Statistical Models & Computing Methods

Lecture 5: Advanced MCMC

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November 5, 2020

- Simple MCMC methods, such as Metropolis algorithm and Gibbs sampler explore the posterior distribution using simple mechanism (e.g., a random walk)
- While this strategy might work well for low-dimensional distributions, it could become very inefficient (e.g., high autocorrelation, missing isolated modes) for high-dimensional distributions
- In this lecture, we discuss several advanced techniques to improve the efficiency of MCMC methods.

Auxiliary Variable Methods

- Auxiliary variable strategies can be used to improving mixing of Markov chains
- When standard MCMC methods mix poorly, one potential remedy is to augment the state space of the variable of interest
- This approach can lead to chains that mix faster and require less tuning than the standard MCMC methods
- Main idea: construct a Markov chain over (X, U) (U is the auxiliary variable) with stationary distribution marginalizes to the target distribution of X
- As we will see later, this includes a large family of modern MCMC methods

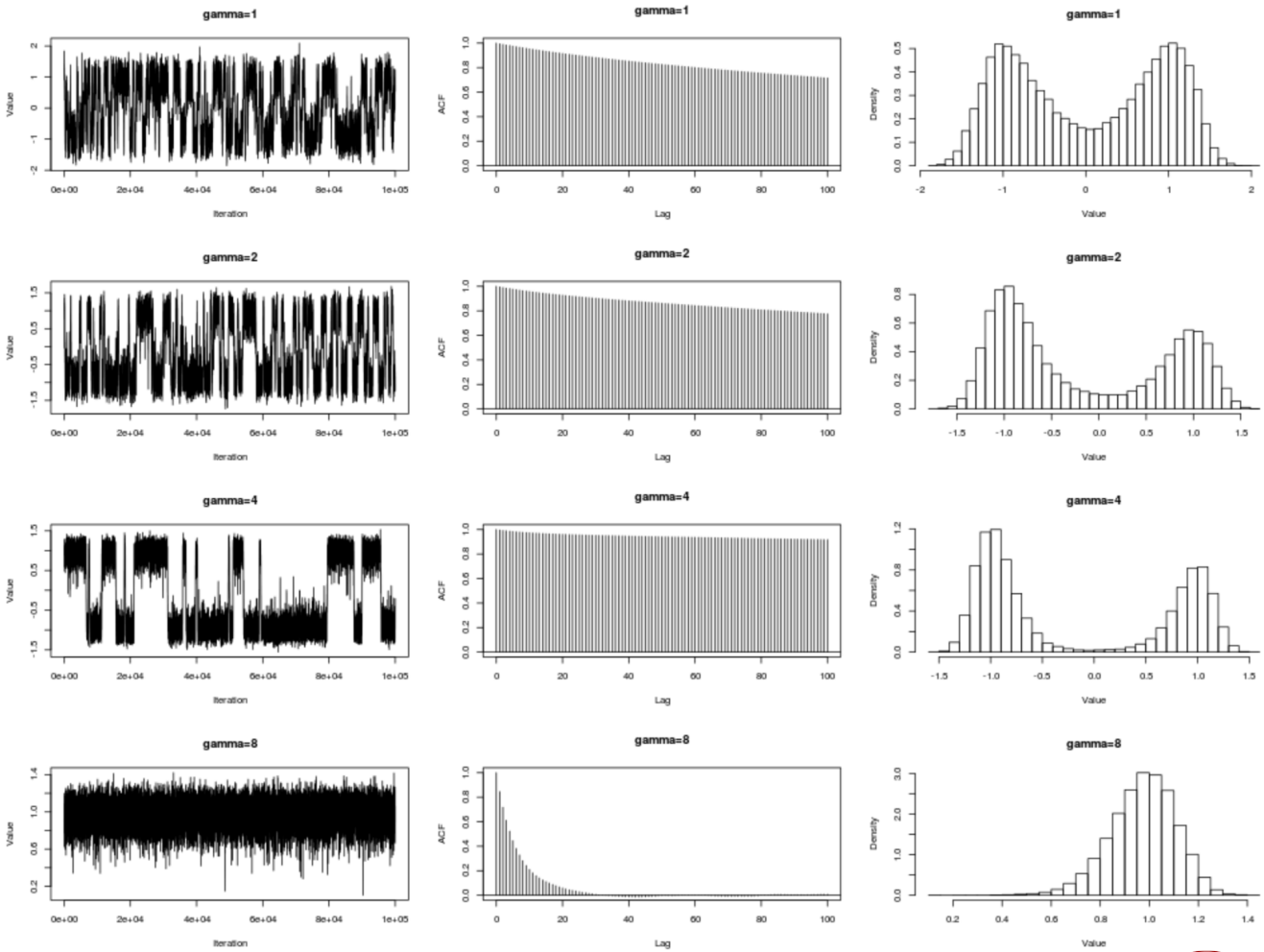
- Suppose that we have a challenging target distribution $f(x) \propto \exp(-U(x))$
- We can introduce temperatures to construct a sequence of distributions that are easier to sample from

$$f_k(x) \propto \exp\left(-U(x)/T_k\right), \quad k = 0, \ldots, K$$

  where $1 = T_0 < T_1 < \ldots < T_K$
- When simulating Markov chains with different temperature T, the chain with high temperature (hot chain) is likely to mix better than the chain with cold temperature (cold chain)
- Therefore, we can run parallel chains and swap states between the chains to improve mixing

Double-well Potential Distribution

$$f_T(x) \propto \exp(-(x^2-1)^2/T), \quad T = 1/\gamma$$



We run parallel Markov chains for distributions with different temperatures. In each iteration

- Follow regular Metropolis steps in each chain to get new states $x_0^{(t)}, \ldots, x_K^{(t)}$
- Select two temperatures, say $(i, j), i < j$, and swap the states

$$x_0^{(t)}, \ldots, x_i^{(t)}, \ldots, x_j^{(t)}, \ldots x_K^{(t)} \to x_0^{(t)}, \ldots, x_j^{(t)}, \ldots, x_i^{(t)}, \ldots x_K^{(t)}$$

- Accept the swapped new states with the following probability

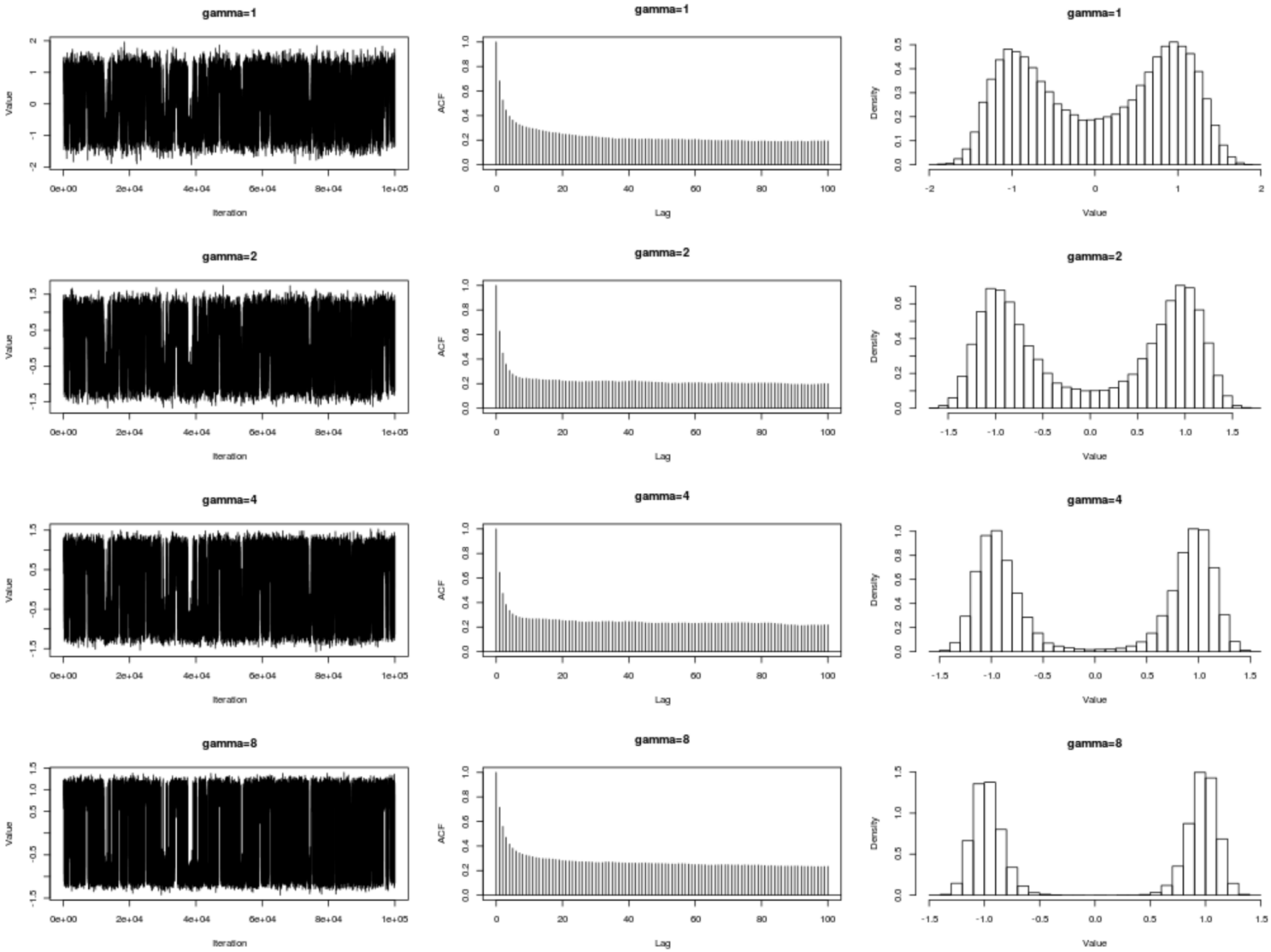
$$\min\left(1, f_i(x_j^{(t)}) f_j(x_i^{(t)}) / f_i(x_i^{(t)}) f_j(x_j^{(t)})\right)$$

