

Bayesian Statistics I

Lecture 9 - HMC, Stan and Variational Inference

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Lecture overview

- Hamiltonian Monte Carlo
- Stan
- Variational Inference

Hamiltonian Monte Carlo

- When $\theta = (\theta_1, \dots, \theta_p)$ is **high-dimensional**, $p(\theta|\mathbf{y})$ usually located in some subregion of \mathbb{R}^p with complicated geometry.
- MH: hard to find good proposal distribution $q(\cdot|\theta^{(i-1)})$.
- MH: use very small step sizes otherwise too many rejections.
- **Hamiltonian Monte Carlo (HMC)**:
 - ▶ distant proposals **and**
 - ▶ high acceptance probabilities.
- HMC: add extra **momentum** parameters $\phi = (\phi_1, \dots, \phi_p)$ and sample from

$$p(\theta, \phi|\mathbf{y}) = p(\theta|\mathbf{y}) p(\phi)$$

.

Hamiltonian Monte Carlo

- Physics: **Hamiltonian** system $H(\theta, \phi) = U(\theta) + K(\phi)$, where U is the **potential energy** and K is the **kinetic energy**.
- **Hamiltonian Dynamics**

$$\begin{aligned}\frac{d\theta_i}{dt} &= \frac{\partial H}{\partial \phi_i} = \frac{\partial K}{\partial \phi_i}, \\ \frac{d\phi_i}{dt} &= -\frac{\partial H}{\partial \theta_i} = -\frac{\partial U}{\partial \theta_i}\end{aligned}$$

- Hockey puck sliding over a friction-less surface: [illustration](#).
- Use $U(\theta) = -\log[p(\theta)p(\mathbf{y}|\theta)]$.
- Use $\phi \sim N(0, \mathbf{M})$ where \mathbf{M} is the mass matrix and

$$K(\phi) = -\log[p(\phi)] = \frac{1}{2}\phi^T \mathbf{M}^{-1}\phi + \text{const}$$

- If we could propose θ in continuous time (spoiler: we can't), the acceptance probability would be one.

Hamiltonian Monte Carlo

■ Hamiltonian Dynamics

$$\begin{aligned}\frac{d\theta_i}{dt} &= [\mathbf{M}^{-1}\phi]_i, \\ \frac{d\phi_i}{dt} &= \frac{\partial \log p(\theta|\mathbf{y})}{\partial \theta_i}\end{aligned}$$

which can be simulated using the **leapfrog algorithm**

$$\begin{aligned}\phi_i\left(t + \frac{\varepsilon}{2}\right) &= \phi_i(t) + \frac{\varepsilon}{2} \frac{\partial \log p(\theta(t)|\mathbf{y})}{\partial \theta_i}, \\ \theta(t + \varepsilon) &= \theta(t) + \varepsilon \mathbf{M}^{-1}\phi(t), \\ \phi_i(t + \varepsilon) &= \phi_i\left(t + \frac{\varepsilon}{2}\right) + \frac{\varepsilon}{2} \frac{\partial \log p(\theta(t)|\mathbf{y})}{\partial \theta_i},\end{aligned}$$

where ε is the step size.

■ **Discretization** \Rightarrow acceptance probability drops with ε .

The Hamiltonian Monte Carlo algorithm

■ Initialize $\theta^{(0)}$ and iterate for $i = 1, 2, \dots$

- 1 Sample the starting **momentum** $\phi_s \sim N(0, \mathbf{M})$
- 2 Simulate new values for (θ_p, ϕ_p) by iterating the **leapfrog algorithm** L times, starting in $(\theta^{(i-1)}, \phi_s)$.
- 3 Compute the **acceptance probability**

$$\alpha = \min \left(1, \frac{p(\mathbf{y}|\theta_p)p(\theta_p)}{p(\mathbf{y}|\theta^{(i-1)})p(\theta^{(i-1)})} \frac{p(\phi_p)}{p(\phi_s)} \right)$$

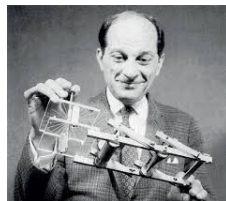
- 4 With probability α set $\theta^{(i)} = \theta_p$ and $\theta^{(i)} = \theta^{(i-1)}$ otherwise.

