Non-reversible Langevin Methods for Sampling Complex Distributions

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Virtual seminar, McMaster University, 18 March 2020

The Need to Sample from Complex Distributions

Very complex, high-dimensional probability distributions arise in

- Statistical physics. The “canonical” distribution at a given temperature is the foundation for deriving the properties of physical systems such as liquids and magnetic materials.
- Bayesian statistics. The “posterior” distribution for unknown quantities is the foundation for statistical inference from data using the Bayesian approach.

By averaging over a random sample of points from these complex distributions, one can get *Monte Carlo* estimates of important quantities. For example,

- The volume of some quantity of a fluid at a given temperature and pressure.
- The predictive mean of a future observation based on past observations.

Markov Chain Sampling

Fast and accurate ways have been devised to randomly sample from many standard univariate distributions — binomial, exponential, etc. Multivariate distributions with a simple dependence structure can also be handled — eg, multivariate Gaussians.

Problem: There is no fast, general method of directly sampling from a high-dimensional distribution for which the joint probability mass or density is some complex function with no special properties.

A general approach: Instead simulate a Markov chain that converges to the desired distribution (from any starting point), in the limit of many transitions.

Surprisingly, this is often much easier than finding a way to sample directly!

Invariance and Reversibility

For a Markov chain to converge to a desired distribution, which has probability density $\pi(x)$, it is necessary for it to leave π *invariant*:

$$\text{For all } x, \quad \int \pi(x)\, T(x'|x)\, dx \;=\; \pi(x')$$

where $T(x'|x)$ is probability density for the Markov chain to move to state x' when it is currently in state x. (Convergence also requires that the Markov chain not get trapped in some subset of the state space.)

Invariance is implied by *reversibility* (also called “detailed balance”) with respect to π:

$$\text{For all } x \text{ and } x', \quad \pi(x)\, T(x'|x) \;=\; \pi(x')\, T(x|x')$$

Just integrate both sides over x to see this.

But reversibility is not *necessary* — non-reversible Markov chains that leave π invariant exist and are useful.

The Metropolis Algorithm

[Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller, 1953]

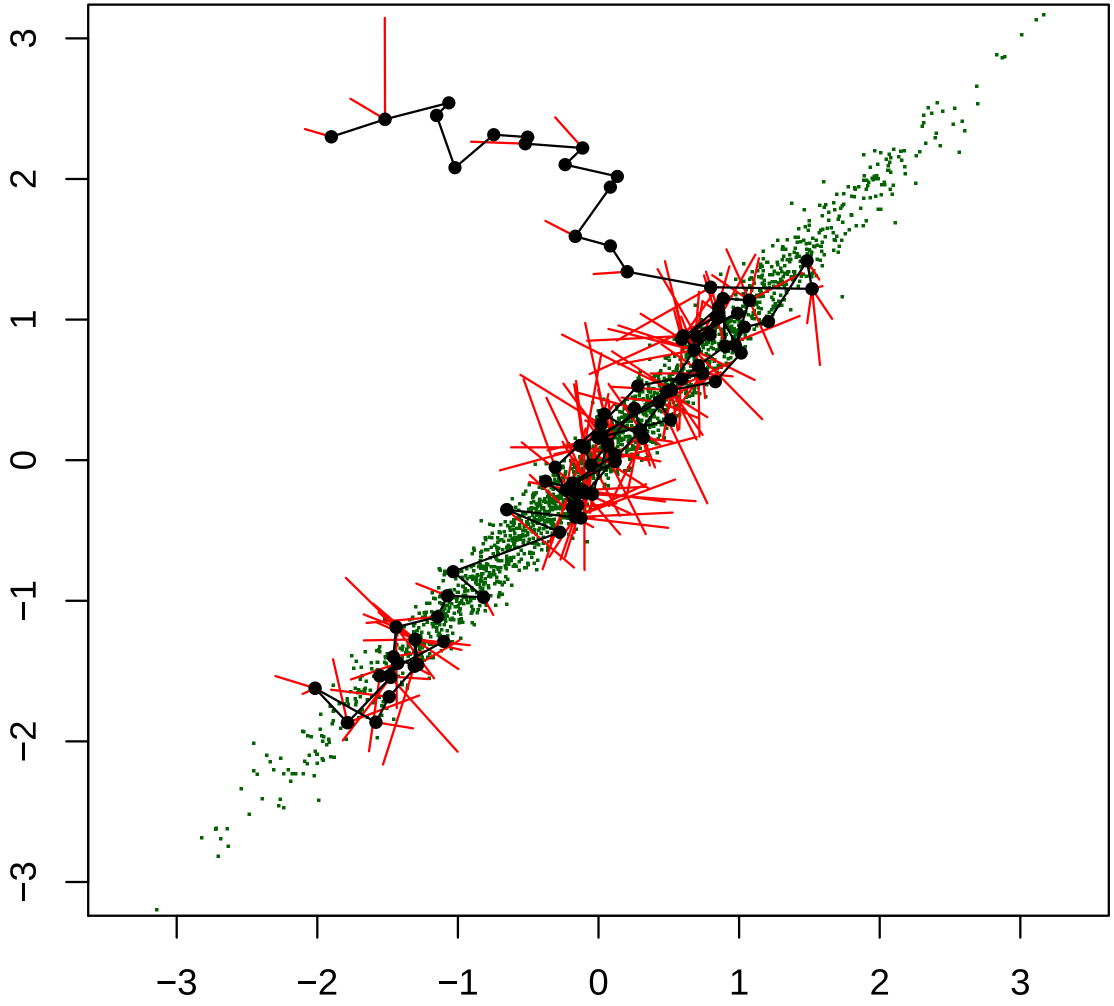
A very general way of defining a transition that's reversible for π was devised by Metropolis, et. al. — *propose* a state, x^*, to move to from x, and then *accept* or *reject* the proposal based on the ratio $\pi(x^*)/\pi(x)$. If we reject the proposal, the new state is the same as the old state.

Let $S(x^*|x)$ be the probability density for proposing to move to x^* when in state x. We require that $S(x^*|x) = S(x|x^*)$.

We accept the proposal x^* with probability $\min[1, \pi(x^*)/\pi(x)]$.
It's easy to show that the resulting transition is reversible with respect to π, and hence leaves π invariant.

Note: We only need the ratio $\pi(x^*)/\pi(x)$, which we can get even if we can only compute an unnormalized density function.

Illustration: Metropolis for Bivariate Gaussian



$$\text{Var}(x_1) \;=\; \text{Var}(x_2) \;=\; 1$$
$$\text{Cov}(x_1, x_2) \;=\; 0.99$$