- Both the within-chain Metropolis updates and the between-chain swap preserves

$$p(x_0, \ldots, x_K) \propto f_0(x_0) f_1(x_1) \ldots f_K(x_K)$$

- Therefore, the joint distribution of $(x_0^{(t)}, \ldots, x_K^{(t)})$ will converge to $p(x)$, and the marginal distribution of x_0 (cold chain) is the target distribution
- There are many ways to swap chains. For example, we can pick a pair of temperatures uniformly at random or only swap chains with successive temperatures
- The design of temperature levels could be crucial for the performance

Example: Double-well Potential Distribution



- Slice sampling was introduced by Neal (2003) to accelerate mixing of Metropolis (or MH)
- It is essentially a Gibbs sampler in the augmented space (X, U) with density

$$f(x, u) = f(x)f(u|x)$$

where U is the auxiliary variable and $f(u|x)$ is designed to be a uniform distribution $\mathcal{U}(0, f(x))$

- For this purpose, slice sampling alternates between two steps:
  - Given the current state of the Markov chain, x, we uniformly sample a new point u from the interval $(0, f(x))$

$$U|x \sim \mathcal{U}(0, f(x))$$

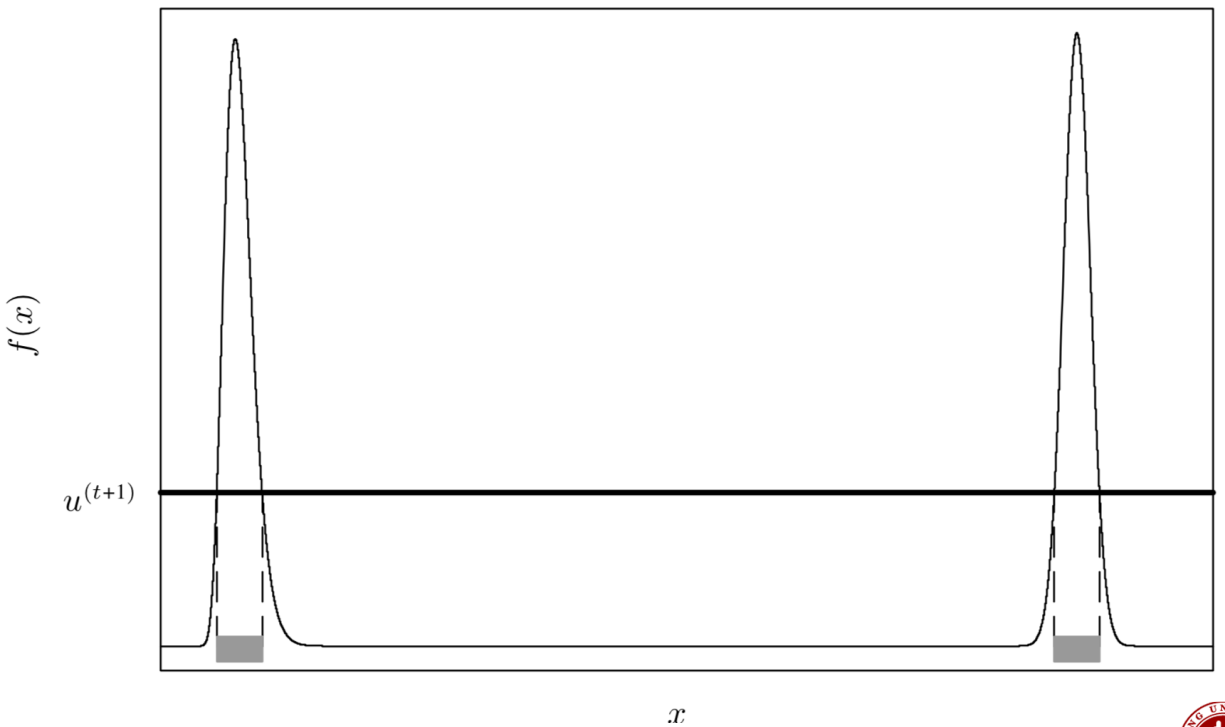
  - Given the current value of u, we uniformly sample from the region $S = \{x : f(x) > u\}$, which is referred to as the *slice* defined by u

$$X|u \sim \mathcal{U}(S)$$

- As mentioned by Neal (2003), in practice it is safer to compute $g(x) = \log(f(x))$, and use the auxiliary variable $z = \log(u) = g(x) - e$, where e has exponential distribution with mean one, and define the slice as $S = \{x : z < g(x)\}$

Move Between Modes with Slice Sampler

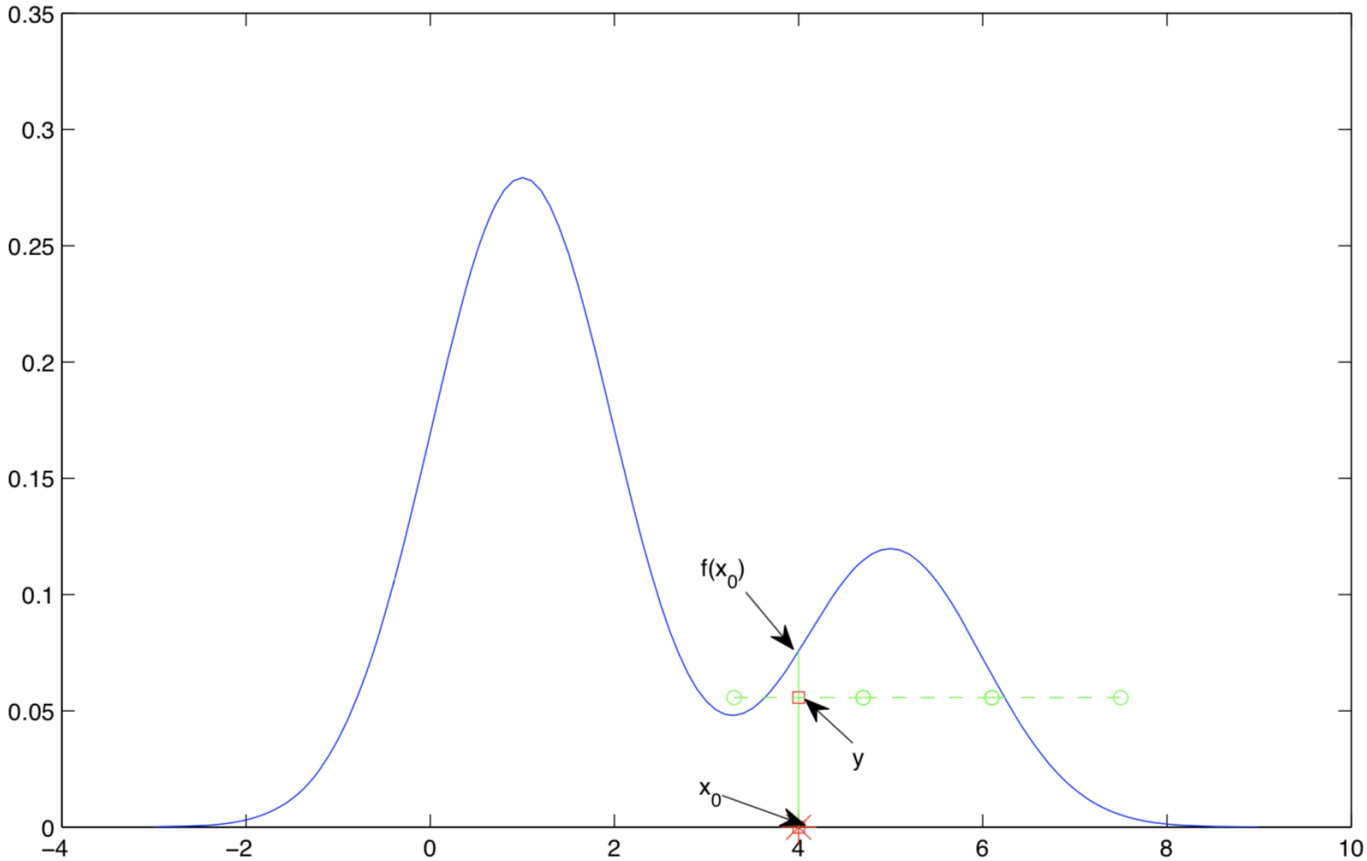
- One advantage of slice sampling is for sampling from multimodal distributions
- Unlike standard Metropolis (or MH) that struggles between distant modes, sampling from the slice allows us to easily jump between different modes



