Bayesian Learning - Lecture 9

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Lecture overview

- **Hamiltonian Monte Carlo**
- **Stan**
- **Variational Bayes**

Hamiltonian Monte Carlo

- **Motivation:** Assume that $\theta = (\theta_1, ..., \theta_p)$. If p is large, then most of the mass of $p(\theta|y)$ is usually located on some subregion in $\mathbb{R}^p$ with complicated geometry.
- Finding a good proposal distribution $q\left(\cdot|\theta^{(i-1)}\right)$ for the MH algorithm might be hard
  $\Rightarrow$ Use very small step sizes or few accepted proposed samples.

Hamiltonian Monte Carlo

- **Motivation:** Assume that $\theta = (\theta_1, ..., \theta_p)$. If p is large, then most of the mass of $p(\theta|y)$ is usually located on some subregion in $\mathbb{R}^p$ with complicated geometry.
- Finding a good proposal distribution $q\left(\cdot|\theta^{(i-1)}\right)$ for the MH algorithm might be hard
  $\Rightarrow$ Use very small step sizes or few accepted proposed samples.
- **Hamiltonian Monte Carlo** (**HMC**) borrows ideas from physics to allow more rapid movements in the posterior distribution.
- HMC adds an auxiliary **momentum** parameter $\phi = (\phi_1, \ldots, \phi_p)$ and samples from $p(\theta, \phi|y) = p(\theta|y)\, p(\phi)$.

Hamiltonian Monte Carlo

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

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

- Use $U(\theta) = -\log\left[p(\theta)\, p(y|\theta)\right]$.
- Use $\phi \sim N(0, M)$ and $K(\phi) = -\log\left[p(\phi)\right] = \frac{1}{2}\phi^T M^{-1}\phi + \text{const}$, where M is the mass matrix (often diagonal).

Hamiltonian Monte Carlo

- This gives the system:

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

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

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

where ε is the step size.

The Hamiltonian Monte Carlo algorithm

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

  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 $\left(\theta^{(i-1)}, \phi_s\right)$.
  3. Compute the **acceptance probability**

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

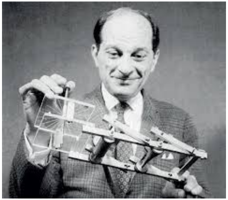
  4. With probability α set $\theta^{(i)} = \theta_p$ and $\theta^{(i)} = \theta^{(i-1)}$ otherwise.

- Imagine a hockey pluck sliding over a friction-less surface: illustration.
- The stepsize ε, number of leapfrog iterations L and mass matrix M are tuning parameters that can be tuned during the burn-in phase.

Stan

- 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`

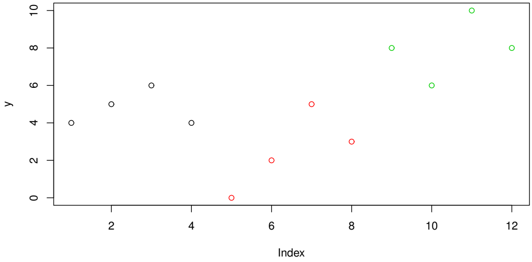
Stan logo



Stanislaw Ulam

Stan - toy example: three plants

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



Stan Model 1: iid normal

$$y_i \overset{iid}{\sim} N\left(\mu, \sigma^2\right)$$

```
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

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

```
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

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

```
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

```r
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 Bayes

- Let $\theta = (\theta_1, ..., \theta_p)$. Approximate the posterior $p(\theta|y)$ with a (simpler) distribution $q(\theta)$.
- We have already seen: $q(\theta) = N\left[\tilde{\theta}, J_{\mathbf{y}}^{-1}(\tilde{\theta})\right]$.
- **Mean field Variational Bayes (VB)**

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

- **Parametric VB**, where $q_\lambda(\theta)$ is a parametric family 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

- Factorization
$$q(\theta) = \prod_{i=1}^{p} q_i(\theta_i)$$
- **No specific functional forms are assumed** for the $q_i(\theta)$.
- **Optimal densities** can be shown to satisfy:
$$q_i(\theta) \propto \exp\left(E_{-\theta_i} \ln p(\mathbf{y}, \theta)\right)$$
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: $q_2^*(\theta_2)$, ..., $q_M^*(\theta_p)$
- Repeat until convergence:
  - $q_1^*(\theta_1) \leftarrow \frac{\exp\left[E_{-\theta_1} \ln p(\mathbf{y},\theta)\right]}{\int \exp\left[E_{-\theta_1} \ln p(\mathbf{y},\theta)\right] d\theta_1}$
  - $\vdots$
  - $q_p^*(\theta_p) \leftarrow \frac{\exp\left[E_{-\theta_p} \ln p(\mathbf{y},\theta)\right]}{\int \exp\left[E_{-\theta_p} \ln p(\mathbf{y},\theta)\right] d\theta_p}$
- Note: we make no assumptions about parametric form of the $q_i(\theta)$, but the optimal $q_i(\theta)$ often turn out to be parametric (normal, gamma etc).
- The updates above then boil down to just updating of hyperparameters in the optimal densities.