$$S(x^*|x) \;=\; N(x^*; x,\, 0.3^2\, I)$$

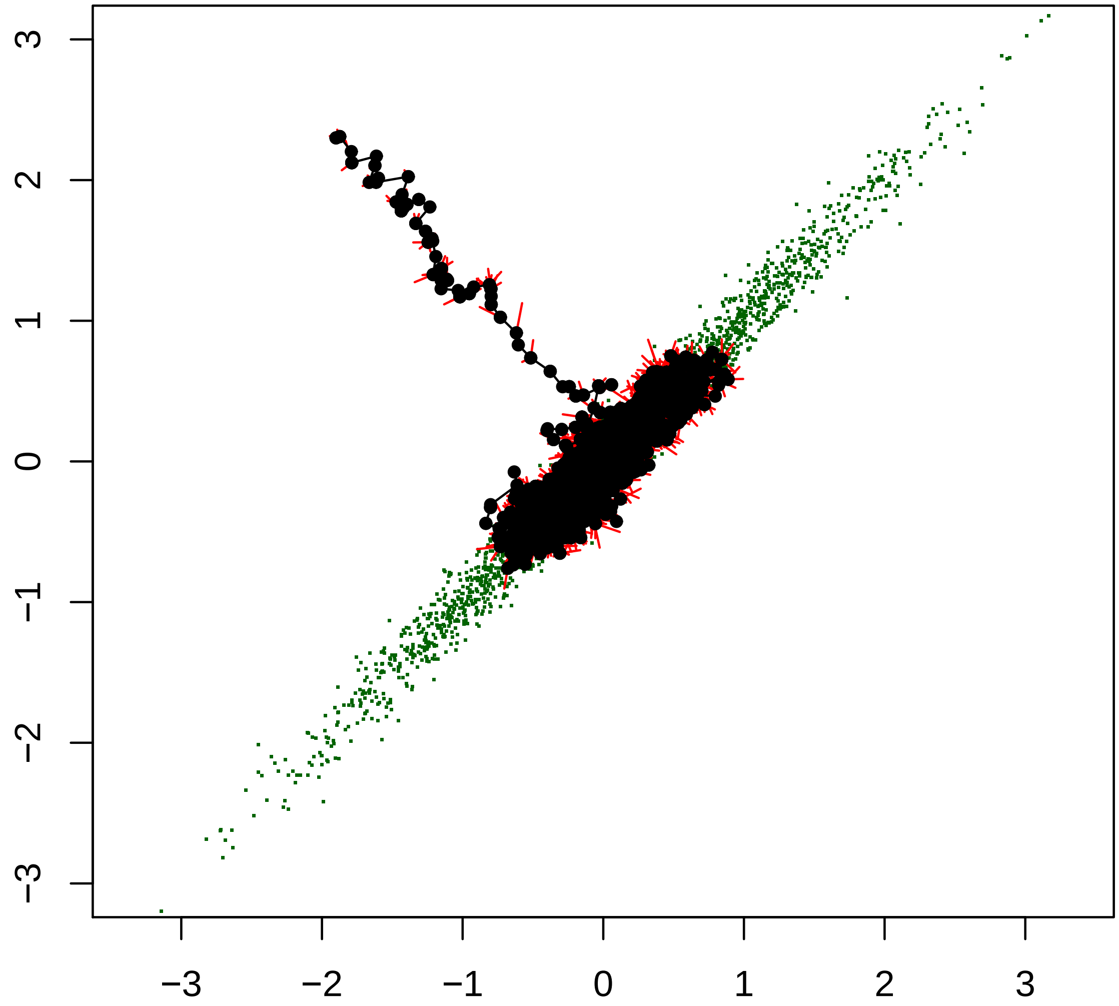
Green points are an i.i.d. sample from $\pi(x)$.

Black points show 250 transitions of the Markov chain

Rejection rate (last 90%) is 0.68. Red lines point to rejected proposals

When started from a low-probability point, the chain moves steadily towards the high-probability region. But once there, it wanders about the distribution in a random walk, often doubling back on itself.

Metropolis for Replicated Bivariate Gaussian



$$\mathrm{Var}(x_i) \;=\; 1,\;\; i = 1, \ldots, 20$$
$$\mathrm{Cov}(x_{2j-1}, x_{2j}) \;=\; 0.99$$

$$S(x^*|x) \;=\; N(x^*; x,\, 0.07^2\, I)$$

Green points are an i.i.d. sample from $\pi(x_1, x_2)$.

Black points show 4500 transitions of the Markov chain

Rejection rate (last 90%) is 0.71. Red lines point to rejected proposals

To get a similar rejection rate with 20 dimensions, a smaller proposal standard deviation is needed. So the random walk takes smaller steps. About 18 times more transitions are needed to move a similar distance.

The Inefficiency of Random Walks

Following an initial period of approach to convergence, reversibility implies that Metropolis transitions that each move only a small distance will explore high-probability regions via a *random walk*, with no tendency to keep going in the same direction.

This is inefficient.

A simple example: Suppose $x_{t+1} = x_t + n_t$, where n_t is a random draw from $N(0,1)$, independently for each t. Then x_{t+K} is likely to be only about $\sqrt{K}$ away from x_t — not about K away, as one might expect if the n_t all had the same sign.

Enormously faster exploration of the distribution can result from avoiding this inefficiency, by either:

- Using transitions that make big rather than small changes, or
- Not doing a random walk (using non-reversible transitions).

Combining Transitions in Sequence

If we have several Markov transitions, $T_1, T_2, \ldots, T_k$, all of which leave the distribution π invariant, then the combined transition that applies each of these T_i in sequence will also leave π invariant.

But even if $T_1, T_2, \ldots, T_k$ are all reversible w.r.t. π, the combination will generally not be reversible.

Gibbs Sampling: For a multivariate state, $x = (x_1, \ldots, x_k)$, each T_i might update only component x_i, replacing it with a random value from its conditional distribution given the other components.

Gibbs sampling is generally not reversible, but the non-reversibility seems to have no important consequences. But in other situations, non-reversible transitions constructed by sequential combinations can be much better than reversible methods.

Hamiltonian Monte Carlo (HMC)

[Duane, Kennedy, Pendleton, and Roweth, 1987]

Simple Metropolis proposals (eg, Gaussian) lead to slow exploration via a random walk. Much better is to make distant proposals by simulating Hamiltonian dynamics for some period of fictitious "time".

We augment the variable of interest, x, with a "momentum" variable, p, of equal dimension, with a Gaussian distribution, independent of x.

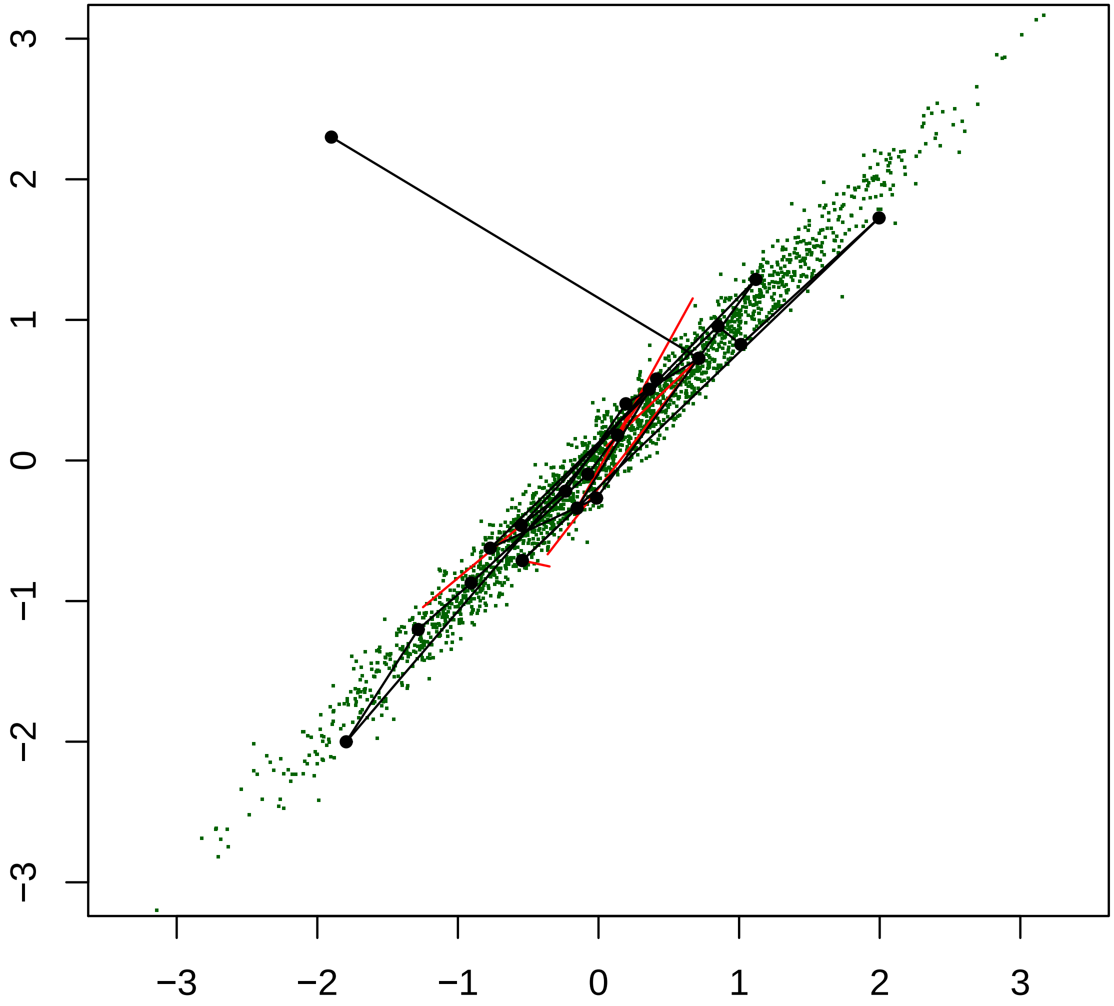
An HMC transition has two parts:

1) Sample p from its distribution (eg, $N(0, I)$).