- Sampling an independent point uniformly from S might be difficult. In practice, we can substitute this step by any update that leaves the uniform distribution over S invariant
- There are several methods to perform this task
- Here, we introduce a simple but effective procedure that consists of two phases:
  - *Stepping-out*. A procedure for finding an interval around the current point
  - *Shrinkage*. A procedure for sampling form the interval obtained
- For a detail description of these methods, see Neal (2003)

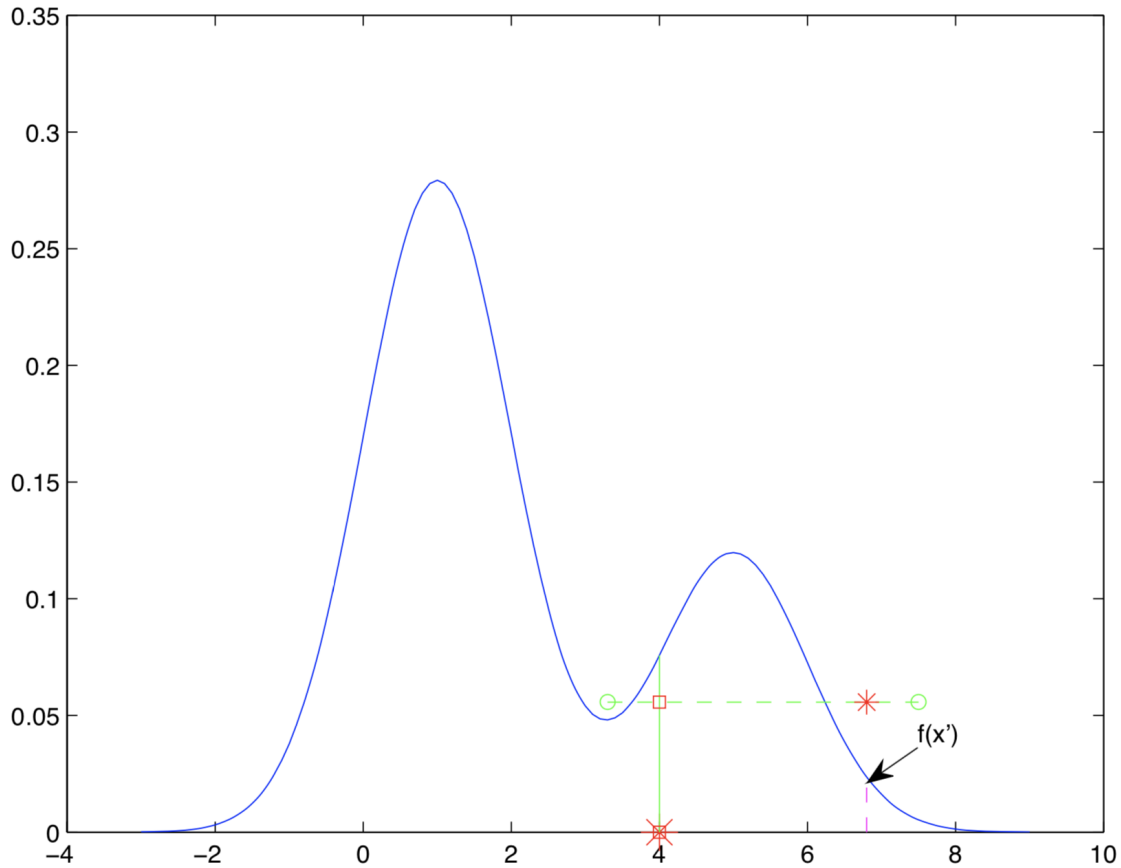
Slice Sampling- Illustration

- Sampling $u \sim \mathcal{U}(0, f(x_0))$ and stepping out (of size w) until we reach points outside the slice



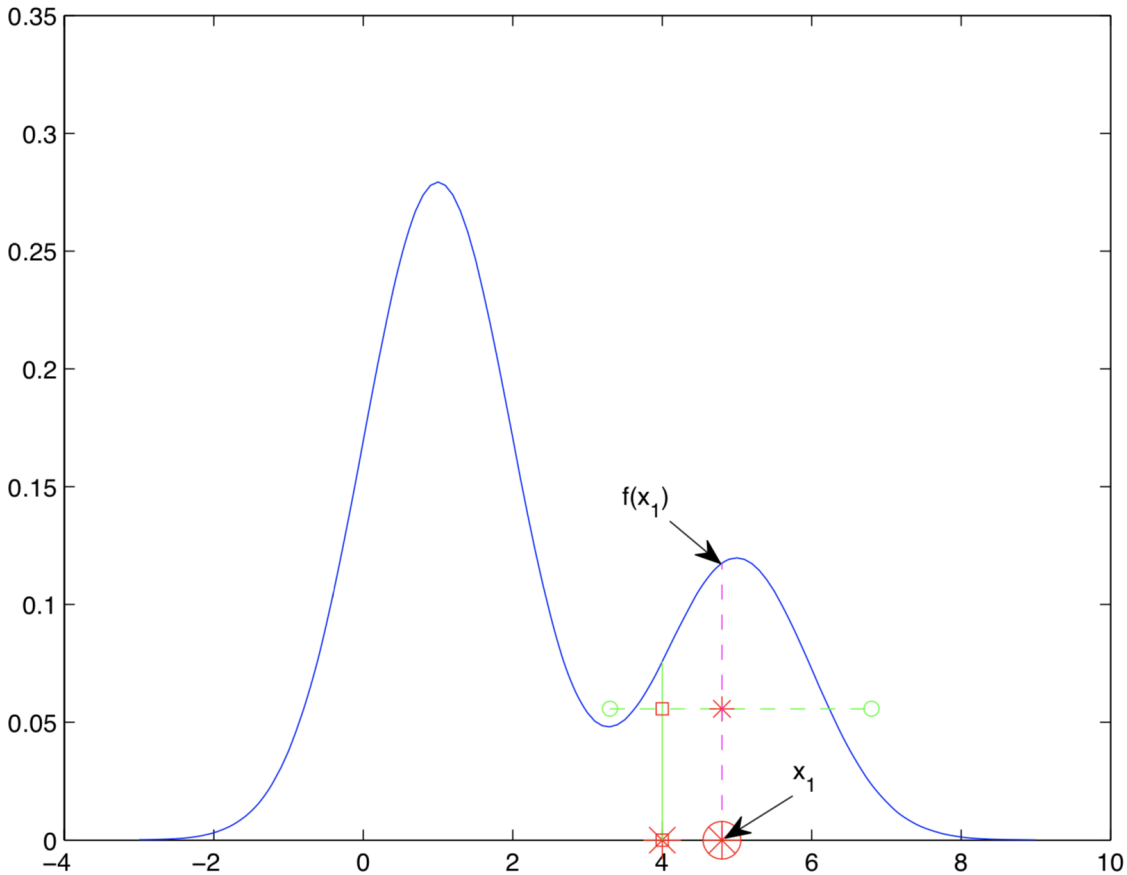
Slice Sampling- Illustration

- Shrinkage of interval to a point, x', which is sampled (uniformly) from the interval but it has $f(x') < y$



Slice Sampling- Illustration

- Continue shrinkage until we reach a point x_1 such that $y < f(x_1)$. We accept x_1 as our new sample



Simple MCMC is Not Enough

Random walk Metropolis (RWM) is struggling with a banana-shaped distribution

Simple MCMC is Not Enough

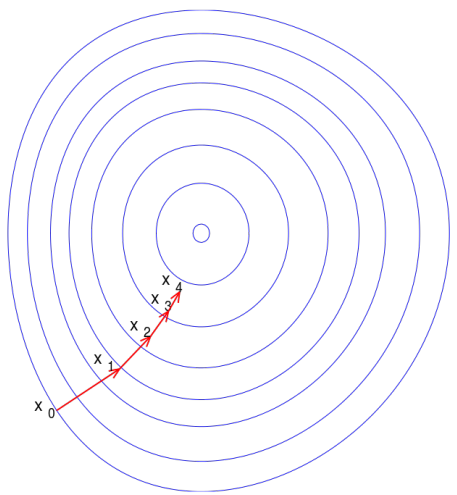
Random walk Metropolis (RWM) is struggling with a banana-shaped distribution

