STA 702: Hamiltonian Monte Carlo

Merlise Clyde

Nov 29, 2022

Gibbs sampling

- Consider model

$$\begin{aligned} \boldsymbol{Y}_1, \ldots, \boldsymbol{Y}_n &\sim N_2\left(\boldsymbol{\theta}, \Sigma\right); \\ \theta_j &\sim N(0,1) \qquad j = 1, 2. \end{aligned}$$

Gibbs sampling

- Consider model

$$\begin{aligned} \boldsymbol{Y}_1, \ldots, \boldsymbol{Y}_n &\sim N_2\left(\boldsymbol{\theta}, \Sigma\right); \\ \theta_j &\sim N(0,1) \qquad j = 1, 2. \end{aligned}$$

- Suppose that the covariance matrix Σ is known and has the form

$$\Sigma = \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}$$

Gibbs sampling

- Consider model

$$\begin{aligned} \boldsymbol{Y}_1, \ldots, \boldsymbol{Y}_n &\sim N_2\left(\boldsymbol{\theta}, \Sigma\right); \\ \theta_j &\sim N(0,1) \qquad j = 1, 2. \end{aligned}$$

- Suppose that the covariance matrix Σ is known and has the form

$$\Sigma = \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}$$

- What happens when $\rho = 0.995$?

Gibbs sampling

- Consider model

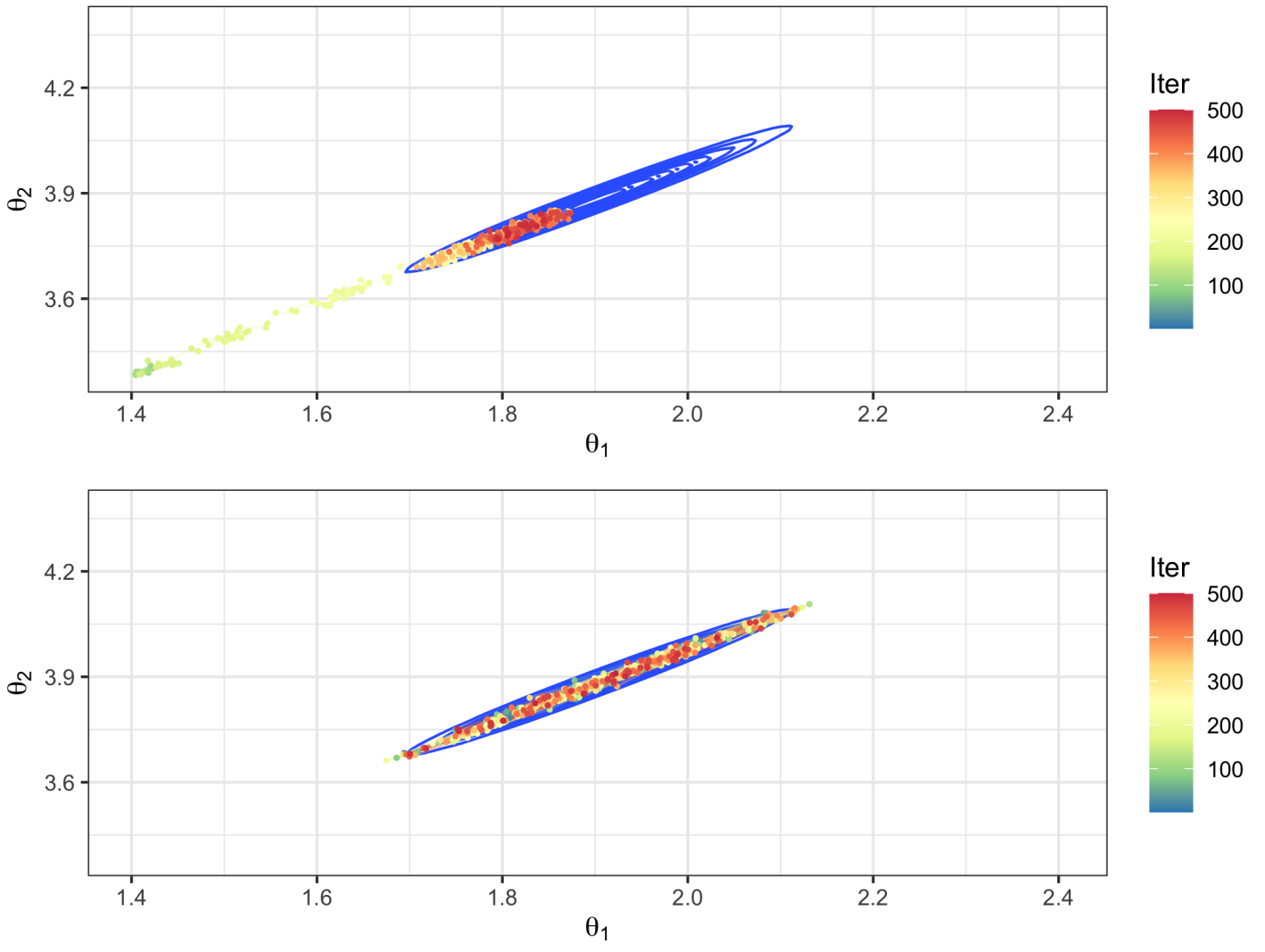
$$\begin{aligned} \boldsymbol{Y}_1, \ldots, \boldsymbol{Y}_n &\sim N_2\left(\boldsymbol{\theta}, \Sigma\right); \\ \theta_j &\sim N(0,1) \qquad j = 1, 2. \end{aligned}$$