■ **Tuning parameters:** 1. **stepsize** ε , 2. **number of leapfrog iterations** L and 3. **mass matrix** M . **No U-turn.**

- **Stan** is a probabilistic programming language based on HMC.
- Allows for Bayesian inference in many models with automatic implementation of the MCMC sampler.
- Named after Stanislaw Ulam (1909-1984), co-inventor of the Monte Carlo algorithm.
- Written in C++ but can be run from R using the package `rstan`



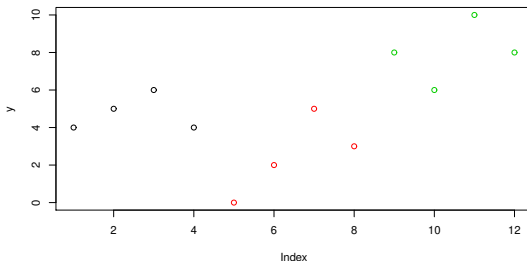
Stan logo



Stanislaw Ulam

Stan - toy example: three plants

- Three plants were observed for four months, measuring the number of flowers



Stan Model 1: iid normal

$$y_i \stackrel{iid}{\sim} N(\mu, \sigma^2)$$

```
library(rstan)
y = c(4,5,6,4,0,2,5,3,8,6,10,8)
N = length(y)

StanModel = '
data {
  int<lower=0> N; // Number of observations
  int<lower=0> y[N]; // Number of flowers
}
parameters {
  real mu;
  real<lower=0> sigma2;
}
model {
  mu ~ normal(0,100); // Normal with mean 0, st.dev. 100
  sigma2 ~ scaled_inv_chi_square(1,2); // Scaled-inv-chi2 with nu 1, sigma 2
  for(i in 1:N)
    y[i] ~ normal(mu,sqrt(sigma2));
}'
```

Stan Model 2: multilevel normal

$$y_{i,p} \sim N(\mu_p, \sigma_p^2), \quad \mu_p \sim N(\mu, \sigma^2)$$

```
StanModel = '  
data {  
  int<lower=0> N; // Number of observations  
  int<lower=0> y[N]; // Number of flowers  
  int<lower=0> P; // Number of plants  
}  
transformed data {  
  int<lower=0> M; // Number of months  
  M = N / P;  
}  
parameters {  
  real mu;  
  real<lower=0> sigma2;  
  real mup[P];  
  real sigmap2[P];  
}  
model {  
  mu ~ normal(0,100); // Normal with mean 0, st.dev. 100  
  sigma2 ~ scaled_inv_chi_square(1,2); // Scaled-inv-chi2 with nu 1, sigma 2  
  for(p in 1:P){  
    mup[p] ~ normal(mu,sqrt(sigma2));  
    for(m in 1:M)  
      y[M*(p-1)+m] ~ normal(mup[p],sqrt(sigmap2[p]));  
  }  
}'
```

Stan Model 3: multilevel Poisson

$$y_{i,p} \sim \text{Poisson}(\mu_p), \quad \mu_p \sim \text{logN}(\mu, \sigma^2)$$

```
StanModel = '  
data {  
  int<lower=0> N; // Number of observations  
  int<lower=0> y[N]; // Number of flowers  
  int<lower=0> P; // Number of plants  
}  
transformed data {  
  int<lower=0> M; // Number of months  
  M = N / P;  
}  
parameters {  
  real mu;  
  real<lower=0> sigma2;  
  real mup[P];  
}  
model {  
  mu ~ normal(0,100); // Normal with mean 0, st.dev. 100  
  sigma2 ~ scaled_inv_chi_square(1,2); // Scaled-inv-chi2 with nu 1, sigma 2  
  for(p in 1:P){  
    mup[p] ~ lognormal(mu,sqrt(sigma2)); // Log-normal  
    for(m in 1:M)  
      y[M*(p-1)+m] ~ poisson(mup[p]); // Poisson  
  }  
}'
```

Stan: fit model and analyze output

```
data = list(N=N, y=y, P=P)
burnin = 1000
niter = 2000
fit = stan(model_code=StanModel, data=data,
           warmup=burnin, iter=niter, chains=4)

# Print the fitted model
print(fit, digits_summary=3)

# Extract posterior samples
postDraws <- extract(fit)

# Do traceplots of the first chain
par(mfrow = c(1,1))
plot(postDraws$mu[1:(niter-burnin)], type="l", ylab="mu", main="Traceplot")

# Do automatic traceplots of all chains
traceplot(fit)

# Bivariate posterior plots
pairs(fit)
```

Stan - useful links

- [Getting started with RStan](#)
- [RStan vignette](#)
- [Stan Modeling Language User's Guide and Reference Manual](#)
- [Stan Case Studies](#)