- Random proposals are likely to be inefficient, since they completely ignore the target distribution
- A better way would be to use information from the target distribution to guide our proposals
- Note that in optimization, the gradient points to an ascent direction, which would also be useful when designing the proposal distributions

$$x' = x + \epsilon \nabla \log p(x)$$

when ϵ is small,

$$\log p(x') > \log p(x)$$

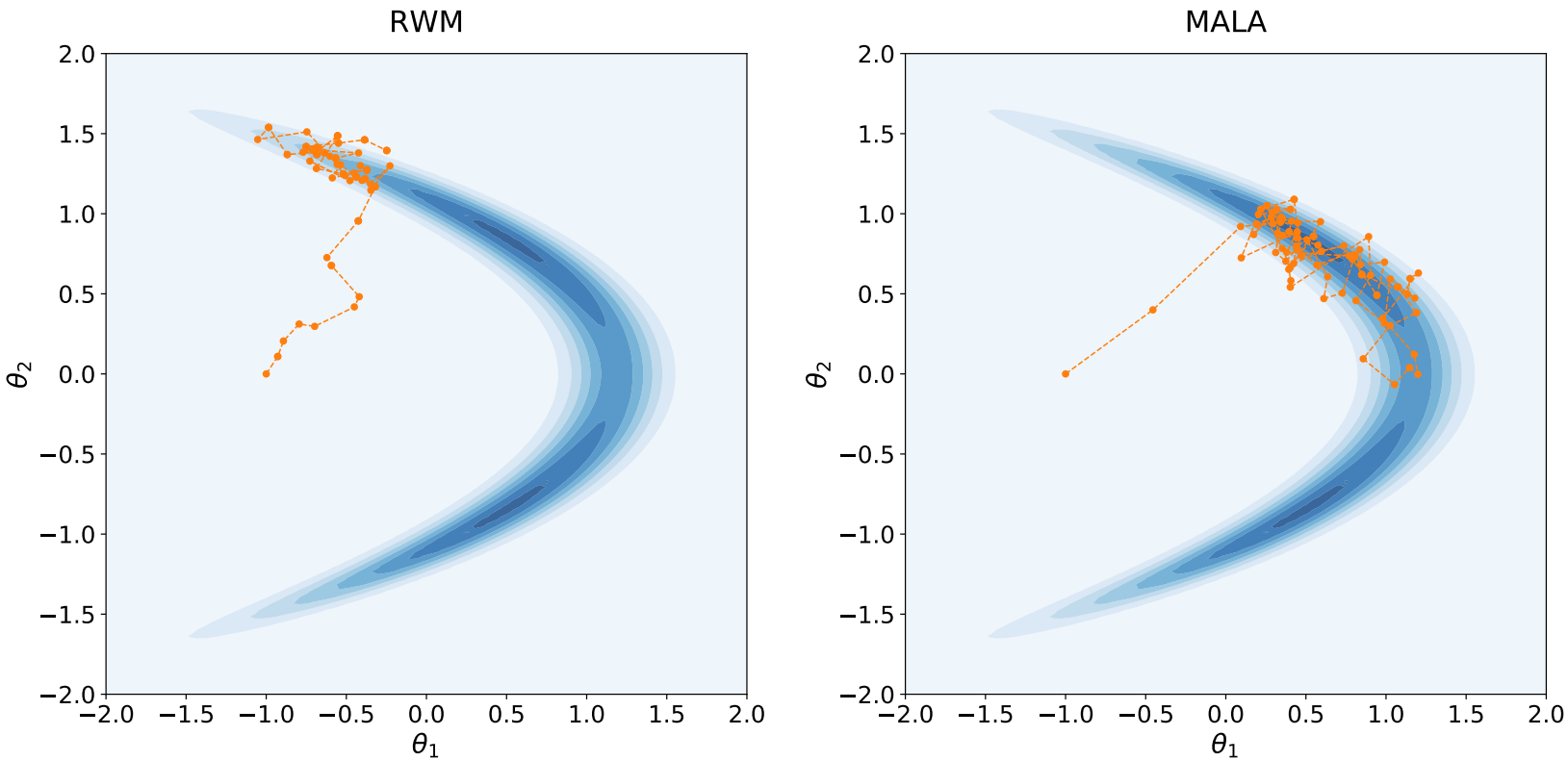


- We can incorporate the gradient information into our proposal distribution
- Let x be the current state, instead of using a random perturbation centered at x (e.g., $\mathcal{N}(x, \sigma^2)$), we can shift toward the gradient direction which leads to the following proposal distribution

$$Q(x'|x) = \mathcal{N}(x + \frac{\sigma^2}{2}\nabla \log p(x), \sigma^2 I)$$

  This looks like GD with noise!
- No longer symmetric, use Metropolis-Hasting instead
- This is called Metropolis Adjusted Langevin Algorithm (MALA)

Metropolis Adjusted Langevin Algorithm



- It turns out that we can combine multiple MALA together, resulting in an algorithm that can generate distant proposals with high acceptance rate
- The new algorithm is based on Hamiltonian dynamics, a system introduced by Alder and Wainwright (1959) to simulate motion of molecules deterministically based on Newton's law of motion
- In 1987, Duane et al. combine the standard MCMC and the Hamiltonian dynamics, and derived a method they called *Hybrid Monte Carlo* (HMC)
- Nowadays, this abbreviation has also been used for Hamiltonian Monte Carlo

- Construct a landscape with *potential energy* $U(x)$

$$p(x) \propto e^{-U(x)}, \quad U(x) = -\log P(x)$$

- Introduce momentum r carrying *kinetic energy* $K(r) = \frac{1}{2} r^T M^{-1} r$, and define **total energy or Hamiltonian** $H(x, r) = U(x) + K(r)$
- Hamiltonian equations

$$\frac{dx}{dt} = \frac{\partial H}{\partial r}, \quad \frac{dr}{dt} = -\frac{\partial H}{\partial x}$$

- Some physics:
  - The two equations are about velocity and force, respectively.
  - Frictionless ball rolling $(x, r) \to (x', r')$ satisfies $H(x', r') = H(x, r)$

- The joint probability of (x, r) is

$$p(x, r) \propto \exp(-H(x, r)) \propto p(x) \cdot \mathcal{N}(r|0, M)$$

- x and r are independent and r follows a Gaussian distribution
- The marginal distribution is the target distribution $p(x)$
- We then use MH to sample from the joint parameter space and x samples are collected as samples from the target distribution
- HMC is an auxiliary variable method

We follow two steps to make proposals in the joint parameter space

- Gibbs sample momentum: $r \sim \mathcal{N}(0, M)$
- Simulate Hamiltonian dynamics and flip the sign of the momentum

$$(x, r) = (x^{(0)}, r^{(0)}) \xrightarrow{\text{HD}} (x^{(t)}, r^{(t)}), \quad (x', r') = (x^{(t)}, -r^{(t)})$$

Important Properties

- Time reversibility: The trajectory is time reversible
- Volume preservation: Hamiltonian flow does not change the volume - the jacobin determinant is 1
- Conservation of Hamiltonian: Total energy is conserved, meaning the proposal will always be accepted

- In practice, Hamiltonian dynamics can not be simulated exactly. We need to use numerical integrators
- **Leap-frog scheme**

$$r(t+\frac{\epsilon}{2}) = r(t) - \frac{\epsilon}{2}\frac{\partial U}{\partial x}(x(t))$$

$$x(t+\epsilon) = x(t) + \epsilon\frac{\partial K}{\partial r}(r(t+\frac{\epsilon}{2}))$$

$$r(t+\epsilon) = r(t+\epsilon/2) - \frac{\epsilon}{2}\frac{\partial U}{\partial x}(x(t+\epsilon))$$