- Suppose that the covariance matrix Σ is known and has the form

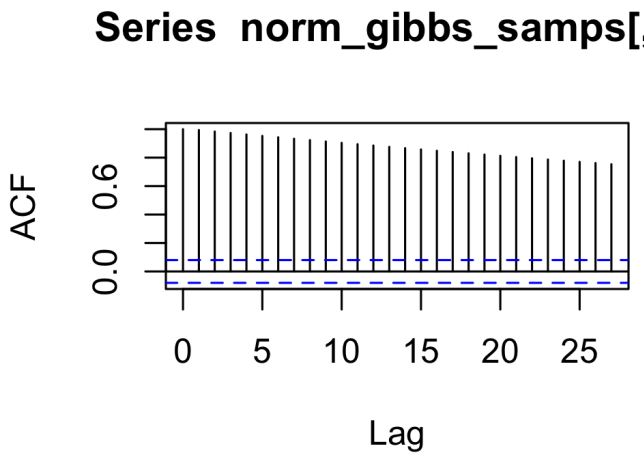
$$\Sigma = \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}$$

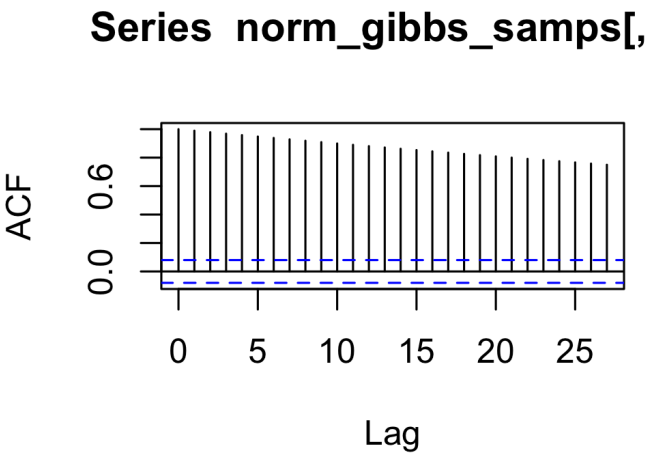
- What happens when $\rho = 0.995$?

