# Bayesian Learning

## Lecture 9 - HMC and Stan

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# Lecture overview

- Hamiltonian Monte Carlo
- Stan

# Hamiltonian Monte Carlo

- When $\theta = (\theta_1, \ldots, \theta_p)$ 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 $q\left(\cdot|\theta^{(i-1)}\right)$.
- 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

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

# 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**

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

- 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

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

# 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 $\varepsilon$ is the step size.

## Discretization $\Rightarrow$ acceptance probability drops with $\varepsilon$.

# The Hamiltonian Monte Carlo algorithm

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

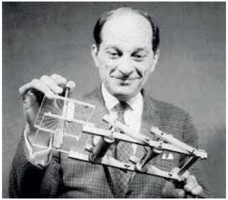
  1. Sample the starting **momentum** $\phi_s \sim N(0, \mathrm{M})$
  2. Simulate new values for $(\theta_p, \phi_p)$ by iterating the **leapfrog algorithm** $L$ times, starting in $\left(\theta^{(i-1)}, \phi_s\right)$.
  3. Compute the **acceptance probability**
  $$\alpha = \min\left(1, \frac{p(\mathrm{y}|\theta_p)p(\theta_p)}{p(\mathrm{y}|\theta^{(i-1)})p(\the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

- **Tuning parameters**: 1. **stepsize** $\varepsilon$, 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`

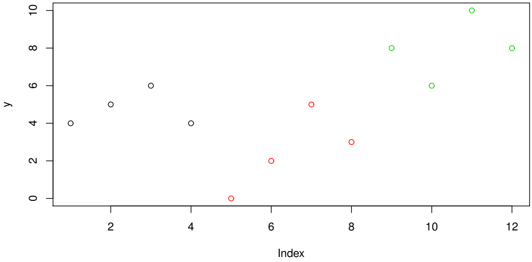
Stan logo



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(file="StanModel.stan", data=data, warmup=warmup, iter=niter, chains=4, cores=2)

# 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-warmup)],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