II

Markov chain Monte Carlo

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Can get a sample estimator for mean, variance and quantiles.

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We also have a Central Limit Theorem, i.e. for large N

$$\widehat{\mathbb{E}}[f(\theta)] \overset{\text{approx}}{\sim} \text{normal}\left(\mathbb{E}f(\theta), \sqrt{\frac{\text{Var}[f(\theta)]}{N}}\right).$$

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- Discard these samples during a burn-in or *warmup* phase.

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    1. Take a random step in the parameter space, from $\theta^{(i)}$ to $\theta^{(i+1)}$ to propose a new sample.
    2. Accept the proposal with probability

$$\Pr = \min\left(\frac{p(\theta^{(i+1)} \mid z)}{p(\theta^{(i)} \mid z)}, 1\right).$$

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3. Return the chain $(\theta^{(1)}, \theta^{(2)}, ..., \theta^{(N)})$.

Example: Metropolis algorithm

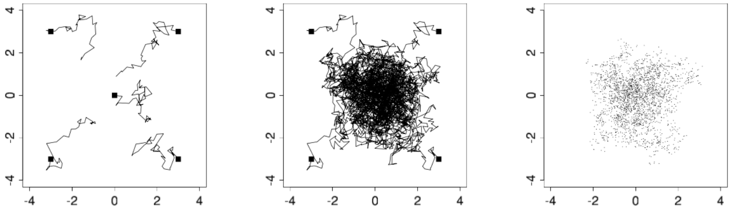

Figure from [Gelman et al., 2013].

Example: Metropolis algorithm

Benefits:

- The algorithm only requires $p(\theta, y) = p(\theta)p(y \mid \theta)$.
- In the asymptotic limit, the algorithm samples from to the true distribution.

Drawbacks:

- In the finite regime, the samples are **biased**.
- The samples are <u>not</u> independent; there are correlated, which **increases the variance** of our Monte Carlo estimators.

Example 2: Continuous diffusion process

In the limit where we take infinitesimally small steps, many MCMC algorithms can be approximated by a random diffusion process [Gelman et al., 1997, Roberts and Rosenthal, 1998].

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$$\theta^{(T)} \sim \text{normal}\left[(\mu_0 - \mu)e^{-T} + \mu, \quad \left(\sigma_0^2 - \sigma^2\right) e^{-2T} + \sigma^2\right].$$

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For T large enough, the bias becomes negligible.

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$$\frac{1}{N} \sum_i f(\theta_n) \overset{\text{approx}}{\sim} \text{Normal}\left(\mathbb{E}[f(\theta)], \frac{\operatorname{Var} f(\theta)}{N_{\text{eff}}} \right)$$

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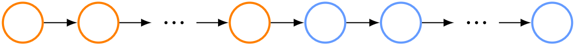
  where n_{eff} is the **effective sample size (ESS)**.
- One definition of ESS is

$$N_{\text{eff}} = \frac{N}{1 + \sum_{t=1}^{\infty} \rho_t}.$$

  Here ρ_t is the chain's autocorrelation for two variables separated by t iterations.

Handling the error of MCMC



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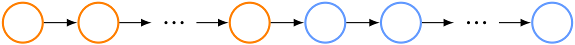

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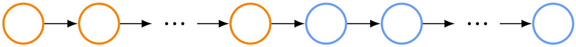


In practice, MCMC proceeds in two phases:

Warmup phase: We run the process for several steps for the <u>bias</u> to become negligible but don't use any of those samples in our Monte Carlo estimator.

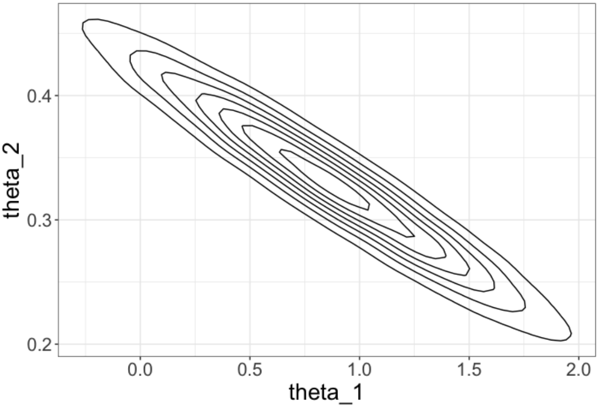
Sampling phase: Collect enough samples to have a large ESS and reduce the <u>variance</u> of the Monte Carlo estimator.

Question: Which transition kernel, Γ, should we choose?

Many choices!

> Metropolis, Metropolis-Hastings, Gibbs, **Hamiltonian Monte Carlo**, Metropolis-adjusted Langevin, ...

