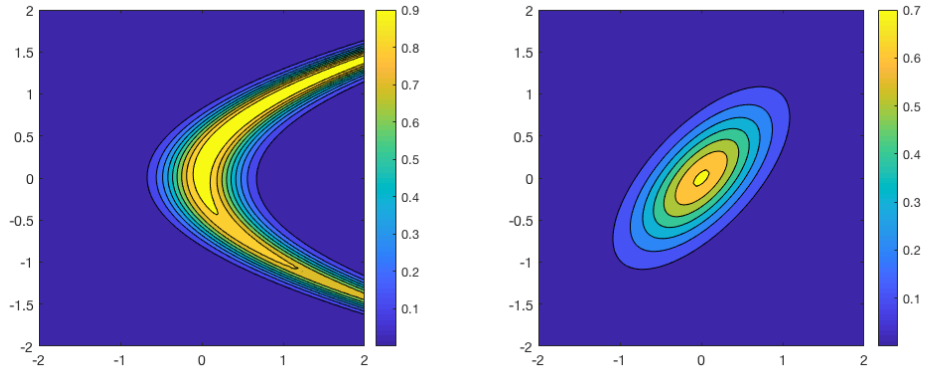


- Connecting to optimisation, a possible way to do this is to use gradient information and propose the next move in the following way

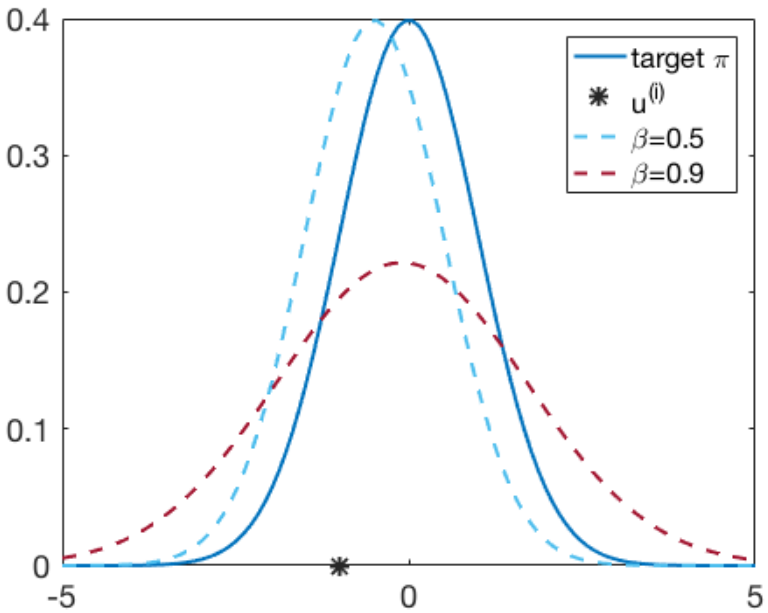
$$u' = u^{(i)} + \beta \nabla \pi(u^{(i)})$$

1. This is a deterministic move (we are losing randomness, and the ability to explore the state space, as we would converge to a local maximum).
2. How can we do this properly?

Metropolis adjusted Langevin algorithm (MALA)

- MALA [Pillai, Stuart, Thiery, 2012]: $P(u) = \mathrm{N}(u + \beta \nabla \log \pi(u), 2\beta \mathrm{I}),\ \beta > 0.$
- For optimal efficiency, step size β tuned s.t. average acceptance rate ≈ 0.574.

$$\Rightarrow \quad \beta \sim \dim(\mathcal{X})^{-1/3}$$



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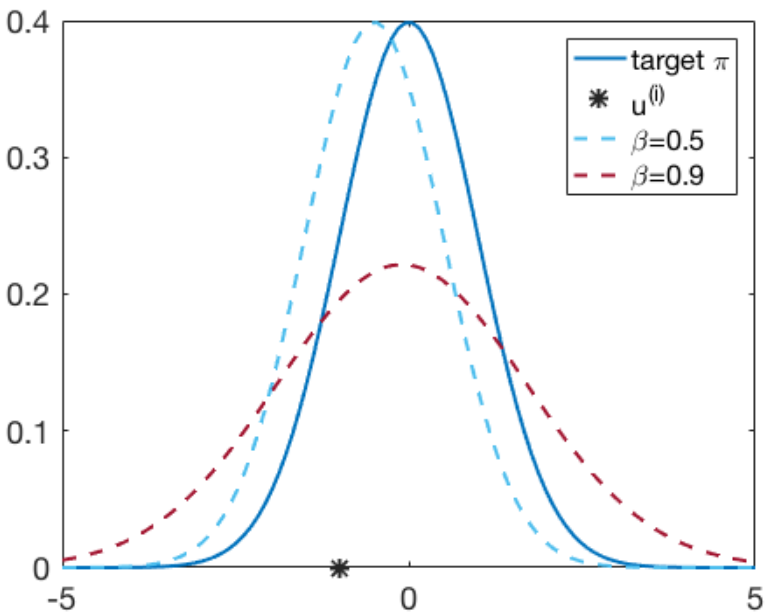