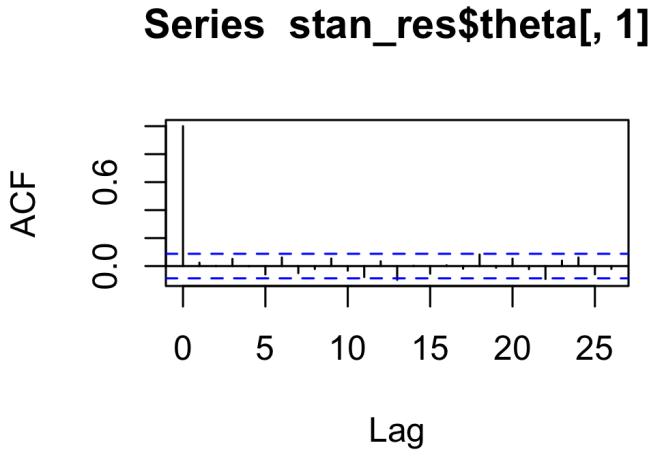
Gibbs vs Stan samples

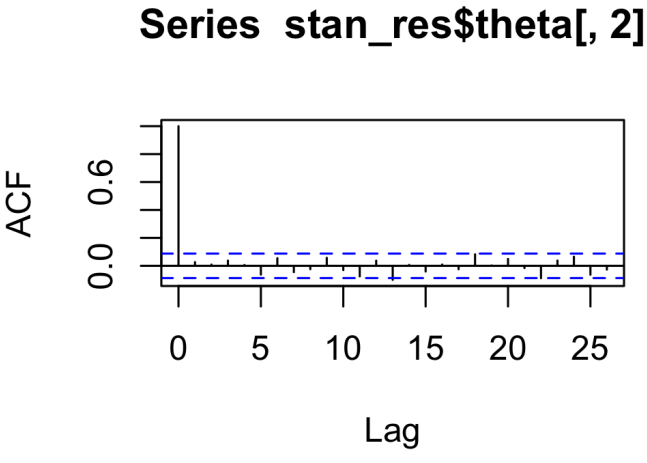


ACF


Series norm_gibbs_samps[, 1]
ACF
0.0
0.6
0
5
10
15
20
25
Lag


Series norm_gibbs_samps[, 2]
ACF
0.0
0.6
0
5
10
15
20
25
Lag


Series stan_res$theta[, 1]
ACF
0.0
0.6
0
5
10
15
20
25
Lag


Series stan_res$theta[, 2]
ACF
0.0
0.6
0
5
10
15
20
25
Lag

Hamiltonian Monte Carlo (HMC)

- HMC creates transitions that *efficiently explore the parameter space* by using concepts from Hamiltonian mechanics.

Hamiltonian Monte Carlo (HMC)

- HMC creates transitions that *efficiently explore the parameter space* by using concepts from Hamiltonian mechanics.
- In Hamiltonian mechanics, a physical system is specified by positions $\mathbf{q}$ and momenta $\mathbf{p}$.

Hamiltonian Monte Carlo (HMC)

- HMC creates transitions that *efficiently explore the parameter space* by using concepts from Hamiltonian mechanics.
- In Hamiltonian mechanics, a physical system is specified by positions $\mathbf{q}$ and momenta $\mathbf{p}$.
- A space defined by these coordinates is called a **phase space**

Hamiltonian Monte Carlo (HMC)

- HMC creates transitions that *efficiently explore the parameter space* by using concepts from Hamiltonian mechanics.
- In Hamiltonian mechanics, a physical system is specified by positions $\mathbf{q}$ and momenta $\mathbf{p}$.
- A space defined by these coordinates is called a **phase space**
- If the parameters of interest in a typical MCMC method are denoted as $q_1, \ldots, q_K$, then HMC introduces auxiliary **momentum** parameters $p_1, \ldots, p_K$ such that the algorithm produces draws from the joint density:

$$\pi(\mathbf{q}, \mathbf{p}) = \pi(\mathbf{p}|\mathbf{q})\pi(\mathbf{q})$$

Hamiltonian Monte Carlo (HMC)

- HMC creates transitions that *efficiently explore the parameter space* by using concepts from Hamiltonian mechanics.
- In Hamiltonian mechanics, a physical system is specified by positions $\mathbf{q}$ and momenta $\mathbf{p}$.
- A space defined by these coordinates is called a **phase space**
- If the parameters of interest in a typical MCMC method are denoted as $q_1, \ldots, q_K$, then HMC introduces auxiliary **momentum** parameters $p_1, \ldots, p_K$ such that the algorithm produces draws from the joint density:

$$\pi(\mathbf{q}, \mathbf{p}) = \pi(\mathbf{p}|\mathbf{q})\pi(\mathbf{q})$$

- marginalizing over the p_k's, we recover the marginal distribution of the q_k's Therefore, if we create a Markov Chain that converges to $\pi(\mathbf{q}, \mathbf{p})$, we have immediate access to samples from $\pi(\mathbf{q})$, which is our target distribution.