Mean field approximation - Normal model

- **Model**: $X_i|\theta,\sigma^2 \overset{iid}{\sim} N(\theta,\sigma^2)$.
- **Prior**: $\theta \sim N(\mu_0,\tau_0^2)$ **independent** of $\sigma^2 \sim Inv-\chi^2(\nu_0,\sigma_0^2)$.
- **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**

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

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

- **Variational density for θ**

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

where

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

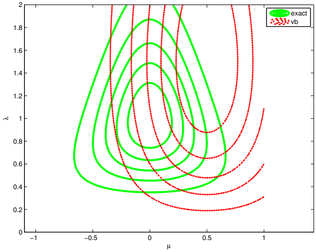
$$\tilde{\mu}_n = \tilde{w}\bar{x} + (1 - \tilde{w})\mu_0,$$

where

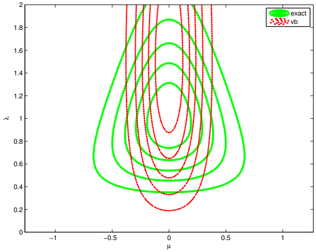
$$\tilde{w} = \frac{\frac{n}{\tilde{\sigma}_n^2}}{\frac{n}{\tilde{\sigma}_n^2} + \frac{1}{\tau_0^2}}$$

NORMAL EXAMPLE FROM MURPHY ($\lambda = 1/\sigma^2$)

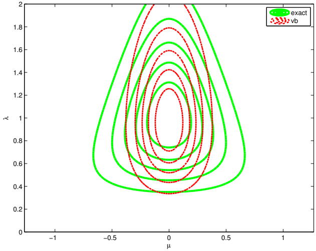
Initial values



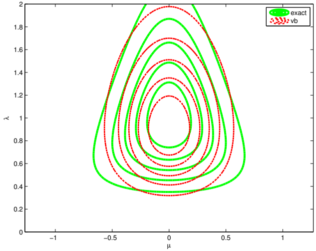
After updating q_μ



After updating q_{σ^2}



At convergence



Probit regression

- **Model**:
$$\Pr(y_i = 1|\mathbf{x}_i) = \Phi(\mathbf{x}_i^T\beta)$$
- **Prior**: $\beta \sim N(0, \Sigma_\beta)$. For example: $\Sigma_\beta = \tau^2 I$.
- **Latent variable formulation** with $u = (u_1, ..., u_n)'$
$$\mathbf{u}|\beta \sim N(\mathbf{X}\beta, 1)$$
and
$$y_i = \begin{cases} 0 & \text{if } u_i \leq 0 \\ 1 & \text{if } u_i > 0 \end{cases}$$
- Factorized **variational approximation**
$$q(\mathbf{u}, \beta) = q_{\mathbf{u}}(\mathbf{u})q_\beta(\beta)$$

VB for probit regression

- VB posterior

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

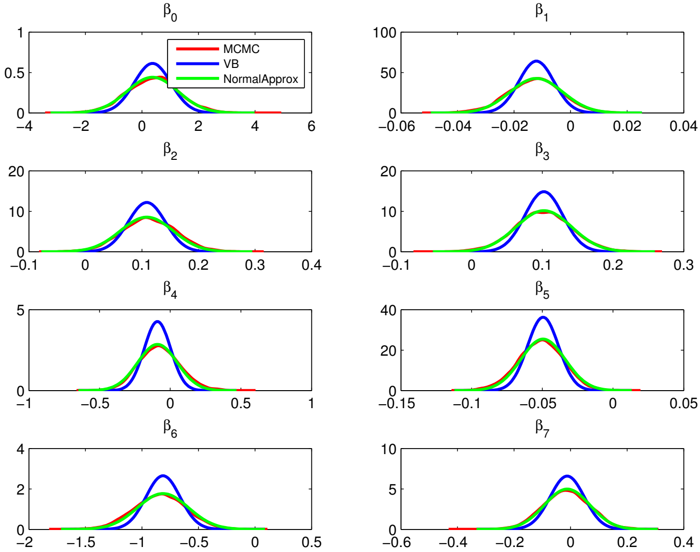
where

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

and

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

PROBIT EXAMPLE (N=200 OBSERVATIONS)



Probit example