2) Do a Metropolis update, with proposal found by simulating Hamiltonian dynamics from (x, p) for some time τ (then negating p so the proposal is symmetrical).

If the dynamical simulation were exact, the proposal would always be accepted — the dynamics preserves the log of the joint density of (x, p). In practice, we simulate the dynamics with L "leapfrog" steps, each for a time $\epsilon = \tau / L$. Since these steps are not exact, rejection is possible.

Illustration: HMC for Bivariate Gaussian



$\text{Var}(x_1) = \text{Var}(x_2) = 1$
$\text{Cov}(x_1, x_2) = 0.99$

$\epsilon = 0.16$, $L = 10$

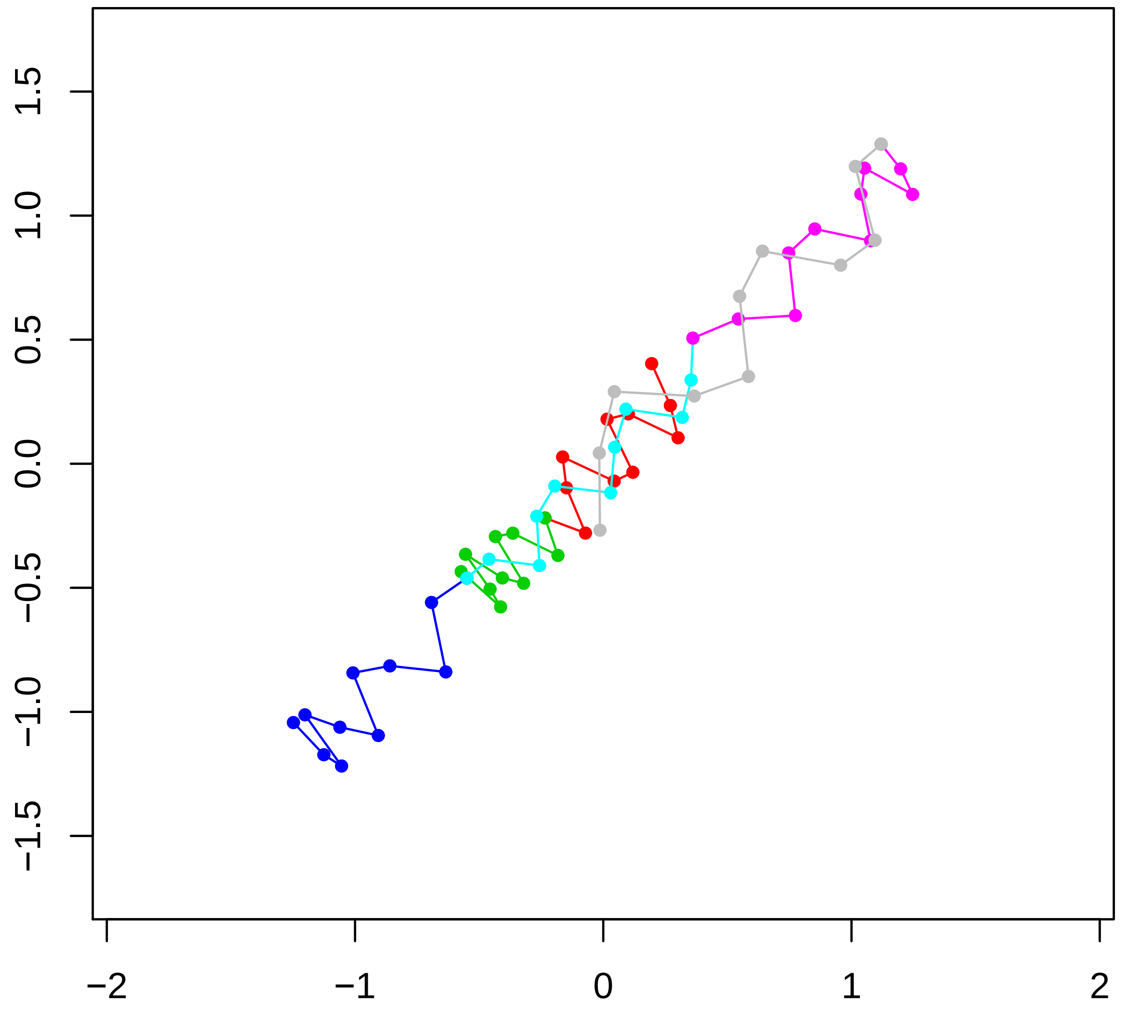
Green points are an i.i.d. sample from $\pi(x)$.

Black points show 25 transitions of the Markov chain

Rejection rate (last 90%) is 0.22. Red lines point to rejected proposals

HMC proposals (as found with suitably long trajectories) are often to states distant from the current state. So even though HMC is reversible, random walks are not a problem.

Some HMC Trajectories for the Bivariate Gaussian



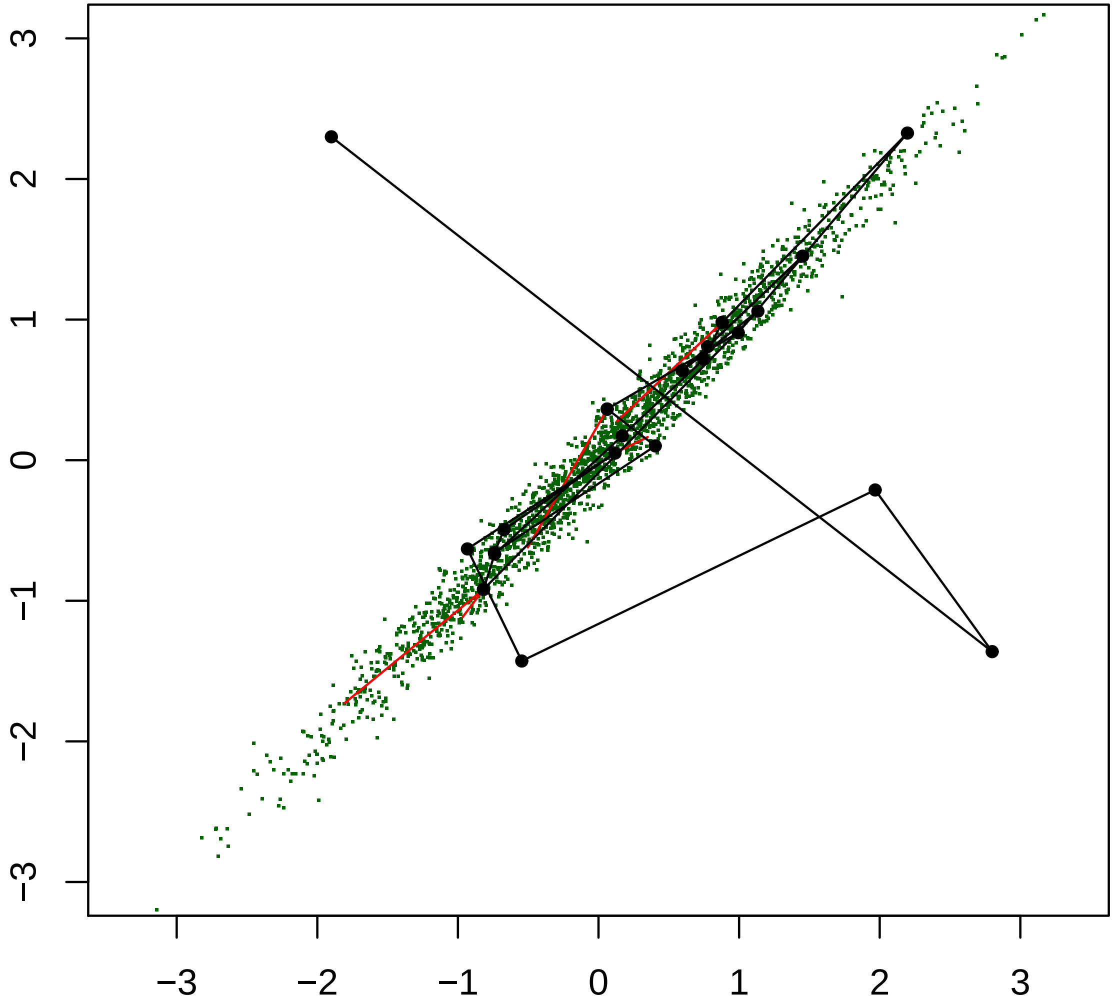
Six successive trajectories (red first) used to produce proposals for HMC (blue rejected, others accepted)