Hamiltonian

- Hamilton's equations describe the time evolution of the system in terms of the **Hamiltonian**, $\mathcal{H}$, which corresponds to the total energy of the system:

$$\mathcal{H}(\mathbf{p}, \mathbf{q}) = K(\mathbf{q}, \mathbf{p}) + U(\mathbf{q})$$

Hamiltonian

- Hamilton's equations describe the time evolution of the system in terms of the **Hamiltonian**, $\mathcal{H}$, which corresponds to the total energy of the system:

$$\mathcal{H}(\mathbf{p}, \mathbf{q}) = K(\mathbf{q}, \mathbf{p}) + U(\mathbf{q})$$

- $K(\mathbf{q}, \mathbf{p})$ represents the **kinetic energy** of the system and is equal to the negative logarithm of the momentum distribution, e.g.

$$K(\mathbf{p}) = \frac{\mathbf{p}^T M^{-1} \mathbf{p}}{2} = \sum_i \frac{p_i^2}{2m_i}$$

- M is the Mass matrix

Hamiltonian

- Hamilton's equations describe the time evolution of the system in terms of the **Hamiltonian**, $\mathcal{H}$, which corresponds to the total energy of the system:

$$\mathcal{H}(\mathbf{p}, \mathbf{q}) = K(\mathbf{q}, \mathbf{p}) + U(\mathbf{q})$$

- $K(\mathbf{q}, \mathbf{p})$ represents the **kinetic energy** of the system and is equal to the negative logarithm of the momentum distribution, e.g.

$$K(\mathbf{p}) = \frac{\mathbf{p}^T M^{-1} \mathbf{p}}{2} = \sum_i \frac{p_i^2}{2m_i}$$

- M is the Mass matrix
- $U(\mathbf{q})$ the **potential energy** of the system; equal to the negative logarithm of the distribution of $\mathbf{q}$.

$$\pi(\mathbf{q}, \mathbf{p}) \propto e^{-\mathcal{H}(\mathbf{q},\mathbf{p})} = e^{-K(\mathbf{p})} e^{-U(\mathbf{q})}$$

Evolution

- At each iteration of the sampling algorithm, HMC implementations make draws from some distribution $\pi(\mathbf{p}|\mathbf{q})$ and then *evolves the system* $(\mathbf{q}, \mathbf{p})$ to obtain the next sample of $\mathbf{q}$.

Evolution

- At each iteration of the sampling algorithm, HMC implementations make draws from some distribution $\pi(\mathbf{p}|\mathbf{q})$ and then *evolves the system* $(\mathbf{q}, \mathbf{p})$ to obtain the next sample of $\mathbf{q}$.
  - To "evolve the system" is to move $(\mathbf{q}, \mathbf{p})$ forward in "time," i.e. to change the values of $(\mathbf{q}, \mathbf{p})$ according to Hamilton's differential equations:

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}} = -\frac{\partial K}{\partial \mathbf{q}} - \frac{\partial U}{\partial \mathbf{q}}$$
$$\frac{d\mathbf{q}}{dt} = +\frac{\partial \mathcal{H}}{\partial \mathbf{p}} = +\frac{\partial K}{\partial \mathbf{p}}$$

Evolution

- At each iteration of the sampling algorithm, HMC implementations make draws from some distribution $\pi(\mathbf{p}|\mathbf{q})$ and then *evolves the system* $(\mathbf{q}, \mathbf{p})$ to obtain the next sample of $\mathbf{q}$.
  - To "evolve the system" is to move $(\mathbf{q}, \mathbf{p})$ forward in "time," i.e. to change the values of $(\mathbf{q}, \mathbf{p})$ according to Hamilton's differential equations:

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}} = -\frac{\partial K}{\partial \mathbf{q}} - \frac{\partial U}{\partial \mathbf{q}}$$
$$\frac{d\mathbf{q}}{dt} = +\frac{\partial \mathcal{H}}{\partial \mathbf{p}} = +\frac{\partial K}{\partial \mathbf{p}}$$

- Defines a mapping T_s from the state at any time t to the state at $t + s$

Evolution

- At each iteration of the sampling algorithm, HMC implementations make draws from some distribution $\pi(\mathbf{p}|\mathbf{q})$ and then *evolves the system* $(\mathbf{q}, \mathbf{p})$ to obtain the next sample of $\mathbf{q}$.
  - To "evolve the system" is to move $(\mathbf{q}, \mathbf{p})$ forward in "time," i.e. to change the values of $(\mathbf{q}, \mathbf{p})$ according to Hamilton's differential equations:

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}} = -\frac{\partial K}{\partial \mathbf{q}} - \frac{\partial U}{\partial \mathbf{q}}$$
$$\frac{d\mathbf{q}}{dt} = +\frac{\partial \mathcal{H}}{\partial \mathbf{p}} = +\frac{\partial K}{\partial \mathbf{p}}$$

- Defines a mapping T_s from the state at any time t to the state at $t + s$

> "The differential change in momentum parameters $\mathbf{p}$ over time is governed in part by the differential information of the density over the target parameters."