Important Properties

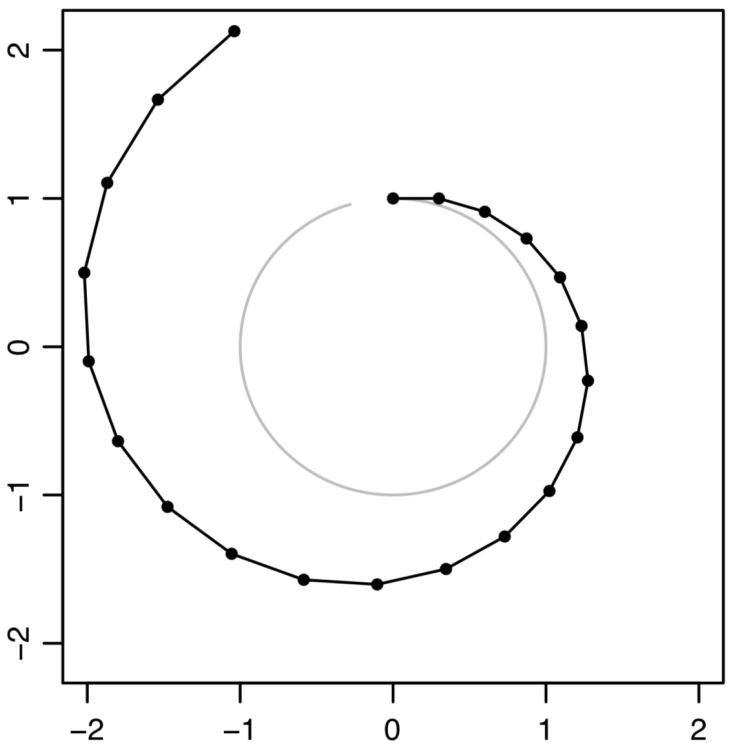
- Reversibility and volume preservation: still hold
- Conservation of Hamiltonian: broken. Acceptance probability becomes

$$a(x', r'|x, r) = \min\left(1, \exp(-H(x', r') + H(x, r))\right)$$

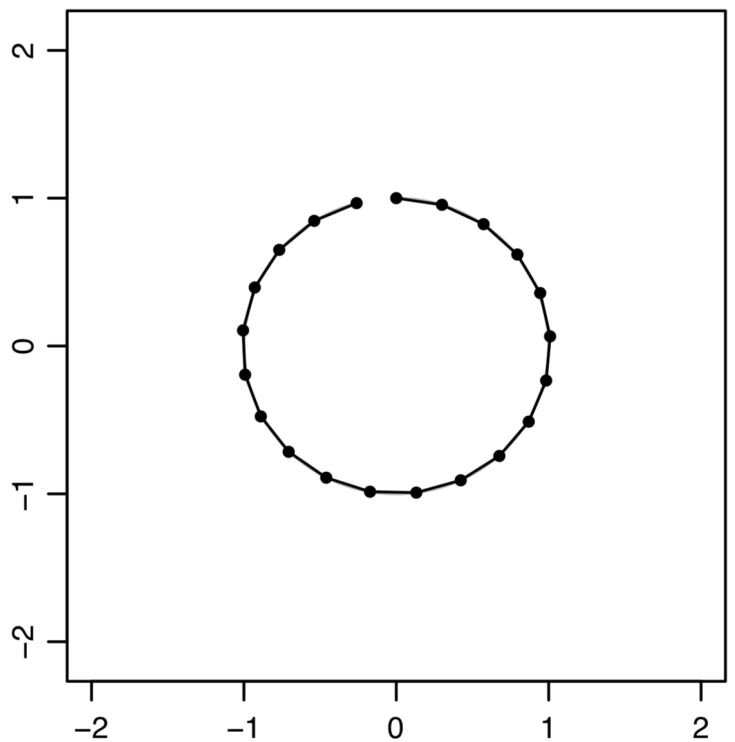
Comparison of Numerical Integrators

$$H(x, r) = \frac{x^2}{2} + \frac{r^2}{2}$$

Euler, $\epsilon = 0.3$



Leap-frog, $\epsilon = 0.3$



Adapted from Neal (2011)

HMC in one iteration

- Sample momentum $r \sim \mathcal{N}(0, M)$
- Run numerical integrators (e.g., leapfrog) for L steps
- Accept new position with probability

$$\min\left(1, \exp(-H(x', r') + H(x, r))\right)$$

HMC in one iteration

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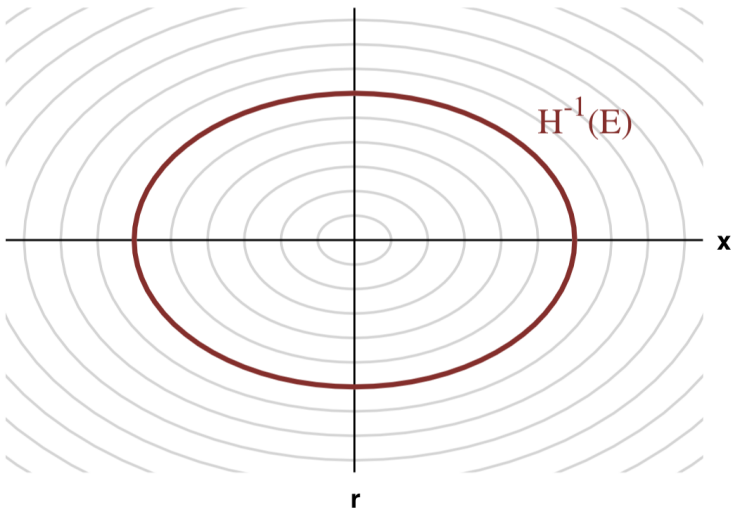
$$\min\left(1, \exp(-H(x', r') + H(x, r))\right)$$

- Since Hamiltonian is conserved, every Hamiltonian trajectory is confined to an energy level set

$$H^{-1}(E) = \{x, r | H(x, r) = E\}$$



Adapted from Betancourt (2017)

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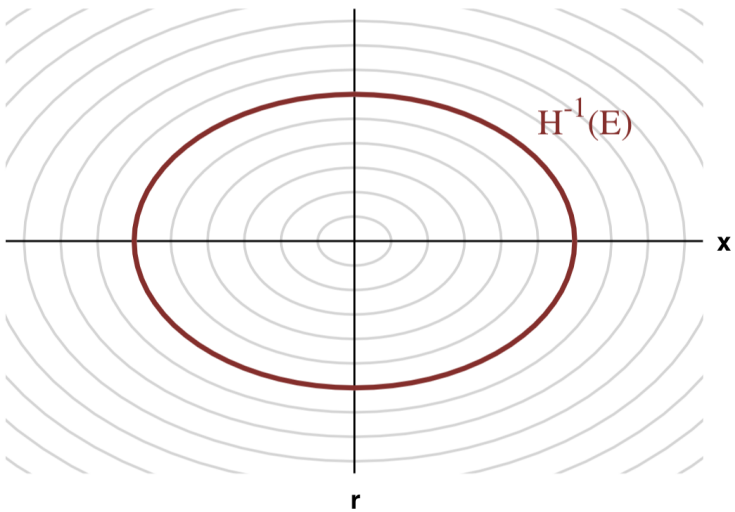
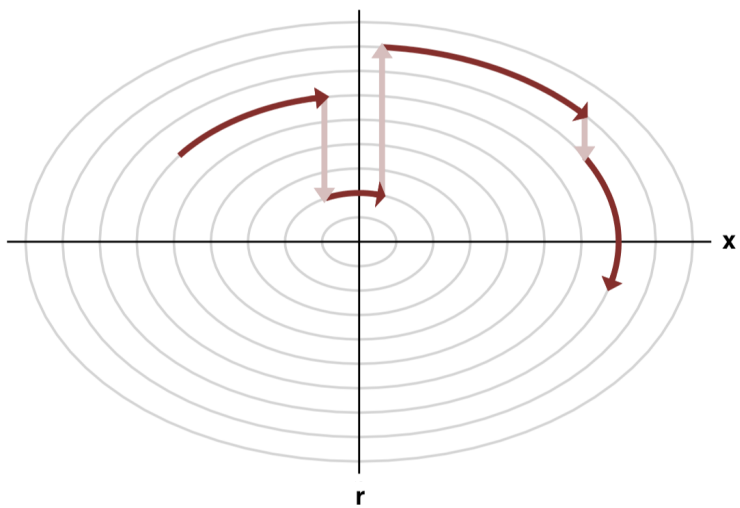




Adapted from Betancourt (2017)

Choice of Kinetic Energy

- The choice of the conditional probability distribution over the momentum, or equivalently, the kinetic energy, affects HMC's behavior over different energy level sets
- Ideally, the kinectic energy will interact with the target distribution to ensure that the energy level sets are uniformly distributed
- In HMC, we often use Euclidean-Gaussain kinetic energy $K(r) = \frac{r^T r}{2}$. This sets $M = I$ and completely ignore local geometric information of the target distribution
- Preconditioning mass matrix may help, but it is also quite limited
- Instead of using a fixed M, how about using an adaptive one?

