Bayesian Learning

Lecture 9 - HMC, Stan and Variational Inference (VI)

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Lecture overview

- Hamiltonian Monte Carlo
- Stan
- Variational Inference

Hamiltonian Monte Carlo

- When $\theta = (\theta_1, \ldots, \theta_p)$ is **high-dimensional**, $p(\theta|\mathrm{y})$ usually located in some subregion of $\mathbb{R}^p$ with complicated geometry.
- MH: hard to find good proposal distribution $q\left(\cdot|\theta^{(i-1)}\right)$.
- 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 $\phi = (\phi_1, \ldots, \phi_p)$ and sample from

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

.

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**

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

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

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

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

Hamiltonian Monte Carlo

- **Hamiltonian Dynamics**

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

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

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

where ε is the step size.

- **Discretization** $\Rightarrow$ acceptance probability drops with ε.

The Hamiltonian Monte Carlo algorithm

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

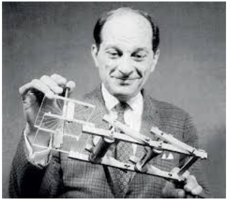
  1. Sample the starting **momentum** $\phi_s \sim N(0, \mathrm{M})$
  2. Simulate new values for (θ_p, ϕ_p) by iterating the **leapfrog algorithm** L times, starting in $\left(\theta^{(i-1)}, \phi_s\right)$.
  3. Compute the **acceptance probability**
  $$\alpha = \min\left(1, \frac{p(\mathrm{y}|\theta_p)p(\theta_p)}{p(\mathrm{y}|\theta^{(i-1)})p(\theta^{(i-1)})}\frac{p(\phi_p)}{p(\phi_s)}\right)$$
  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

- 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`

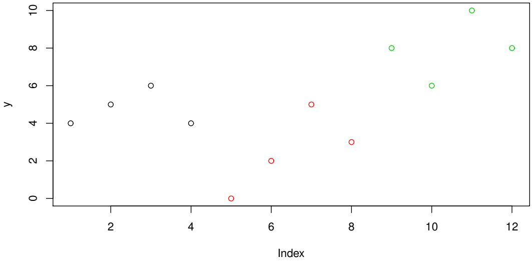
Stan logo



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

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

```
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

$$y_{t,p} \sim Poisson\left(\mu_p\right),\ \mu_p \sim logN\left(\mu, \sigma^2\right)$$

```
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];
}
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)
warmup <- 1000
niter <- 2000
fit <- stan(model_code=StanModel,data=data, warmup=warmup,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 $\theta = (\theta_1, ..., \theta_p)$. Approximate the posterior $p(\theta|y)$ with a (simpler) distribution $q(\theta)$.
- Before: **Normal approximation** from optimization: $q(\theta) = N\left[\tilde{\theta}, J_{\mathrm{y}}^{-1}(\tilde{\theta})\right]$.
- **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:

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

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

Mean field approximation - algorithm

- Initialize: $q_2^*(\theta_2), ..., q_p^*(\theta_p)$
- Repeat until convergence:
  - $q_1^*(\theta_1) \leftarrow \frac{\exp\left[E_{-\theta_1} \ln p(y,\theta)\right]}{\int \exp\left[E_{-\theta_1} \ln p(y,\theta)\right] d\theta_1}$
  - $\vdots$
  - $q_p^*(\theta_p) \leftarrow \frac{\exp\left[E_{-\theta_p} \ln p(y,\theta)\right]}{\int \exp\left[E_{-\theta_p} \ln p(y,\theta)\right] d\theta_p}$
- 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**: $X_i|\theta, \sigma^2 \overset{iid}{\sim} N(\theta, \sigma^2)$.
- **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

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

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 ($\lambda = 1/\sigma^2$)