Key Properties

1) **Reversibility** The mapping of the state at time t $(\mathbf{p}(t), \mathbf{q}(t))$ to the state at $t + s$ $(\mathbf{p}(t + s), \mathbf{q}(t + s))$ is one-to-one and we have an inverse T_{-s} - obtained by negating the derivatives; $K(\mathbf{p}) = K(-\mathbf{p})$
MCMC updates using the dymamics don't modify invariant distribution!

Key Properties

1) **Reversibility** The mapping of the state at time t $(\mathbf{p}(t), \mathbf{q}(t))$ to the state at $t + s$ $(\mathbf{p}(t + s), \mathbf{q}(t + s))$ is one-to-one and we have an inverse T_{-s} - obtained by negating the derivatives; $K(\mathbf{p}) = K(-\mathbf{p})$ MCMC updates using the dymamics don't modify invariant distribution!

2) **Invariance/Conservation** the dymamics keep the Hamiltonian invariant - if we use the dynamics to generate proposals, the acceptance probability of MH is equal to one if $\mathcal{H}$ is kept invariant!

Key Properties

1) **Reversibility** The mapping of the state at time t $(\mathbf{p}(t), \mathbf{q}(t))$ to the state at $t + s$ $(\mathbf{p}(t + s), \mathbf{q}(t + s))$ is one-to-one and we have an inverse T_{-s} - obtained by negating the derivatives; $K(\mathbf{p}) = K(-\mathbf{p})$ MCMC updates using the dymamics don't modify invariant distribution!

2) **Invariance/Conservation** the dymamics keep the Hamiltonian invariant - if we use the dynamics to generate proposals, the acceptance probability of MH is equal to one if $\mathcal{H}$ is kept invariant!

3) **Volume Preservation/Symplectiness** the mapping T_s of a region R to $T_s(R)$ preserves volume -- means that we do not need to compute Jacobians

Key Properties

1) **Reversibility** The mapping of the state at time t $(\mathbf{p}(t), \mathbf{q}(t))$ to the state at $t+s$ $(\mathbf{p}(t+s), \mathbf{q}(t+s))$ is one-to-one and we have an inverse T_{-s} - obtained by negating the derivatives; $K(\mathbf{p}) = K(-\mathbf{p})$ MCMC updates using the dymamics don't modify invariant distribution!

2) **Invariance/Conservation** the dymamics keep the Hamiltonian invariant - if we use the dynamics to generate proposals, the acceptance probability of MH is equal to one if $\mathcal{H}$ is kept invariant!

3) **Volume Preservation/Symplectiness** the mapping T_s of a region R to $T_s(R)$ preserves volume -- means that we do not need to compute Jacobians

in practice we need to use approximations to solve the PDE's so won't have exact invariance etc so acceptance probability is not 1!

Approximate Solutions to Differential Equations

- Discretize time into steps ϵ

Approximate Solutions to Differential Equations

- Discretize time into steps ϵ
- Euler's Method for ith coordinate

$$p_i(t+\epsilon) = p_i(t) + \epsilon \frac{dp_i}{t}(t) = p_i(t) - \epsilon \frac{\partial U(q_i(t))}{\partial q_i}$$

$$q_i(t+\epsilon) = q_i(t) + \epsilon \frac{dq_i}{t}(t) = q_i(t) + \epsilon \frac{\partial K(p_i(t))}{\partial p_i} = q_i(t) + \epsilon \frac{p_i(t)}{m_i}$$

Approximate Solutions to Differential Equations

- Discretize time into steps ϵ
- Euler's Method for ith coordinate

$$p_i(t+\epsilon) = p_i(t) + \epsilon \frac{dp_i}{t}(t) = p_i(t) - \epsilon \frac{\partial U(q_i(t))}{\partial q_i}$$

$$q_i(t+\epsilon) = q_i(t) + \epsilon \frac{dq_i}{t}(t) = q_i(t) + \epsilon \frac{\partial K(p_i(t))}{\partial p_i} = q_i(t) + \epsilon \frac{p_i(t)}{m_i}$$