Only x is shown (not p)

$\epsilon = 0.16$, $L = 10$

The dynamics confines the trajectories to the high-probability region, while keeping them going in the same direction (except turning at an end). But each trajectory has a random initial direction.

HMC for Replicated Bivariate Gaussian



$$\mathrm{Var}(x_i) \;=\; 1,\; i=1,\ldots,20$$
$$\mathrm{Cov}(x_{2j-1},x_{2j}) \;=\; 0.99$$

$\epsilon \;=\; 0.1,\, L \;=\; 16$

Green points are an i.i.d. sample from $\pi(x)$.

Black points show 25 transitions of the Markov chain

Rejection rate (last 90%) is 0.22. Red lines point to rejected proposals

With 20 dimensions, ϵ needs to be smaller, and so L needs to be larger to compensate. But the scaling of HMC with dimensionality is substantially better than for simple Metropolis methods.

Langevin Monte Carlo

[Rossky, Doll, and Friedman, 1978; others later]

Doing only one leapfrog step in HMC is equivalent to “Langevin” Monte Carlo. A Langevin transition goes as follows:

- Sample p (of same dimension as x) from the $N(0, I)$ distribution.
- Compute a proposal (x^*, p^*) with one leapfrog step, as follows:

$$\begin{aligned} p^\circ &= p \;-\; (\epsilon/2)\, \nabla \log \pi(x) \\ x^* &= x \;+\; \epsilon\, p^\circ \\ p^* &= -\,[\, p^\circ \;-\; (\epsilon/2)\, \nabla \log \pi(x^*)\,] \end{aligned}$$

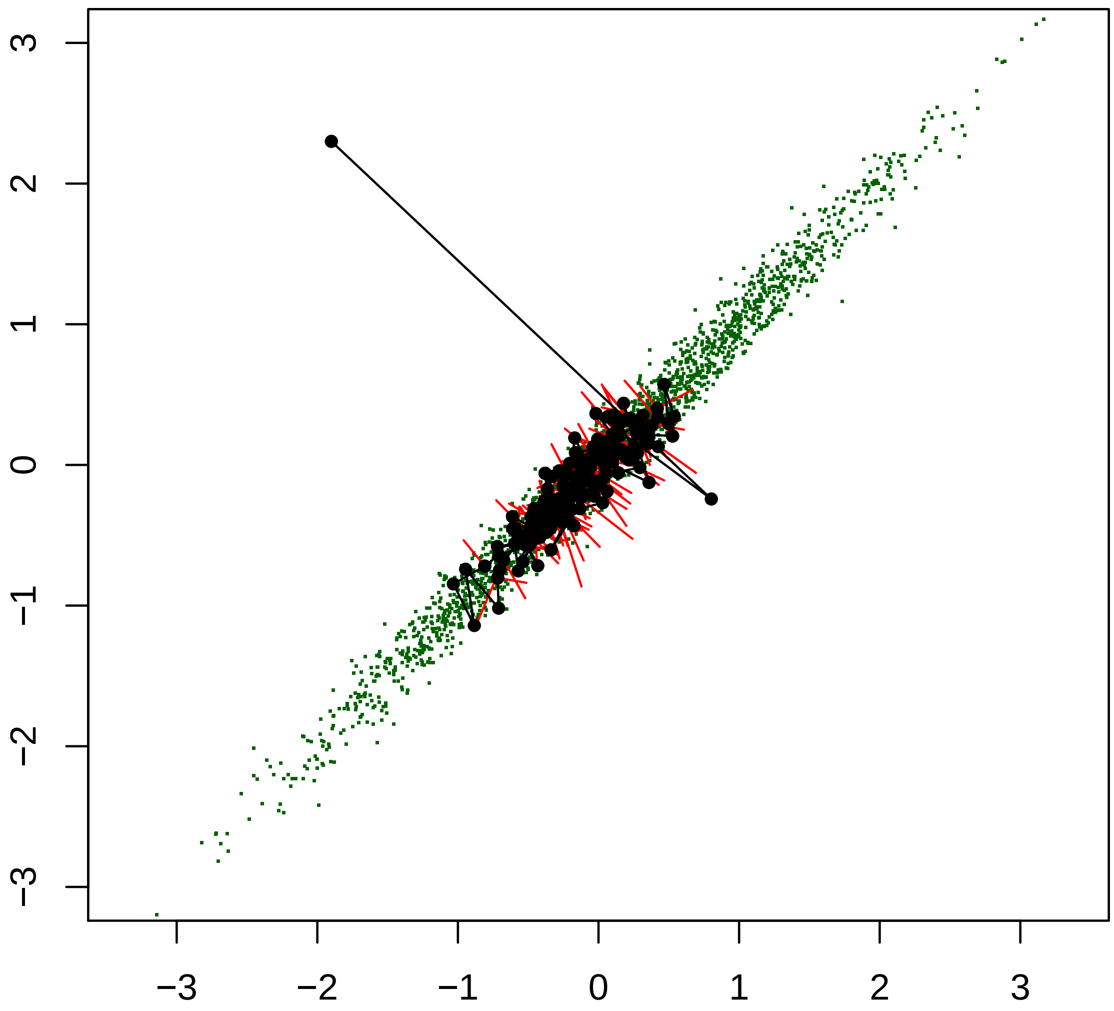
- Accept (x^*, p^*) as the new state with probability

$$\min\,[1,\ \pi(x^*)\phi(p^*)\,/\,\pi(x)\phi(p)]$$

  where $\phi(p)$ is the probability density for the $N(0, I)$ distribution. If (x^*, p^*) is not accepted, the new state is the same as the old.

Note: we can write x^* as $x + (\epsilon^2/2)\nabla \log \pi(x) + \epsilon n$, with $n \sim N(0, I)$.

