

Bayesian Statistics I

Lecture 9 - HMC and Variational Inference

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Lecture overview

- Hamiltonian Monte Carlo
- Variational Inference

Hamiltonian Monte Carlo

- When $\theta = (\theta_1, \dots, \theta_p)$ is **high-dimensional**, $p(\theta|y)$ 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

$$p(\theta, \phi|y) = p(\theta|y) p(\phi)$$

.

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 $U(\theta) = -\log[p(\theta)p(y|\theta)]$.
- Use $\phi \sim N(0, M)$ where M is the mass matrix and

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

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

Hamiltonian Monte Carlo

■ Hamiltonian Dynamics

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

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

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

where ε is the step size.

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

The Hamiltonian Monte Carlo algorithm

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

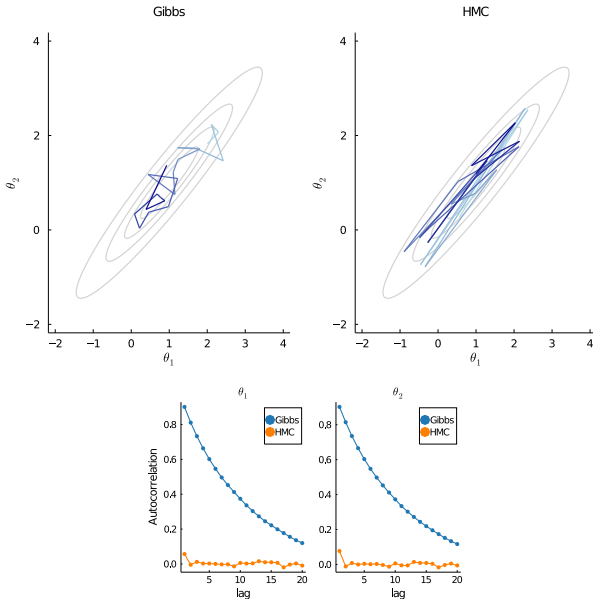
- 1 Sample the starting **momentum** $\phi_s \sim N(0, M)$
- 2 Simulate new values for (θ_p, ϕ_p) by iterating the **leapfrog algorithm** L times, starting in $(\theta^{(i-1)}, \phi_s)$.
- 3 Compute the **acceptance probability**

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

- 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**.

Gibbs vs HMC on bivariate normal



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:

$$q(\theta) = \prod_{j=1}^p q_j(\theta_j)$$

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

$$q_j(\theta_j) \propto \exp \left(E_{-\theta_j} \ln p(y, \theta) \right)$$

where $E_{-\theta_j}(\cdot)$ is the expectation with respect to $\prod_{k \neq j} q_k(\theta_k)$.

- **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:
 - ▶ $q_1^*(\theta_1) \leftarrow \frac{\exp[E_{-\theta_1} \ln p(y, \theta)]}{\int \exp[E_{-\theta_1} \ln p(y, \theta)] d\theta_1}$
 - ▶ \vdots
 - ▶ $q_p^*(\theta_p) \leftarrow \frac{\exp[E_{-\theta_p} \ln p(y, \theta)]}{\int \exp[E_{-\theta_p} \ln p(y, \theta)] d\theta_p}$
- 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:** $X_i | \theta, \sigma^2 \stackrel{\text{iid}}{\sim} N(\theta, \sigma^2)$.
- **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

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

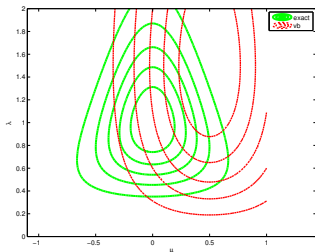
$$\tilde{\mu}_n = \tilde{w} \bar{x} + (1 - \tilde{w}) \mu_0,$$

where

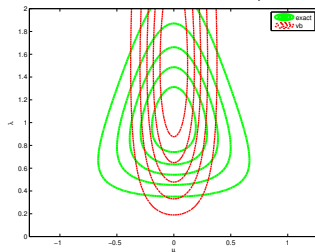
$$\tilde{w} = \frac{\frac{n}{\tilde{\sigma}_n^2}}{\frac{n}{\tilde{\sigma}_n^2} + \frac{1}{\tau_0^2}}$$

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

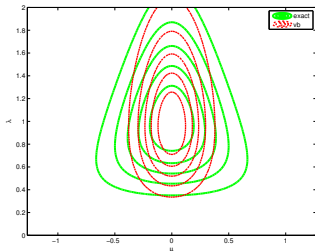
Initial values



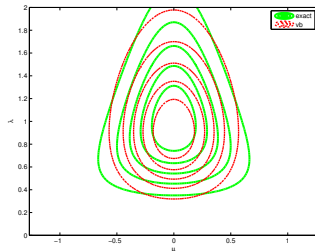
After updating q_μ



After updating q_{σ^2}



At convergence



Probit regression

- **Model:**

$$\Pr(y_i = 1|x_i) = \Phi(x_i^T \beta)$$

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

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

$$u|\beta \sim N(X\beta, 1)$$

and

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

- Factorized **variational approximation**

$$q(u, \beta) = q_u(u)q_\beta(\beta)$$

VI for probit regression

■ VI posterior

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

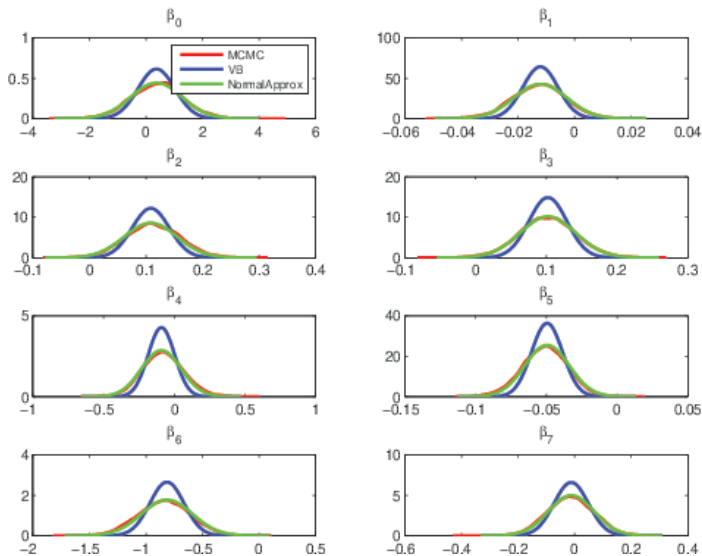
where

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

and

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

Probit example (n=200 observations)



Probit example