- Modified Euler method

$$p_i(t+\epsilon) = p_i(t) - \epsilon \frac{\partial U(q_i(t))}{\partial q_i}$$

$$q_i(t+\epsilon) = q_i(t) + \epsilon \frac{p_i(t+\epsilon)}{m_i}$$

Leapfrog

- Divide into half steps

Leapfrog

- Divide into half steps
- apply Modified Euler

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

$$q_i(t + \epsilon) = q_i(t) + \epsilon \frac{p_i(t + \epsilon/2)}{m_i}$$

$$p_i(t + \epsilon) = p_i(t) - \frac{\epsilon}{2} \frac{\partial U(q_i(t + \epsilon))}{\partial q_i}$$

Leapfrog

- Divide into half steps
- apply Modified Euler

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

$$q_i(t + \epsilon) = q_i(t) + \epsilon \frac{p_i(t + \epsilon/2)}{m_i}$$

$$p_i(t + \epsilon) = p_i(t) - \frac{\epsilon}{2} \frac{\partial U(q_i(t + \epsilon))}{\partial q_i}$$

- Preserves volume exactly

Leapfrog

- Divide into half steps
- apply Modified Euler

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

$$q_i(t + \epsilon) = q_i(t) + \epsilon \frac{p_i(t + \epsilon/2)}{m_i}$$

$$p_i(t + \epsilon) = p_i(t) - \frac{\epsilon}{2} \frac{\partial U(q_i(t + \epsilon))}{\partial q_i}$$

- Preserves volume exactly
- Reversible

Leapfrog

- Divide into half steps
- apply Modified Euler

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

$$q_i(t+\epsilon) = q_i(t) + \epsilon\frac{p_i(t+\epsilon/2)}{m_i}$$

$$p_i(t+\epsilon) = p_i(t) - \frac{\epsilon}{2}\frac{\partial U(q_i(t+\epsilon))}{\partial q_i}$$

- Preserves volume exactly
- Reversible
- We don't get exact invariance (so probability of acceptance is not 1)

Leapfrog

- Divide into half steps
- apply Modified Euler

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

$$q_i(t+\epsilon) = q_i(t) + \epsilon\frac{p_i(t+\epsilon/2)}{m_i}$$

$$p_i(t+\epsilon) = p_i(t) - \frac{\epsilon}{2}\frac{\partial U(q_i(t+\epsilon))}{\partial q_i}$$

- Preserves volume exactly
- Reversible
- We don't get exact invariance (so probability of acceptance is not 1)
- Step size and number of steps is still important!

MCMC with HMC

Steps: replace $\mathbf{q}$ with $\boldsymbol{\theta}$

MCMC with HMC

Steps: replace $\mathbf{q}$ with $\boldsymbol{\theta}$

1) sample a new value for the momentum $\mathbf{p}^{(t)} \sim N(0, M)$

MCMC with HMC

Steps: replace $\mathbf{q}$ with $\boldsymbol{\theta}$

1) sample a new value for the momentum $\mathbf{p}^{(t)} \sim N(0, M)$

2) Metropolis: from current state $(\mathbf{q}^{(t-1)}, \mathbf{p}^{(t)})$ simulate proposal $(\mathbf{q}^{*}, \mathbf{p}^{*})$ using Hamiltonian dynamics by applying Leapfrog with step size ϵ for L steps (tuning parameters)

MCMC with HMC

Steps: replace $\mathbf{q}$ with $\boldsymbol{\theta}$

1) sample a new value for the momentum $\mathbf{p}^{(t)} \sim N(0, M)$

2) Metropolis: from current state $(\mathbf{q}^{(t-1)}, \mathbf{p}^{(t)})$ simulate proposal $(\mathbf{q}^{*}, \mathbf{p}^{*})$ using Hamiltonian dynamics by applying Leapfrog with step size ϵ for L steps (tuning parameters)

3) Accept or reject acceptance probability is

$$\min\{1, \exp(-\mathcal{H}(\mathbf{q}^{*}, \mathbf{p}^{*}) + \mathcal{H}(\mathbf{q}^{(t-1)}, \mathbf{p}^{(t)})\}$$

Tuning

- in addition to tuning ϵ and L, we can tune M

Tuning

- in addition to tuning ϵ and L, we can tune M
- $\mathrm{Cov}(\mathbf{q}) = V$ can be highly variable

Tuning

- in addition to tuning ϵ and L, we can tune M
- $\text{Cov}(\mathbf{q}) = V$ can be highly variable
- Consider reparameterization $A\mathbf{q} = \mathbf{q}'$ so that $\text{Cov}(A\mathbf{q}) = AVA^T = I_d$; $A = V^{-1/2}$

Tuning

- in addition to tuning ϵ and L, we can tune M
- $\mathrm{Cov}(\mathbf{q}) = V$ can be highly variable
- Consider reparameterization $A\mathbf{q} = \mathbf{q}'$ so that $\mathrm{Cov}(A\mathbf{q}) = AVA^T = I_d$; $A = V^{-1/2}$
- eliminates posterior correlation!