Illustration: Langevin for Bivariate Gaussian



$$\mathrm{Var}(x_1) \;=\; \mathrm{Var}(x_2) \;=\; 1$$
$$\mathrm{Cov}(x_1, x_2) \;=\; 0.99$$

$\epsilon \;=\; 0.17.$

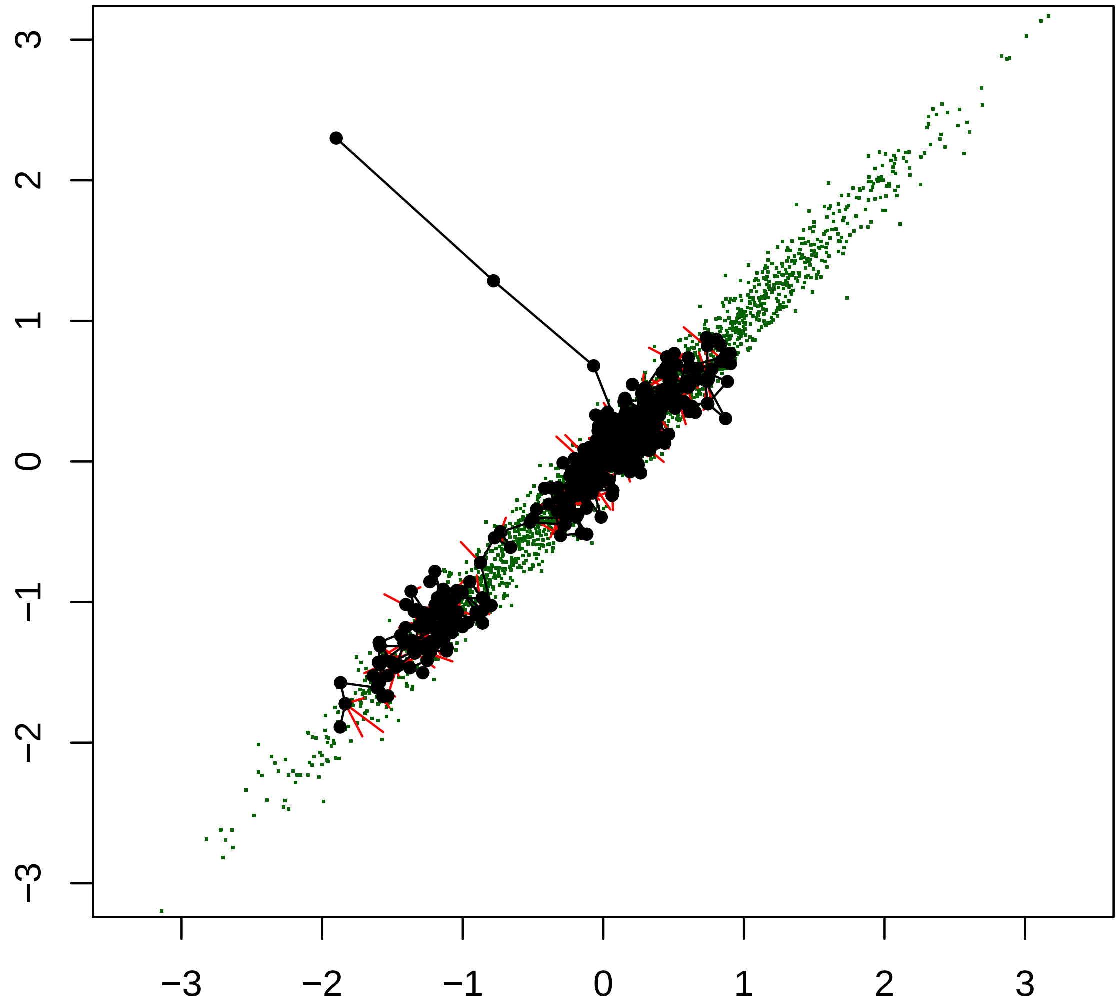
Green points are an i.i.d. sample from $\pi(x)$.

Black points show 250 transitions of the Markov chain

Rejection rate (last 90%) is 0.37. Red lines point to rejected proposals

Langevin benefits from using gradient information, but since it is reversible, and (typically) takes small steps, it still suffers from the inefficiency of a random walk.

Langevin for Replicated Bivariate Gaussian



$\text{Var}(x_i) \;=\; 1,\; i = 1, \ldots, 20$

$\text{Cov}(x_{2j-1}, x_{2j}) \;=\; 0.99$

$\epsilon \;=\; 0.11.$

Green points are an i.i.d. sample from $\pi(x)$.

Black points show 600 transitions of the Markov chain

Rejection rate (last 90%) is 0.39. Red lines point to rejected proposals

Langevin's scaling with dimensionality is better than for simple Metropolis, but worse than for HMC.

Langevin Monte Carlo with Persistent Momentum

[Horowitz, 1991]

A transition from (x, p) to the next state has three steps:

1) Update p to $\alpha p + \sqrt{1-\alpha^2}\, n$, where α is slightly less than 1 and n is a $N(0, I)$ random variable.

2) Propose a new state by doing one leapfrog step from (x, p) and then negating p. Accept or reject this proposal the usual way.

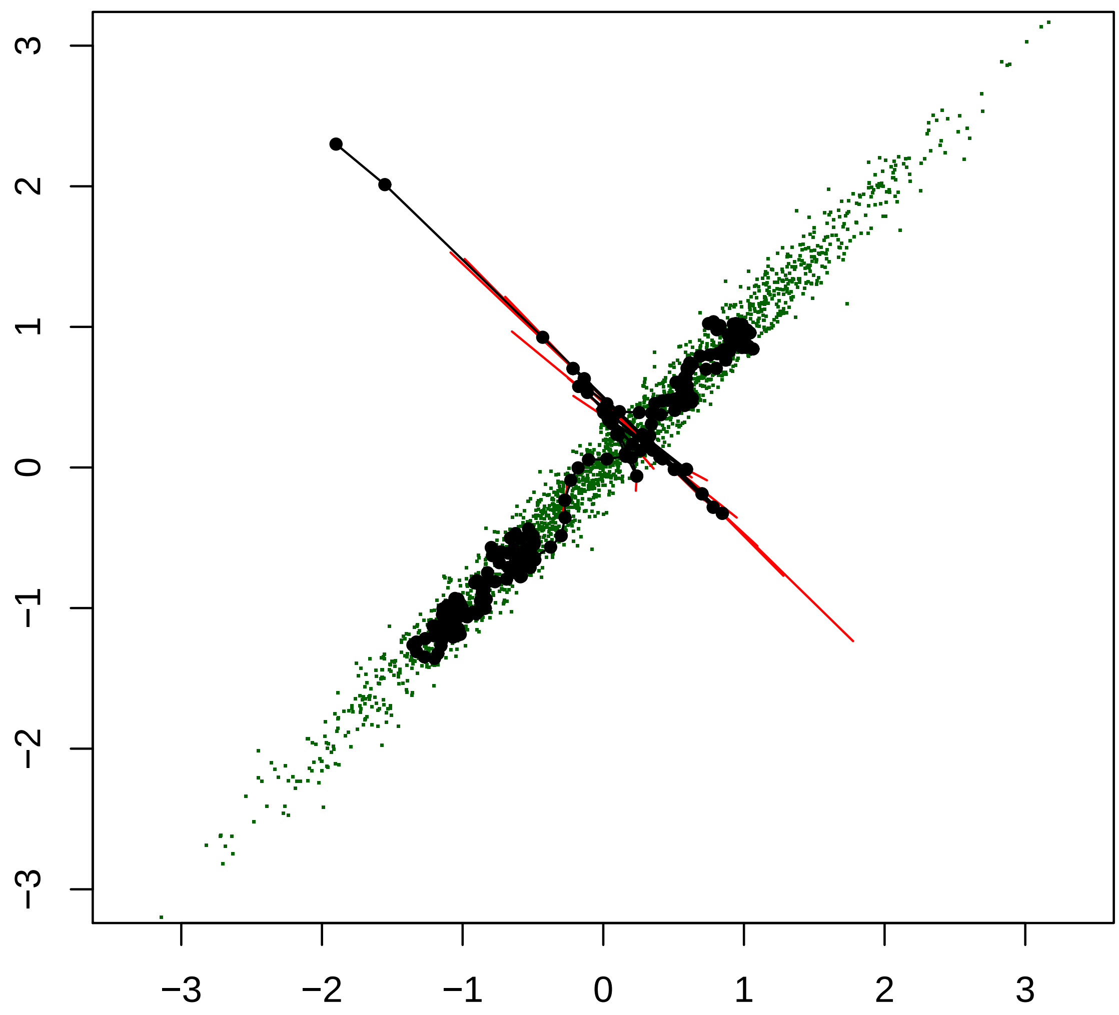
3) Negate p.