Variational Inference

- Let $\theta = (\theta_1, \dots, \theta_p)$. Approximate the posterior $p(\theta|y)$ with a (simpler) distribution $q(\theta)$.
- Before: **Normal approximation** from optimization:
 $q(\theta) = N[\tilde{\theta}, J_y^{-1}(\tilde{\theta})]$.
- **Mean field Variational Inference (VI)**: $q(\theta) = \prod_{i=1}^p q_i(\theta_i)$
- **Parametric VI**: Parametric family $q_\lambda(\theta)$ with parameters λ
- Find the $q(\theta)$ that **minimizes the Kullback-Leibler distance** between the true posterior p and the approximation q :

$$KL(q, p) = \int q(\theta) \ln \frac{q(\theta)}{p(\theta|y)} d\theta = E_q \left[\ln \frac{q(\theta)}{p(\theta|y)} \right].$$

Mean field approximation

- **Mean field VI** is based on factorized approximation:

$$q(\theta) = \prod_{i=1}^p q_i(\theta_i)$$

- **No specific functional forms** are assumed for the $q_i(\theta)$.
- **Optimal densities** can be shown to satisfy:

$$q_i(\theta) \propto \exp(E_{-\theta_i} \ln p(\mathbf{y}, \theta))$$

where $E_{-\theta_i}(\cdot)$ is the expectation with respect to $\prod_{i \neq j} q_j(\theta_j)$.

- **Structured mean field approximation**. Group subset of parameters in tractable blocks. Similar to Gibbs sampling.

Mean field approximation - algorithm

■ Initialize: $q_2^*(\theta_2), \dots, q_M^*(\theta_p)$

■ Repeat until convergence:

▶ $q_1^*(\theta_1) \leftarrow \frac{\exp[E_{-\theta_1} \ln p(\mathbf{y}, \theta)]}{\int \exp[E_{-\theta_1} \ln p(\mathbf{y}, \theta)] d\theta_1}$

▶ \vdots

▶ $q_p^*(\theta_p) \leftarrow \frac{\exp[E_{-\theta_p} \ln p(\mathbf{y}, \theta)]}{\int \exp[E_{-\theta_p} \ln p(\mathbf{y}, \theta)] d\theta_p}$

■ Note: no assumptions about parametric form of the $q_i(\theta)$.

■ Optimal $q_i(\theta)$ often **turn out** to be parametric (normal etc).

■ Just update hyperparameters in the optimal densities.

Mean field approximation - Normal model

- **Model:** $X_i | \theta, \sigma^2 \stackrel{iid}{\sim} N(\theta, \sigma^2)$.
- **Prior:** $\theta \sim N(\mu_0, \tau_0^2)$ independent of $\sigma^2 \sim \text{Inv} - \chi^2(\nu_0, \sigma_0^2)$.
- **Mean-field approximation:** $q(\theta, \sigma^2) = q_\theta(\theta) \cdot q_{\sigma^2}(\sigma^2)$.
- Optimal densities

$$q_\theta^*(\theta) \propto \exp \left[E_{q(\sigma^2)} \ln p(\theta, \sigma^2, \mathbf{x}) \right]$$
$$q_{\sigma^2}^*(\sigma^2) \propto \exp \left[E_{q(\theta)} \ln p(\theta, \sigma^2, \mathbf{x}) \right]$$

Normal model - VB algorithm

■ Variational density for σ^2

$$\sigma^2 \sim \text{Inv} - \chi^2 (\tilde{\nu}_n, \tilde{\sigma}_n^2)$$

where $\tilde{\nu}_n = \nu_0 + n$ and $\tilde{\sigma}_n^2 = \frac{\nu_0 \sigma_0^2 + \sum_{i=1}^n (x_i - \tilde{\mu}_n)^2 + n \cdot \tilde{\tau}_n^2}{\nu_0 + n}$

■ Variational density for θ

$$\theta \sim N(\tilde{\mu}_n, \tilde{\tau}_n^2)$$

where

$$\tilde{\tau}_n^2 = \frac{1}{\frac{n}{\tilde{\sigma}_n^2} + \frac{1}{\tau_0^2}}$$