- Note that this is one Euler-Maruyama step applied to the Langevin SDE

$$dX = \nabla \log \pi(X) dt + \sqrt{2} dW$$

$$X_{n+1} = X_n + \beta \nabla \log \pi(X_n) + \sqrt{2\beta}\xi_n$$

with $\xi_n \sim \mathcal{N}(0, \mathrm{I})$.

- The stationary distribution of the Langevin SDE is π.

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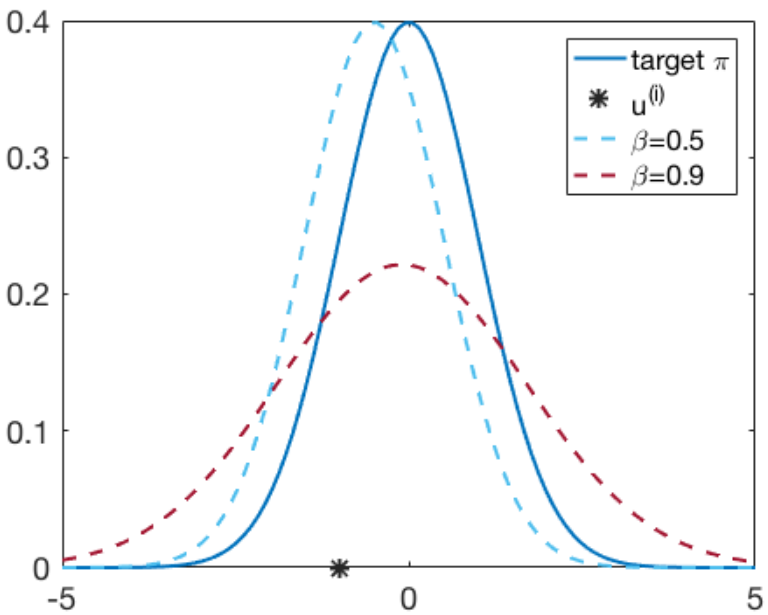

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- Can also include **Hessian** (2^{nd}-order) information. [Girolami, Calderhead, 2011], [Cui , Law, Marzouk, 2016], [Rudolf, Sprungk, 2018], ...

Surrogate transition method [Liu, 2001]

- This method uses a surrogate posterior $\pi^*(u)$ to pre-screen proposals.

Surrogate transition method

- At state u, sample a proposal v^* from proposal density $p^*(u, \cdot)$.
- Set $v = v^*$ with probability

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- Accept v with probability

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- **Important.** $\Phi(v)$ only evaluated for proposals that were accepted for π^*.
- The surrogate π^* can be, e.g., the posterior associated with a coarser discretisation ($h^* > h$ and/or $s^* < s$)

$\Rightarrow$ Multilevel MCMC [Dodwell, Ketelsen **RS**, Teckentrup, 2015], [Lykkegaard et al, 2023]

Summary – Part II

- MH algorithm with random walk or pCN proposals agnostic about the data and the likelihood.
- Better proposals are available that incorporate gradient or Hessian information abot the negative log-likelihood: **MALA, HMC, DILI, ...**
- To reduce cost we can 'prescreen' proposals with a cheaper surrogate using the **surrogate transition method** [Liu, 2001].
- Two particularly efficient methods of this type are the **multilevel MCMC method** [Dodwell, Ketelsen **RS**, Teckentrup, 2015] and the **multilevel delayed-acceptance algorithm** [Lykkegaard, Dodwell, Fox, Mingas, **RS**, 2023].
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Thank you very much!

Main References and other Useful Literature

R Scheichl & J Zech, *Numerical Methods for Bayesian Inverse Problems*, Lecture Notes, Heidelberg University, 2021. Available in the git repository and at `https://katana.iwr.uni-heidelberg.de/pdfs/NM4BIP21_notes.pdf`

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Some recent more advanced publications

- T Cui, G Detommaso & R Scheichl, Multilevel dimension-independent likelihood- Informed MCMC for large-scale inverse problems, *Inverse Prob* **40**, 2024
- T Cui, S Dolgov, R Scheichl, Deep importance sampling using tensor-trains with application to a priori and a posteriori rare event estimation, *SIAM J Sci Comput*, **46**, 2024
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