All steps leave the desired distribution invariant and are reversible.

Their sequential combination leaves the desired distribution invariant but is not reversible.

For α near 1, Step (1) only slightly changes p. If Step (2) accepts, the negation in the proposal is canceled by the negation in Step (3). But a rejection will reverse p, and the chain will almost double back on itself.

Illustration: Persistent Langevin for Bivariate Gaussian



$\mathrm{Var}(x_1) = \mathrm{Var}(x_2) = 1$

$\mathrm{Cov}(x_1, x_2) = 0.99$

$\epsilon = 0.062$, $\alpha = 0.94$

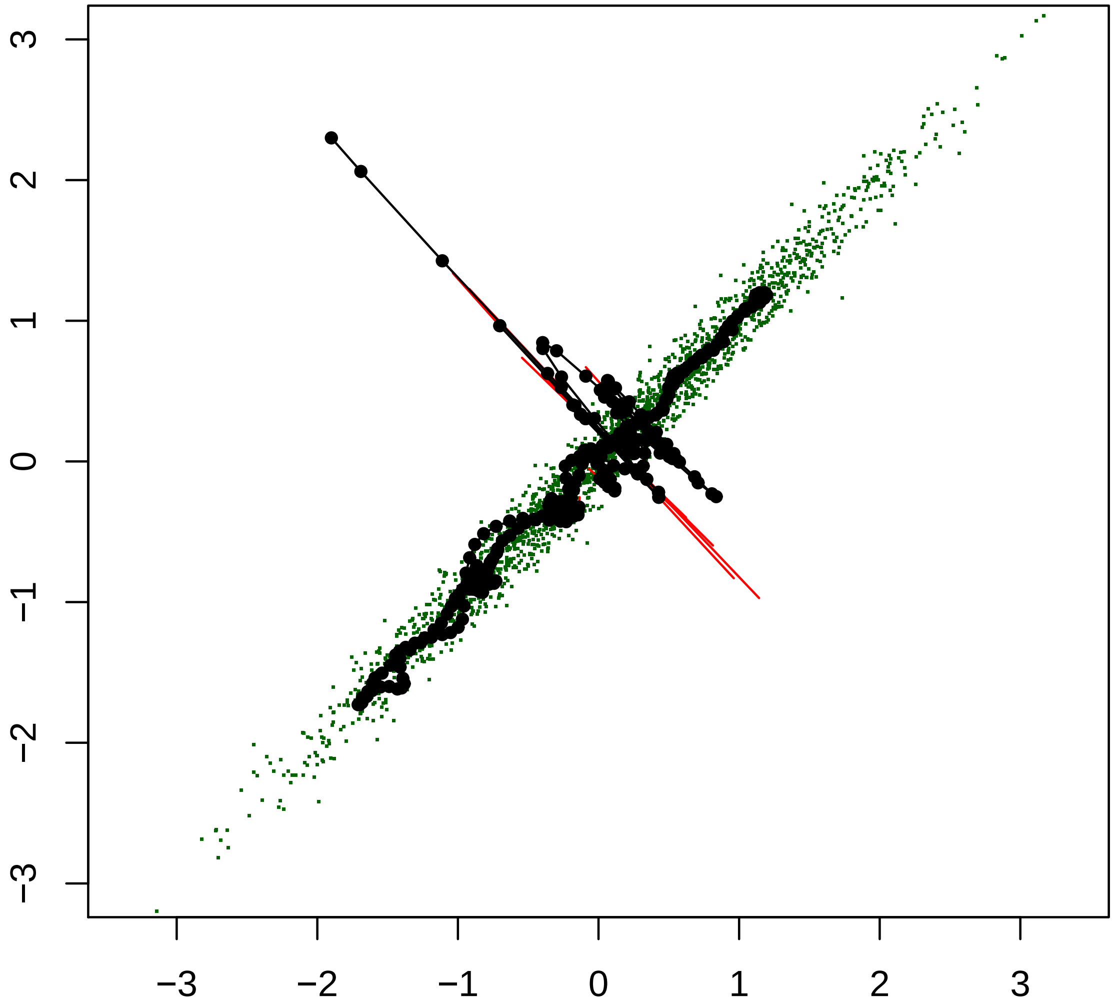
Green points are an i.i.d. sample from $\pi(x)$.

Black points show 250 transitions of the Markov chain

Rejection rate (last 90%) is 0.044. Red lines point to rejected proposals

By only slightly changing p each iteration, persistent Langevin can suppress random walk behaviour. Unfortunately, for this to work, the rejection rate must be small (comparable to or less than $1-\alpha$).

Persistent Langevin for Replicated Bivariate Gaussian



$\mathrm{Var}(x_i) \; = \; 1, \; i = 1, \ldots, 20$
$\mathrm{Cov}(x_{2j-1}, x_{2j}) \; = \; 0.99$

$\epsilon \; = \; 0.045, \; \alpha \; = \; 0.95$

Green points are an i.i.d. sample from $\pi(x)$.

Black points show 345 transitions of the Markov chain

Rejection rate (last 90%) is 0.035. Red lines point to rejected proposals

As dimensionality increases, ϵ must be made even smaller in order to keep the rejection rate very small.

Avoiding Reversals $\Rightarrow$ Inefficient Small Stepsize

Unfortunately, though persistent Langevin can avoid random walks, it does so only *only* if the rejection rate is small. This requires a small ϵ, which slows speed of exploration.

So it's not as good as Hamiltonian Monte Carlo, which can use a comparatively large ϵ even when the number of leapfrog steps, L, needs to be quite large in order to avoid random walks.

The new innovation: As well as the non-reversibility from not completely replacing p, also introduce non-reversibility into the *acceptance decision.*

Non-Reversible Form of the Acceptance Decision

To decide on accepting a Metropolis proposal to move from x to x^*, we can check if $u < \pi(x^*)/\pi(x)$, with u a random uniform over $[0, 1]$.

Equivalently, we can check whether $\pi(x^*) > s$, where s is a random uniform over $[0, \pi(x)]$.

Rather than choosing s randomly, we can make it, or $u = s/\pi(x)$, part of the state, and update it in any way that leaves the joint distribution invariant.

One possible update: For some constant δ, add/subtract δs to s, reflecting off the boundaries at 0 and $\pi(x)$.

Implementation details: We let $s = \pi(x)|v|$, with v having the uniform(-1,$+1$) distribution. We update v by adding δ, and then subtracting 2 if $v > 1$. If x changes to x', we make a corresponding change of v to $v' = v\pi(x)/\pi(x')$, which keeps s unchanged.

Non-Reversible Acceptance Can Cluster Rejections, Avoid Random Walks at a Higher Rejection Rate

If the rejection rate is not high, $\pi(x^*)/\pi(x)$ will usually be close to one. So u will mostly change as a result of adding δ (reflecting off 0 and 1). If δ is small, u will be near 0 for a while, then near 1 for a while, etc.

Rejections will tend to be *clustered*, and acceptances will be too. (Overall rejection rate will be same as for the standard method.)

Clustering of rejections produces *less random walk behaviour*.

Compare: If each accept moves d in same direction, each reject randomizes direction, then $20K$ iterations of the following form:

4 accepts, 1 reject, 4 accepts, 1 reject, . . .