Tuning

- in addition to tuning ϵ and L, we can tune M
- $\text{Cov}(\mathbf{q}) = V$ can be highly variable
- Consider reparameterization $A\mathbf{q} = \mathbf{q}'$ so that $\text{Cov}(A\mathbf{q}) = AVA^T = I_d; A = V^{-1/2}$
- eliminates posterior correlation!
- general trick of reparameterizing to reduce posterior correlation is often called **pre-conditioning** - improves efficiency!

Tuning

- in addition to tuning ϵ and L, we can tune M
- $\text{Cov}(\mathbf{q}) = V$ can be highly variable
- Consider reparameterization $A\mathbf{q} = \mathbf{q}'$ so that $\text{Cov}(A\mathbf{q}) = AVA^T = I_d; A = V^{-1/2}$
- eliminates posterior correlation!
- general trick of reparameterizing to reduce posterior correlation is often called **pre-conditioning** - improves efficiency!
- use $M = I_d$

Tuning

- in addition to tuning ϵ and L, we can tune M
- $\text{Cov}(\mathbf{q}) = V$ can be highly variable
- Consider reparameterization $A\mathbf{q} = \mathbf{q}'$ so that $\text{Cov}(A\mathbf{q}) = AVA^T = I_d; A = V^{-1/2}$
- eliminates posterior correlation!
- general trick of reparameterizing to reduce posterior correlation is often called **pre-conditioning** - improves efficiency!
- use $M = I_d$
- Automatic tuning is achieved by the No-U-Turn-Sampler (NUTS)
- bit complicated, but used by STAN

Tuning

- in addition to tuning ϵ and L, we can tune M
- $\text{Cov}(\mathbf{q}) = V$ can be highly variable
- Consider reparameterization $A\mathbf{q} = \mathbf{q}'$ so that $\text{Cov}(A\mathbf{q}) = AVA^T = I_d; A = V^{-1/2}$
- eliminates posterior correlation!
- general trick of reparameterizing to reduce posterior correlation is often called **pre-conditioning** - improves efficiency!
- use $M = I_d$
- Automatic tuning is achieved by the No-U-Turn-Sampler (NUTS)
- bit complicated, but used by STAN
- other variations Metropolis-Adjusted Langevin Algorithm (MALA)

Hybrid Approaches

- Recall mixed effects model

$$Y_{ij} = x_{ij}^T B + z_{ij}^T \beta_j + \epsilon_{ij} \qquad \epsilon_{ij} \sim N(0, \sigma^2)$$

Hybrid Approaches

- Recall mixed effects model

$$Y_{ij} = x_{ij}^T B + z_{ij}^T \beta_j + \epsilon_{ij} \qquad \epsilon_{ij} \sim N(0, \sigma^2)$$

- random effects $\beta_j \sim N_d(0, \Psi)$ (diagonal Ψ)

Hybrid Approaches

- Recall mixed effects model

$$Y_{ij} = x_{ij}^T B + z_{ij}^T \beta_j + \epsilon_{ij} \qquad \epsilon_{ij} \sim N(0, \sigma^2)$$

- random effects $\beta_j \sim N_d(0, \Psi)$ (diagonal Ψ)
- marginalize over the random effects

Hybrid Approaches

- Recall mixed effects model

$$Y_{ij} = x_{ij}^T B + z_{ij}^T \beta_j + \epsilon_{ij} \qquad \epsilon_{ij} \sim N(0, \sigma^2)$$

- random effects $\beta_j \sim N_d(0, \Psi)$ (diagonal Ψ)
- marginalize over the random effects

$$Y_j = N(X_j B, Z_j \Psi Z_j^T + \sigma^2 I)$$

Hybrid Approaches

- Recall mixed effects model

$$Y_{ij} = x_{ij}^T B + z_{ij}^T \beta_j + \epsilon_{ij} \qquad \epsilon_{ij} \sim N(0, \sigma^2)$$