Geometric structure in the distribution



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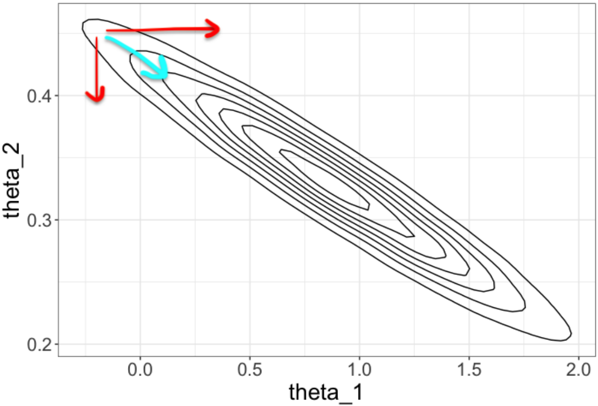

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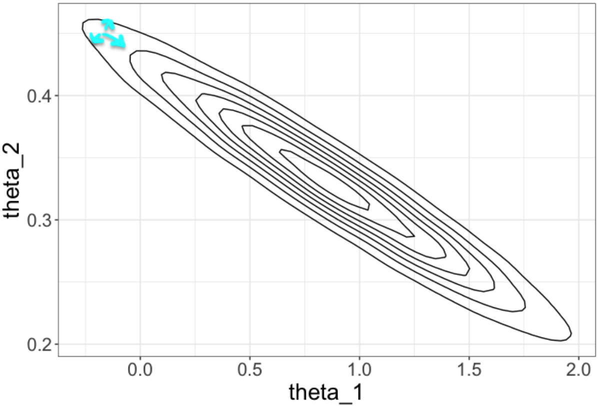

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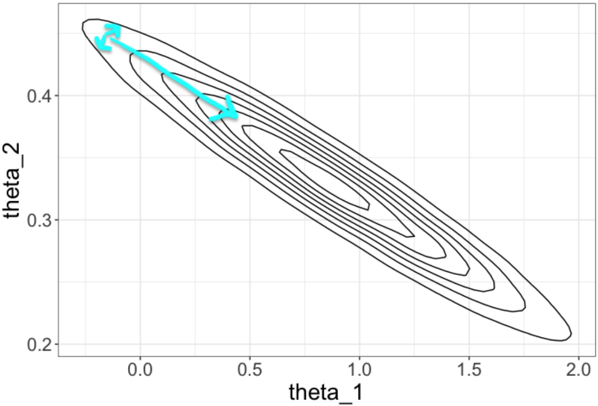

Hamiltonian Monte Carlo

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- Treat the Markov chain as a physical *particle* with mass matrix, M.

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- Treat the Markov chain as a physical *particle* with mass matrix, M.
- Instead of a random step, give the particle a random shove, by endowing the particle with a *momentum* ξ,

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- Treat the negative log density as a physical *potential*,

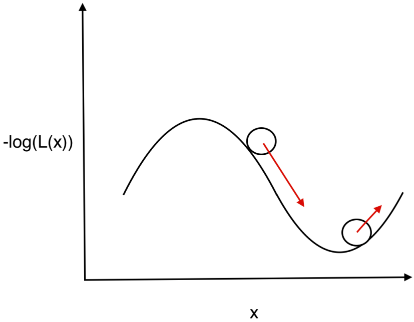
$$U(\theta) = -\log p(\theta \mid y).$$

- Simulate a the laws of classical mechanics for a time T,

$$\mathcal{Q} : (\theta_0, \xi_0) \to (\theta_T, \xi_T).$$

Hamiltonian Dynamics

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = M^{-1}\xi; \quad \frac{\mathrm{d}\xi}{\mathrm{d}t} = -\nabla_\theta \log p(\theta \mid y).$$



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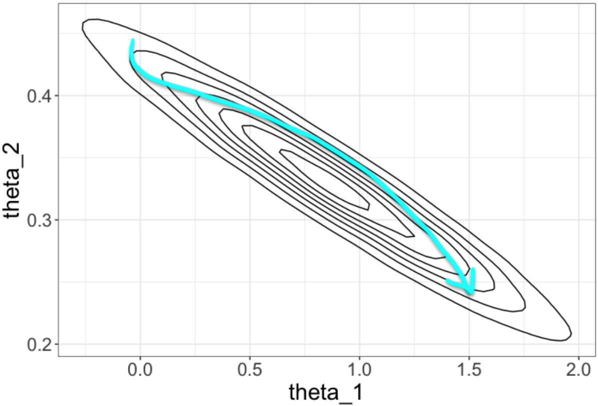

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  - The No U-Turn Sampler [Hoffman and Gelman, 2014] adaptively tunes these parameters during the warmup phase.

Comparison between sampling methods

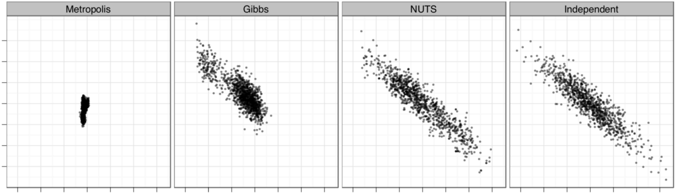

Figure from [Hoffman and Gelman, 2014].

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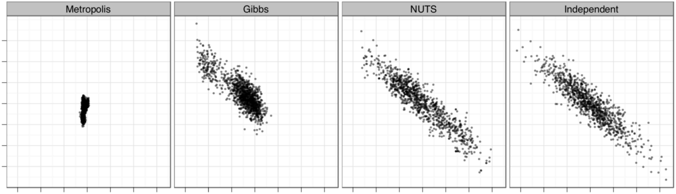

Figure from [Hoffman and Gelman, 2014].

For a thorough treatment of Hamiltonian Monte Carlo, see *A Conceptual introduction to HMC* [Betancourt, 2017].

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