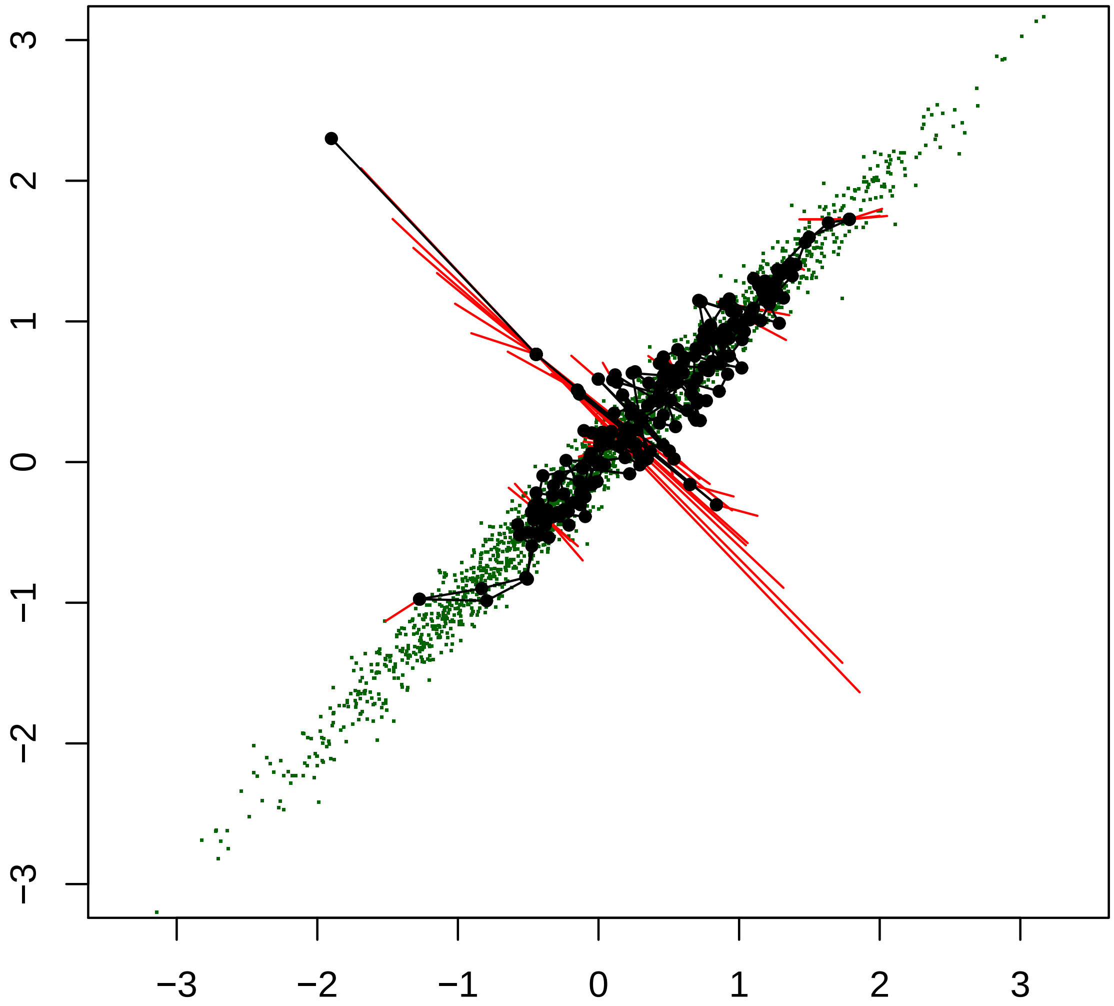
move on average a distance of $4d\sqrt{4K} \;=\; 8d\sqrt{K}$.

But $20K$ iterations of the form:

16 accepts, 4 rejects, 16 accepts, 4 rejects, . . .

move on average a distance of $16d\sqrt{K}$.

Illustration: Persistent Langevin with Non-Reversible Acceptance for Bivariate Gaussian



$\mathrm{Var}(x_1) = \mathrm{Var}(x_2) = 1$
$\mathrm{Cov}(x_1, x_2) = 0.99$

$\epsilon = 0.12,\ \alpha = 0.92,\ \delta = 0.05$

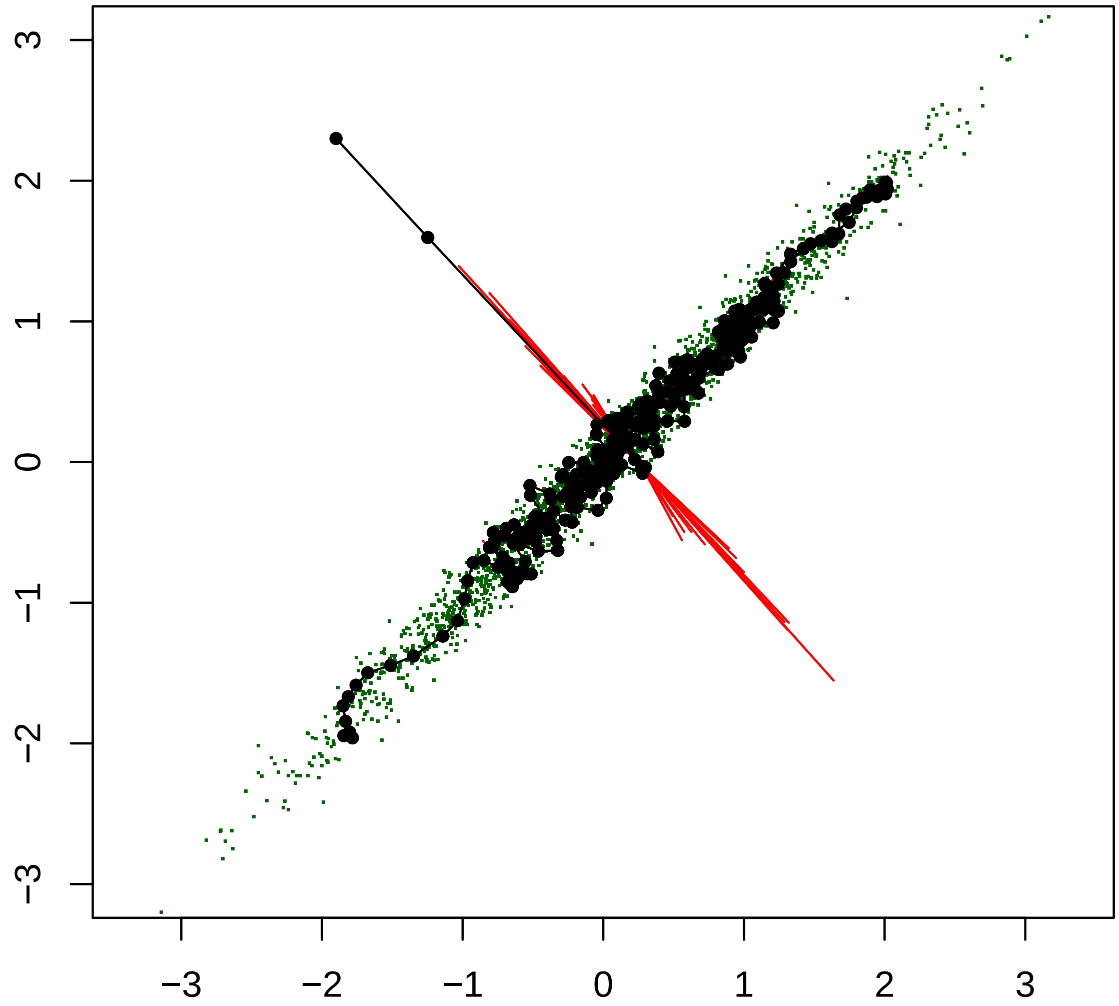
Green points are an i.i.d. sample from $\pi(x)$.