- Consider the symmetric KL divergence between two densities p and q

$$D_{\mathrm{KL}}^{\mathcal{S}}(p\|q) = D_{\mathrm{KL}}(p\|q) + D_{\mathrm{KL}}(q\|p)$$

- Let $p(y|x)$ be the likelihood. Then $D_{\mathrm{KL}}^{\mathcal{S}}(p(y|x+\delta x)\|p(y|x))$ is approximately

$$\delta x^T \mathbb{E}_{y|x}\left(\nabla_x \log p(y|x) \nabla_x \log p(y|x)^T\right) \delta x = \delta x^T G(x) \delta x$$

where $G(x)$ is the **Fisher Information** matrix

- This induces a **Riemannian manifold** (Amari 2000) over the parameter space of a statistical model, which defines the natural geometric structure of density $p(x)$

- Based on the Riemannian manifold formulation, Girolami and Calderhead (2011) introduce a new method, called Riemannian manifold HMC (RMHMC)
- Hamiltonian on a Riemannian manifold

$$H(x,r) = U(x) + \frac{1}{2}\log((2\pi)^d|G(x)|) + \frac{1}{2}r^T G(x)^{-1} r$$

- The joint probability is

$$p(x,r) \propto \exp(-H(x,r)) \propto p(x) \cdot \mathcal{N}(r|0, G(x))$$

- x and r now are correlated, and the conditional distribution of r given x follows a Gaussian distribution
- The marginal distribution is the target distribution

- The resulting dynamics is non-separable, so instead of the standard leapfrog we need to use the *generalized* leapfrog method (Leimkuhler and Reich, 2004)
- **The generalized leapfrog scheme**

$$
\begin{aligned}
r(t+\frac{\epsilon}{2}) &= r(t) - \frac{\epsilon}{2}\nabla_x H(x(t), r(t+\frac{\epsilon}{2})) \\
x(t+\epsilon) &= x(t) + \frac{\epsilon}{2}\big(G(x(t))^{-1} + G(x(t+\epsilon))^{-1}\big) r(t+\frac{\epsilon}{2}) \\
r(t+\epsilon) &= r(t+\frac{\epsilon}{2}) - \frac{\epsilon}{2}\nabla_x H(x(t+\epsilon), r(t+\frac{\epsilon}{2}))
\end{aligned}
$$

- The above scheme is time reversible and volume preserving. However, the first two equations are defined implicitly (can be solved via several fixed point iterations)

Examples: Banana Shape Distribution

- Consider a 2D banana-shaped posterior distribution as follows

$$y_i \sim \mathcal{N}(\theta_1 + \theta_2^2, \sigma_y^2), \quad \theta = (\theta_1, \theta_2) \sim \mathcal{N}(0, \sigma_\theta^2 I)$$

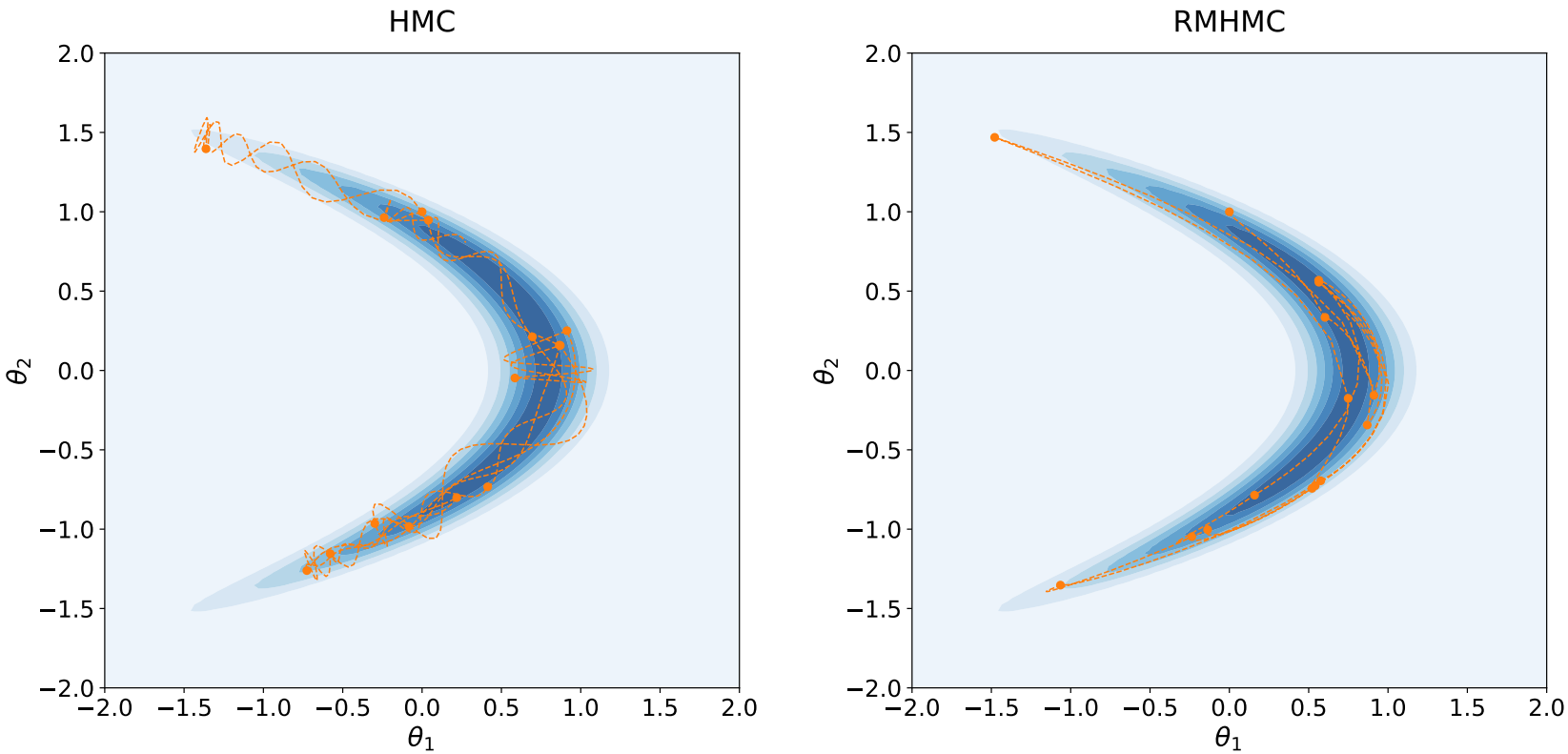
- the log-posterior is (up to an ignorable constant)

$$\log p(\theta | Y, \sigma_y^2, \sigma_\theta^2) = -\frac{\sum_i (y_i - \theta_1 - \theta_2^2)^2}{2\sigma_y^2} - \frac{\theta_1^2 + \theta_2^2}{2\sigma_\theta^2}$$

- Fisher information for the joint likelihood

$$G(\theta) = \mathbb{E}_{Y|\theta}\left(-\nabla_\theta^2 \log p(Y, \theta)\right) = \frac{n}{\sigma_y^2}\begin{bmatrix} 1 & 2\theta_2 \\ 2\theta_2 & 4\theta_2^2 \end{bmatrix} + \frac{1}{\sigma_\theta^2} I$$

Examples: Banana Shape Distribution



Examples: Bayesian Logistic Regression

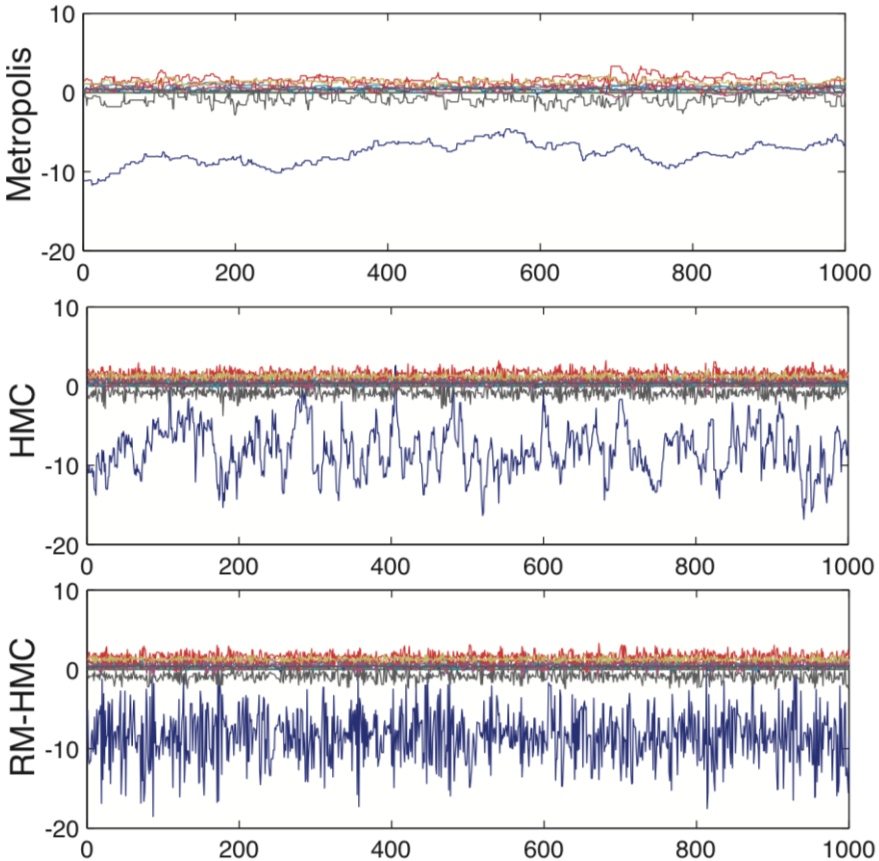
- Consider a Bayesian logistic regression model with design matrix X and regression coefficients $\beta \in \mathbb{R}^d$, with a simple prior $\beta \sim \mathcal{N}(0, \alpha I_d)$
- Neglecting constants, the log-posterior is