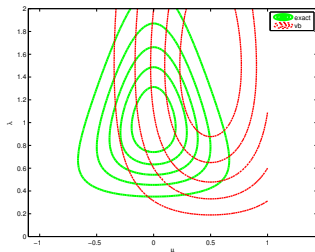
$$\tilde{\mu}_n = \tilde{w} \bar{x} + (1 - \tilde{w}) \mu_0,$$

where

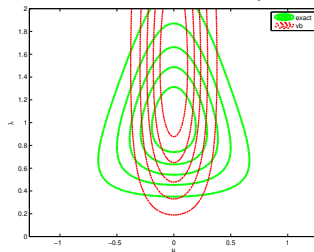
$$\tilde{w} = \frac{\frac{n}{\tilde{\sigma}_n^2}}{\frac{n}{\tilde{\sigma}_n^2} + \frac{1}{\tau_0^2}}$$

Normal example from Murphy ($\lambda = 1/\sigma^2$)

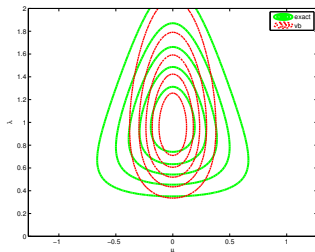
Initial values



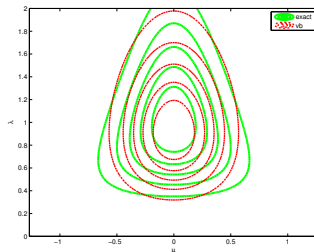
After updating q_μ



After updating q_{σ^2}



At convergence



Probit regression

- **Model:**

$$\Pr(y_i = 1 | \mathbf{x}_i) = \Phi(\mathbf{x}_i^T \boldsymbol{\beta})$$

- **Prior:** $\boldsymbol{\beta} \sim N(0, \Sigma_{\boldsymbol{\beta}})$. For example: $\Sigma_{\boldsymbol{\beta}} = \tau^2 I$.

- **Latent variable formulation** with $\mathbf{u} = (u_1, \dots, u_n)'$

$$\mathbf{u} | \boldsymbol{\beta} \sim N(\mathbf{X}\boldsymbol{\beta}, 1)$$

and

$$y_i = \begin{cases} 0 & \text{if } u_i \leq 0 \\ 1 & \text{if } u_i > 0 \end{cases}$$

- Factorized **variational approximation**

$$q(\mathbf{u}, \boldsymbol{\beta}) = q_{\mathbf{u}}(\mathbf{u})q_{\boldsymbol{\beta}}(\boldsymbol{\beta})$$

VI for probit regression

■ VI posterior

$$\beta \sim N \left(\tilde{\mu}_\beta, \left(\mathbf{X}^T \mathbf{X} + \Sigma_\beta^{-1} \right)^{-1} \right)$$

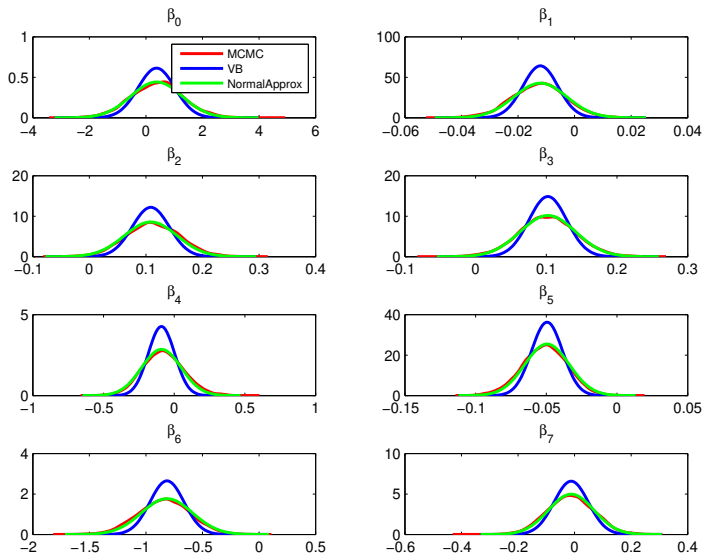
where

$$\tilde{\mu}_\beta = \left(\mathbf{X}^T \mathbf{X} + \Sigma_\beta^{-1} \right)^{-1} \mathbf{X}^T \tilde{\mu}_\mathbf{u}$$

and

$$\tilde{\mu}_\mathbf{u} = \mathbf{X} \tilde{\mu}_\beta + \frac{\phi(\mathbf{X} \tilde{\mu}_\beta)}{\Phi(\mathbf{X} \tilde{\mu}_\beta)^y [\Phi(\mathbf{X} \tilde{\mu}_\beta) - 1_n]^{1_n - y}}.$$

Probit example (n=200 observations)



Probit example