Black points show 250 transitions of the Markov chain

Rejection rate is 0.13; red lines point to rejected proposals

Compare to standard acceptance, with $\epsilon = 0.062$ and rejection rate of 0.044. Here, random walks are mostly suppressed despite a rejection rate of 0.13, and the larger ϵ of 0.12 leads to more movement.

Persistent Langevin with Non-Reversible Acceptance for Replicated Bivariate Gaussian



$\text{Var}(x_i) \;=\; 1,\; i = 1, \ldots, 20$

$\text{Cov}(x_{2j-1}, x_{2j}) \;=\; 0.99$

$\epsilon = 0.08,\ \alpha = 0.94,\ \delta = 0.05$

Green points are an i.i.d. sample from $\pi(x)$.

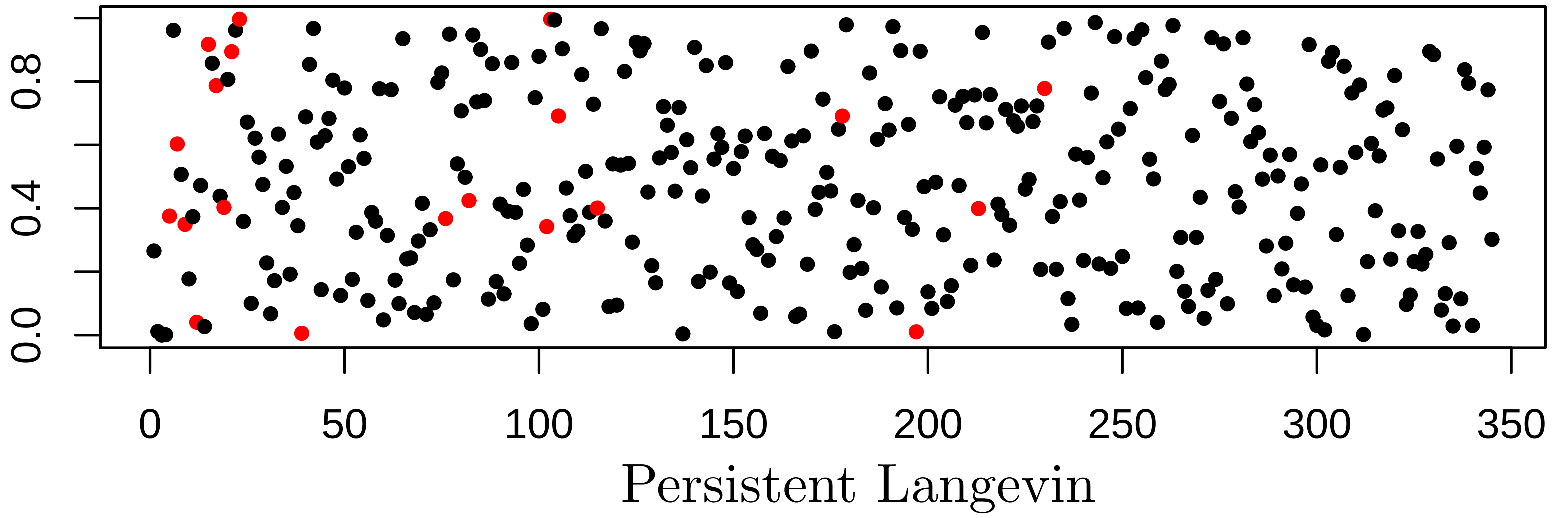
Black points show 345 transitions of the Markov chain

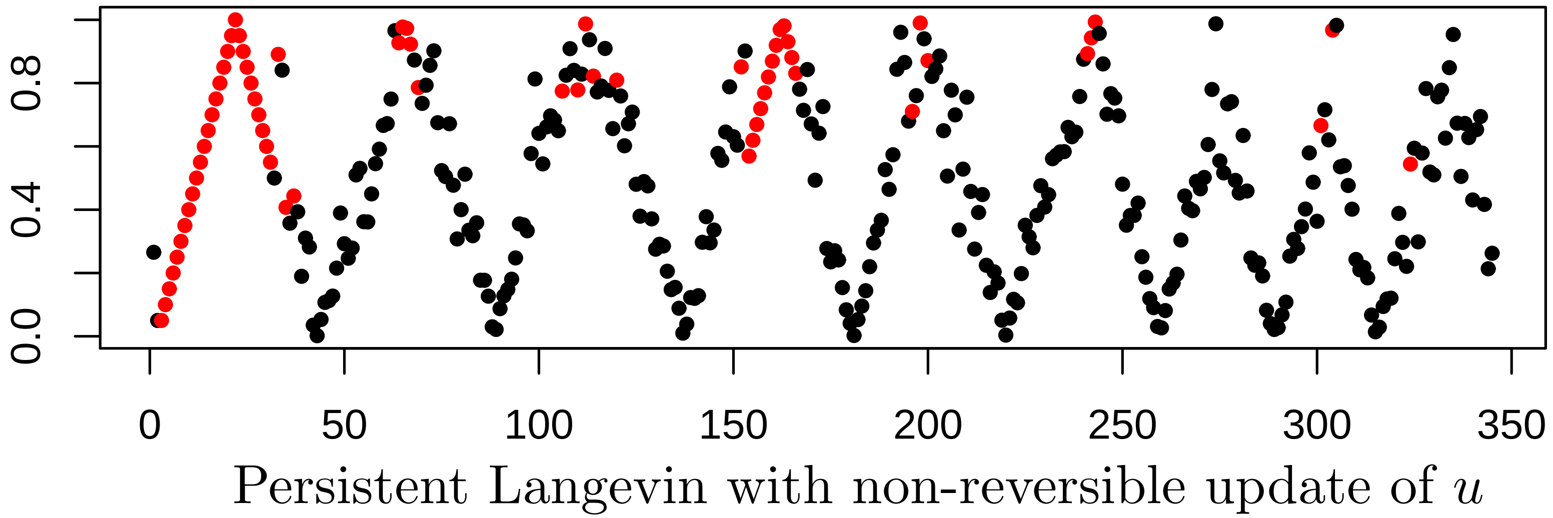
Rejection rate is 0.11; red lines point to rejected proposals

A smaller ϵ is needed in higher dimensions, then α needs to be closer to 1 for the same random walk suppression. Choosing δ to be roughly $1-\alpha$ seems about right. Performance here seems comparable to HMC.

Changes to u and Clustering of Rejections

Plots of u values for each accept/reject decision, with values leading to rejection in red, for sampling from replicated bivariate Gaussian:





Advantage for Models with Discrete Variables

With non-reversible acceptance, persistent Langevin can be made about as efficient as HMC. But does it have any advantage over HMC?

It can be better when the state consists of both continuous and discrete variables — then HMC or Langevin updates must be combined (eg, in sequence) with updates such as Gibbs sampling for the discrete variables.

If HMC does L leapfrog steps, the discrete variables can be updated only once every L steps. But a Langevin method can update them more often — possibly after every step, though a bigger interval may sometimes be better.

Advantage for Models with Variance Hyperparameters

Langevin's advantage over HMC of allowing more frequent updates of other sorts also applies to Bayesian models with variance hyperparameters — eg, prior variances for groups of weights in a Bayesian neural network model.

Even though variance hyperparameters are continuous, they can cause problems if updated with other continuous variables. Consider:

$$\begin{aligned} y_i \mid x_i,\, \beta,\, \sigma &\sim N(\beta^T x_i, \sigma^2) \\ \beta \mid \tau &\sim N(0, \tau^2 I) \\ \tau,\, \sigma &\sim \ldots\text{something}\ldots \end{aligned}$$

Using an HMC or Langevin method for sampling β alone, with σ and τ temporarily fixed, can work well, perhaps using an ϵ that is set based on the current σ and τ. But including σ and τ (or their logs) in the state makes setting ϵ very difficult. It may be better to update them separately (eg, with Gibbs sampling or Metropolis).

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