- random effects $\beta_j \sim N_d(0, \Psi)$ (diagonal Ψ)
- marginalize over the random effects

$$Y_j = N(X_j B, Z_j \Psi Z_j^T + \sigma^2 I)$$

- we could use Gibbs on the conditional model, but we may get slow mixing (i.e. due to updating variance components)

Hybrid Approaches

- Recall mixed effects model

$$Y_{ij} = x_{ij}^T B + z_{ij}^T \beta_j + \epsilon_{ij} \qquad \epsilon_{ij} \sim N(0, \sigma^2)$$

- random effects $\beta_j \sim N_d(0, \Psi)$ (diagonal Ψ)
- marginalize over the random effects

$$Y_j = N(X_j B, Z_j \Psi Z_j^T + \sigma^2 I)$$

- we could use Gibbs on the conditional model, but we may get slow mixing (i.e. due to updating variance components)
- run HMC within Gibbs to update the variance components Ψ and σ^2 using the marginal model given B

Hybrid Approaches

- Recall mixed effects model

$$Y_{ij} = x_{ij}^T B + z_{ij}^T \beta_j + \epsilon_{ij} \qquad \epsilon_{ij} \sim N(0, \sigma^2)$$

- random effects $\beta_j \sim N_d(0, \Psi)$ (diagonal Ψ)
- marginalize over the random effects

$$Y_j = N(X_j B, Z_j \Psi Z_j^T + \sigma^2 I)$$

- we could use Gibbs on the conditional model, but we may get slow mixing (i.e. due to updating variance components)
- run HMC within Gibbs to update the variance components Ψ and σ^2 using the marginal model given B
- HMC in its basic form doesn't like constraints so reparameterize to use log transformations

Advantages & Disadvantages

- HMC can produce samples with low correlation and high acceptance ratio!

Advantages & Disadvantages

- HMC can produce samples with low correlation and high acceptance ratio!
- driven by step size (larger time steps mean values are farther away but may lead to lower acceptance- error is $O(\epsilon^2)$ for the leapfrog method)

Advantages & Disadvantages

- HMC can produce samples with low correlation and high acceptance ratio!
- driven by step size (larger time steps mean values are farther away but may lead to lower acceptance- error is $O(\epsilon^2)$ for the leapfrog method)
- number of steps (more steps reduces correlation; to avoid U turns stan uses NUTS)

Advantages & Disadvantages

- HMC can produce samples with low correlation and high acceptance ratio!
- driven by step size (larger time steps mean values are farther away but may lead to lower acceptance- error is $O(\epsilon^2)$ for the leapfrog method)
- number of steps (more steps reduces correlation; to avoid U turns stan uses NUTS)
- most implementations limited to continuous variables (need gradients of log densities)

Advantages & Disadvantages

- HMC can produce samples with low correlation and high acceptance ratio!
- driven by step size (larger time steps mean values are farther away but may lead to lower acceptance- error is $O(\epsilon^2)$ for the leapfrog method)
- number of steps (more steps reduces correlation; to avoid U turns stan uses NUTS)
- most implementations limited to continuous variables (need gradients of log densities)
- need to calculate gradients (automatic differentiation methods)

Advantages & Disadvantages

- HMC can produce samples with low correlation and high acceptance ratio!
- driven by step size (larger time steps mean values are farther away but may lead to lower acceptance- error is $O(\epsilon^2)$ for the leapfrog method)
- number of steps (more steps reduces correlation; to avoid U turns stan uses NUTS)
- most implementations limited to continuous variables (need gradients of log densities)
- need to calculate gradients (automatic differentiation methods)
- can mix Gibbs (for discrete) and HMC (for continuous)

Advantages & Disadvantages

- HMC can produce samples with low correlation and high acceptance ratio!
- driven by step size (larger time steps mean values are farther away but may lead to lower acceptance- error is $O(\epsilon^2)$ for the leapfrog method)
- number of steps (more steps reduces correlation; to avoid U turns stan uses NUTS)
- most implementations limited to continuous variables (need gradients of log densities)
- need to calculate gradients (automatic differentiation methods)
- can mix Gibbs (for discrete) and HMC (for continuous)
- Nishimura et al (2020 Biometrika) for HMC with discrete targets