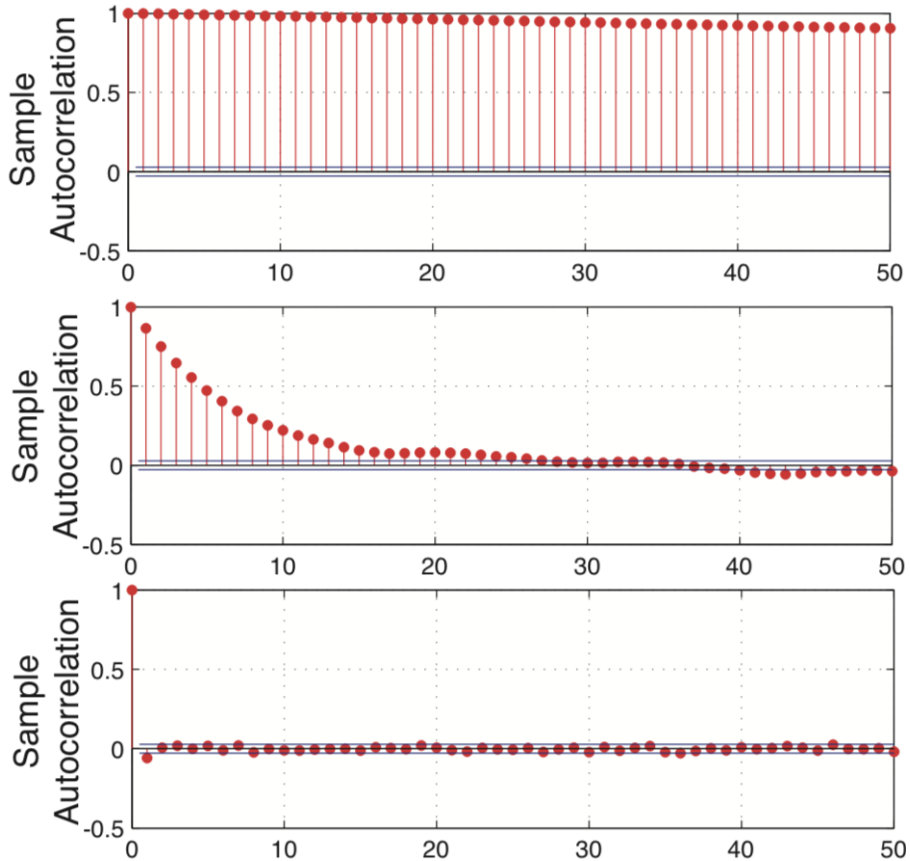
$$\begin{aligned}\log p(\beta|X, Y, \alpha) &= L(\beta) - \frac{1}{2\alpha}\beta^T\beta \\ &= \beta^T X^T Y - \sum_i \log(1 + \exp(x_i^T\beta)) - \frac{1}{2\alpha}\beta^T\beta\end{aligned}$$

- Use the joint likelihood to compute the fisher information

$$G(\beta) = \mathbb{E}_{Y|X,\beta,\alpha}\left(-\nabla^2_\beta L(\beta) + \frac{1}{\alpha}I_d\right) = X^T W X + \frac{1}{\alpha}I_d$$

Examples: Bayesian Logistic Regression





Adapted form Girolami and Calderhead (2011)

Choice of Integration Time

- Integration time determines the exploration efficiency of Hamiltonian trajectory in each energy level set
  - Too short integration time lose the advantage of the coherent exploration of the Hamiltonian trajectory (e.g., one step HMC is equivalent to MALA)
  - Too long integration time wastes computation since trajectories are likely to return to explored regions
- The No-U-Turn Sampler (Hoffman and Gelman, 2011).
  - Idea: use the distance to the initial position as a criteria for selecting integration time - avoid U-Turn
  - Naive implementation is not time reversible. Use a strategy similar to the doubling procedure in slice sampling (Neal 2003).

Adaptive MCMC

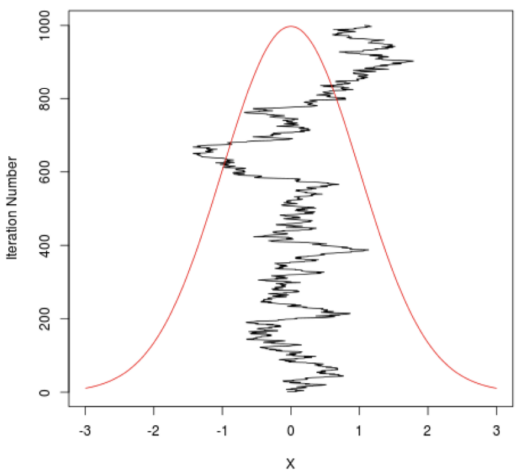
- Generally speaking, the efficiency of MCMC depends on its proposal distribution, which usually involves several hyper-parameters
- Most MCMC algorithms, therefore, need tuning to be efficient and reliable in large scale applications
- However, tuning could be painful and sometimes not practical (requires computing time, human time, and typically expert knowledge, too many variables, when to stop tuning, tuning criterion not clear, etc)
- Adaptive MCMC is about tuning MCMC without human intervention
- It uses the trajectory so far to tune the sampling kernel on the fly (so it is not a Markov chain anymore)

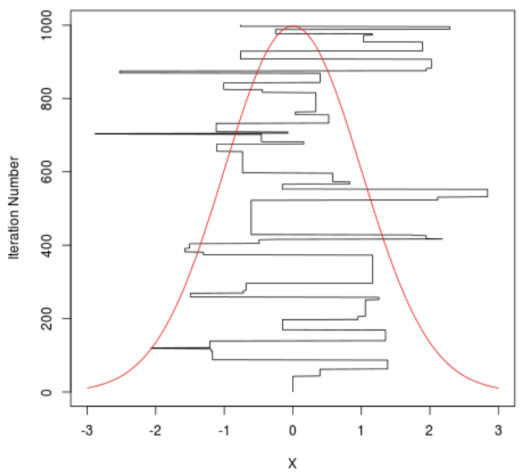
Examples: Random Walk Metropolis

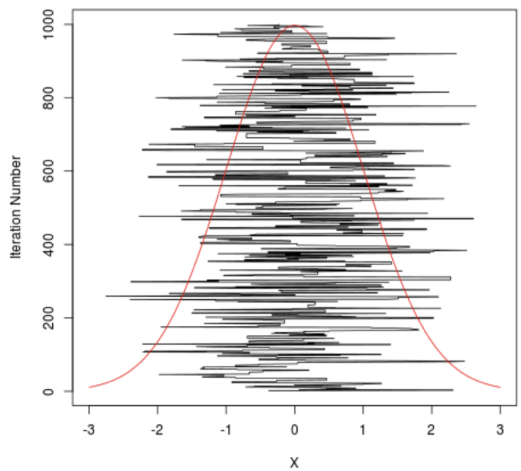
- Proposal distribution:

