MATH 598: TOPICS IN STATISTICS
HAMILTONIAN MCMC: 1D EXAMPLE

Example: Suppose $Y \equiv Gamma(\alpha, 1)$, and consider the pdf of $X = \log Y$. Then for $x \in \mathbb{R}$

$$f_X(x) = e^x f_Y(e^x) = \frac{1}{\Gamma(\alpha)} \exp\{\alpha x - e^x\}.$$

We set $\pi_X(x) \equiv f_X(x)$ so that

$$\log \pi_X(x) = \alpha x - e^x - \log \Gamma(\alpha)$$

and hence

$$U(x) = -\alpha x + e^x + \text{constant}$$

with the constant chosen to that $U(x) \geq 0$ for all x. As

$$\dot{U}(x) = -\alpha + e^x$$

the function $U(x)$ is minimized at $x = \log \alpha$, so we define

$$U(x) = -\alpha x + e^x + \alpha \log \alpha - \alpha.$$

Define also

$$K(v) = \frac{1}{2} v^2.$$

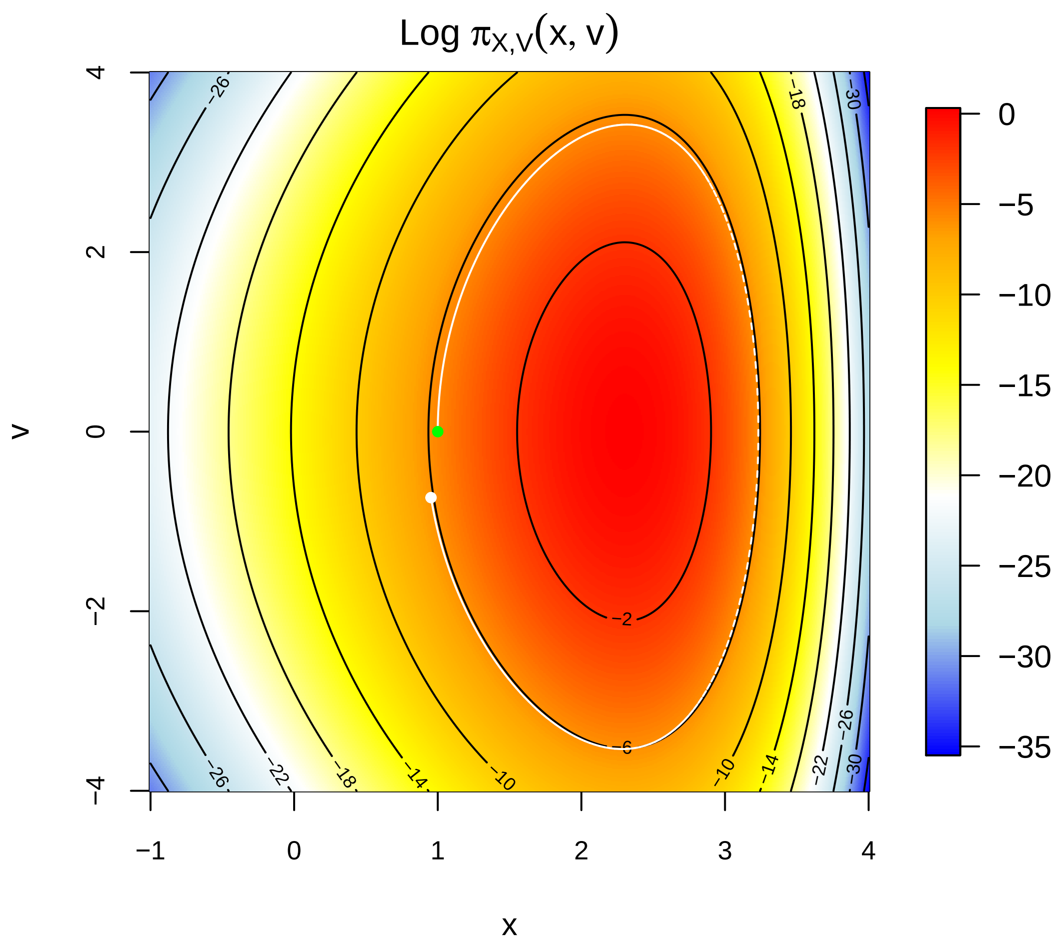
We consider the leapfrog algorithm for proposing moves on the joint pdf

