## Hamiltonian MC Exercise

DUE: in class on Friday October 11

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## Intro

You are already familiar with Metropolis-Hastings and Gibbs sampling routines in the context of MCMC sampling. The stan software package utilizes a different routine called NUTS which is more generally based on Hamiltonian Monte Carlo (HMC). This assignment will get you familiar with the basics of HMC.

## Hamiltonian MC Idea

Assume we want draws from the posterior distribution  $p(\phi|y)$ . The principle of HMC is equivalent to rolling a large number of balls on a potential field of  $-\log(p(\phi|y))$  and sampling the locations  $(\phi \text{ values})$  of those balls. Those sampled locations are samples from  $p(\phi|y)$ . In the case that  $\phi$  is one or two dimensional, it is pretty easy to think about:  $-\log(p(\phi|y))$  is a deformed surface or hill on which a ball can roll. The analogue is the same in higher dimensions, but not easy to envision.

1. Consider an observation y from the binomial likelihood,  $y \sim \text{binomial}(n, \pi)$  with n known. If  $\phi = \log\left(\frac{\pi}{1-\pi}\right)$  (ie the exponential family canonical parameter of the binomial likelihood), and we choose a prior on  $\phi$  of a normal distribution with a mean of  $\mu$  and standard deviation of  $\sigma$ , show that the posterior of  $\phi$  based on an observation of y is proportional to

$$f(\phi) = \exp(\phi)^y \left(1 + \exp(\phi)\right)^{-n} \exp\left(-\frac{(\phi - \mu)^2}{2\sigma^2}\right)$$

Write an R function that calculates the above expression given inputs  $\phi$ , y, n,  $\mu$ , and  $\sigma$ . Plot it as a function of  $\phi$  for y = 5, n = 10,  $\mu = 0$ ,  $\sigma = 2$ . (Does this problem sound familiar?)

- 2. Plot  $(-\log(f(\phi)))$ .
- 3. A ball sitting on the potential field  $-\log(p(\phi|y))$  at position  $\phi$  will accelerate at a rate

proportional to the gradient of the field. In one-dimension we simply find this by:

$$\frac{d}{d\phi} \left( -\log(p(\phi|y)) \right).$$

Typically, we just write down  $p(\phi|y)$  up to a multiplicative constant like our  $f(\phi)$ . Show that we only need to know the posterior up to a multiplicative factor to calculate the derivative above. Calculate the derivative for our scenario in terms of y, n,  $\mu$ , and  $\sigma$ . Write an R function that evaluates the derivative and plot it.

4. If you have written R functions to calculate f (problem 1) and the derivative of the negative log of f (problem 3) and both take as inputs  $\phi$ , y, n,  $\mu$ , and  $\sigma$  in that order, you can run the following two lines of code to watch a ball roll around:

```
source("roll.R") #check directory
roll(0, grad, dens)
```

where 0 is the initial  $\phi$  value (location to start the ball), grad is the name of your function from problem 3 and dens is the name of your function from problem 1.