$$x' \sim Q_\sigma(\cdot|x) = x + \sigma\mathcal{N}(0, I_d)$$

- Plots for different σ - Goldilock's principle

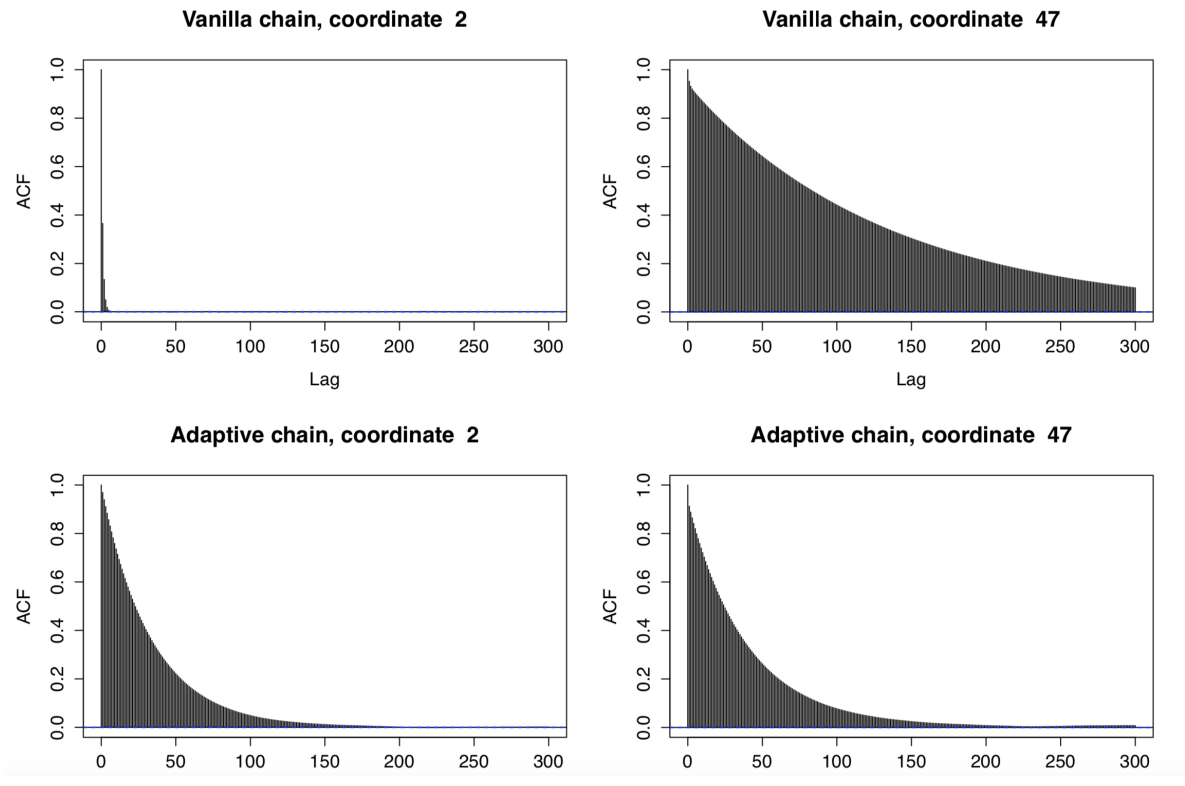






Examples: Random Scan Gibbs Sampler

- Random Scan Gibbs Sampler for 50-d Truncated Multivariate Normals. Are uniform $1/d$ selection probabilities optimial?



- First, we need a parameterized family of proposal distributions for a given MCMC class
- We also need an optimization rule that is mathematically sound and computationally cheap
- We need it to work in practice

Ergodicity of Adaptive MCMC

- How do we know that the chain will converge to the target distribution if it is not even Markovian?
- **Two conditions** (see Roberts and Rosenthal 2007):
  - *Diminishing adaption*: the dependency on ealier states of the chain goes to zero
  - *Bounded convergence*: convergence times for all adapted transition kernels are bounded in probablity

- Consider random walk Metropolis for a d-dimensional target distribution with proposal $Q(x'|x_n) = \mathcal{N}(x_n, \sigma^2\Sigma^{(n)})$
- If the target distribution is Gaussian with covariance Σ, the optimal proposal is $\mathcal{N}(x_n, \frac{2.38^2}{d}\Sigma)$, which leads to an acceptance rate $\alpha^* \approx 0.23$ (see Gelman et al 1996)
- This gives a simple criterion for random walk Metropolis in practice
- We can use it to design an adaptive Metropolis algorithm

- Draw proposal

$$x' \sim Q(\cdot|x_n) = x_n + \sigma_n \mathcal{N}(0, I_d)$$

- select the value x_{n+1} according to the Metropolis acceptance rate $\alpha_n = \alpha(x'|x_n)$
- Update scale by

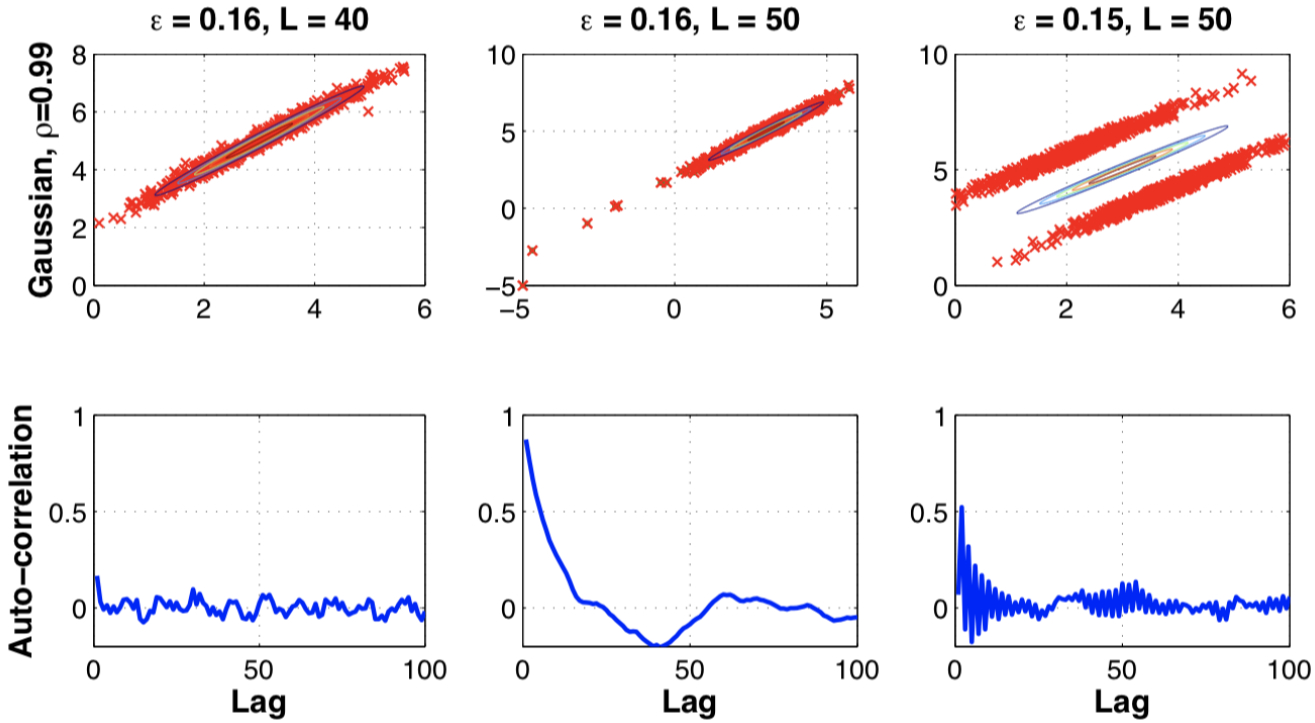
$$\log \sigma_{n+1} = \log \sigma_n + \gamma_n(\alpha_n - \alpha^*)$$

where the adaptation parameter $\gamma_n \to 0$

- Optimal scaling is not the whole story. In fact, the optimal proposal suggests to learn the covariance matrix of the target distribution (e.g., use the empirical estimates)
- The algorithm runs as follows:
  - Sample a candidate value from $\mathcal{N}(x_n, \frac{2.38^2}{d}\Sigma_n)$
  - Select the value x_{n+1} as in the usual Metropolis (or MH)
  - Update the proposal distribution in two steps:

$$\mu_{n+1} = \mu_n + \gamma_{n+1}(x_{n+1} - \mu_n)$$
$$\Sigma_{n+1} = \Sigma_n + \gamma_{n+1}\left((x_{n+1} - \mu_n)(x_{n+1} - \mu_n)^T - \Sigma_n\right)$$

  where $\gamma_n \to 0$
- Many variants exist (e.g., adapting the scale, block updates, and batch adaption, etc)



- The performance of HMC would be sensitive to its hyperparameters, mainly the stepsize ϵ and trajectory length L

- Optimal acceptance rate strategy might not work well. The example shown on the previous slides all have similar acceptance rate
- Effective sample size is impractical since high order auto-correlation are hard to estimate
- Wang et al (2013) uses normalized expected squared jumping distance (ESJD)

$$\text{ESJD}_\gamma = \mathbb{E}_\gamma \|x^{(t+1)} - x^{(t)}\|^2 / \sqrt{L}$$

where $\gamma = (\epsilon, L)$

- Update γ via Bayesian optimization, with an annealing adapting rate

- Instead of using a fixed trajectory length L, we can sample it from some distribution (e.g., $\mathcal{U}(1, L_{\max})$)
- Split the Hamiltonian

$$H(x, r) = H_1(x, r) + H_2(x, r) + \cdots + H_k(x, r)$$

  simulate Hamiltonian dynamics on each H_i (sequentially or randomly) give the Hamiltonian dynamics on H. Can save computation if some of the H_i are analytically solvable
- Partial momentum refreshment
- Acceptance using windows of states
- See Neal (2010) for more complete and detailed discussion

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