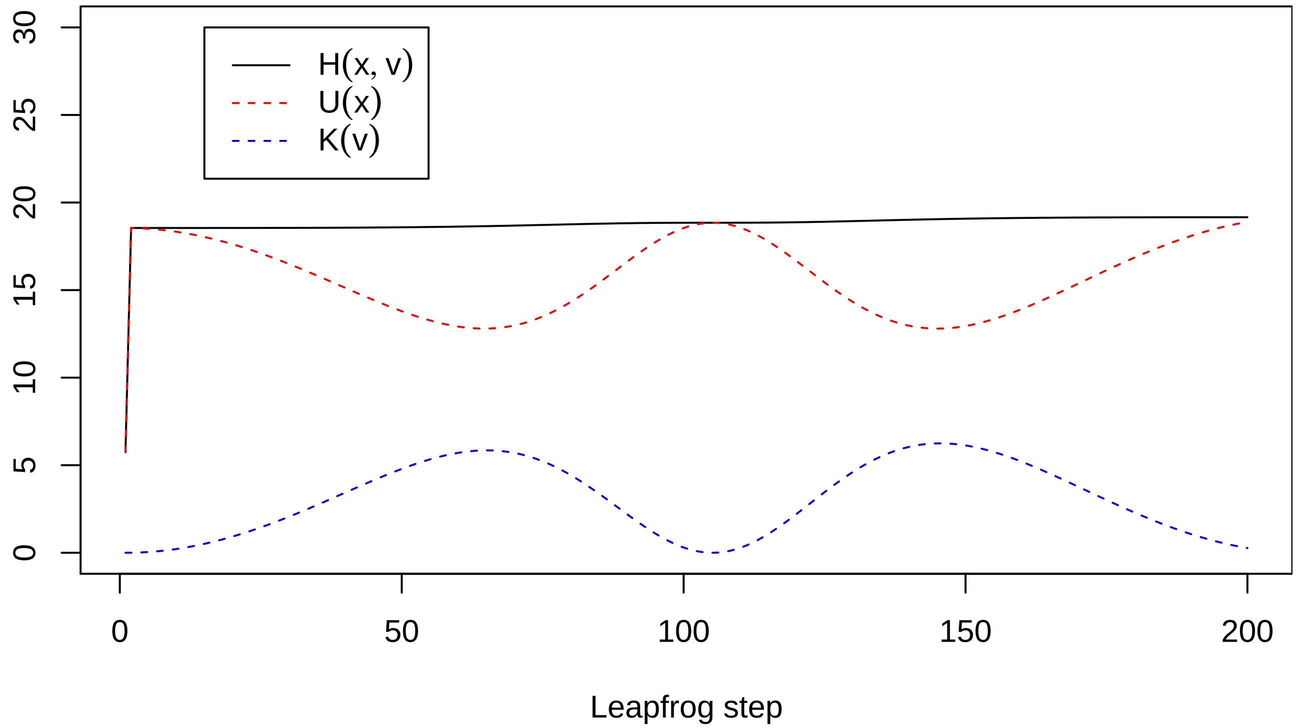
$$\pi_{X,V}(x, v) \propto \exp\{-U(x) - K(v)\} \propto \exp\left\{\alpha x - e^x - \frac{1}{2} v^2\right\}$$

We take $\alpha = 10$, and implement the Leapfrog algorithm from the same fixed starting point $x = 1$, $v = 0$ for different settings of δ and $L = 500$. The path traced out by the leapfrog algorithm is plotted in white.

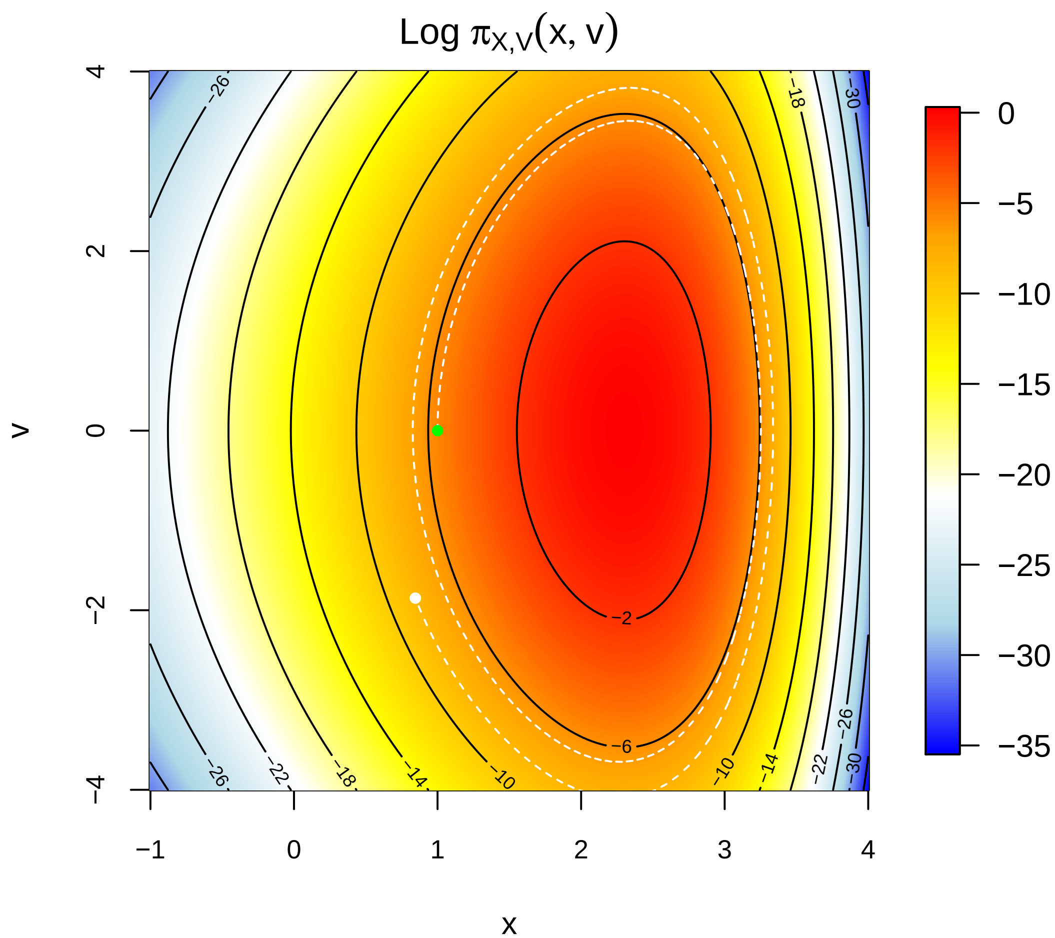
```
set.seed(23984)
al<-10

library(mvnfast,fields,quietly=TRUE)
xvec<-seq(-1,4,by=0.01)
yvec<-seq(-4,4,by=0.01)
dfunc<-function(xv,vv,av){
    dval<-av*xv -exp(xv) - lgamma(av) - 0.5*vv^2
}
f <- Vectorize(dfunc,vectorize.args=c("xv","vv"))
zmat<-outer(xvec,yvec,f,av=al)
par(pty='s',mar=c(4,3,2,2))
colfunc <- colorRampPalette(c("blue","lightblue","white","yellow","orange","red"))
image.plot(xvec,yvec,zmat,col=colfunc(200),
           xlab=expression(x),ylab=expression(v),cex.axis=0.8)
contour(xvec,yvec,zmat,add=T,levels=seq(-50,0,by=4))
title(expression(paste('Log ',pi[paste(X,',',V,sep='')](x,v))))
#Leapfrog run from fixed starting position
L<-200
del<-0.01
x<-1
v<-0
xpath<-matrix(0,nrow=L,ncol=2)
Ham<-U<-K<-rep(0,L)
xpath[1,]<-c(x,v)
U[1]<--al*x+exp(x)+al*log(al)-al
K[1]<-0.5*v^2
Ham[1]<-U[1]+K[1]
```

```
for(l in 1:(L-1)){
    vstar<-v-0.5*del*(-1)*(al-exp(x))
    xnew<-x+del*vstar
    vnew<-vstar-0.5*del*(-1)*(al-exp(x))
    x<-xnew
    v<-vnew
    xpath[l+1,]<-c(x,v)
    U[l+1]<--(al*x-exp(x)-lgamma(al))+al*log(al)-al
    K[l+1]<-0.5*v^2
    Ham[l+1]<-U[l+1]+K[l+1]
}
for(i in 2:L){lines(xpath[c(i-1,i),1],xpath[c(i-1,i),2],lty=2,col='white')}
points(xpath[1,1],xpath[1,2],col='green',pch=20)
points(xpath[L,1],xpath[L,2],col='white',pch=20);
```



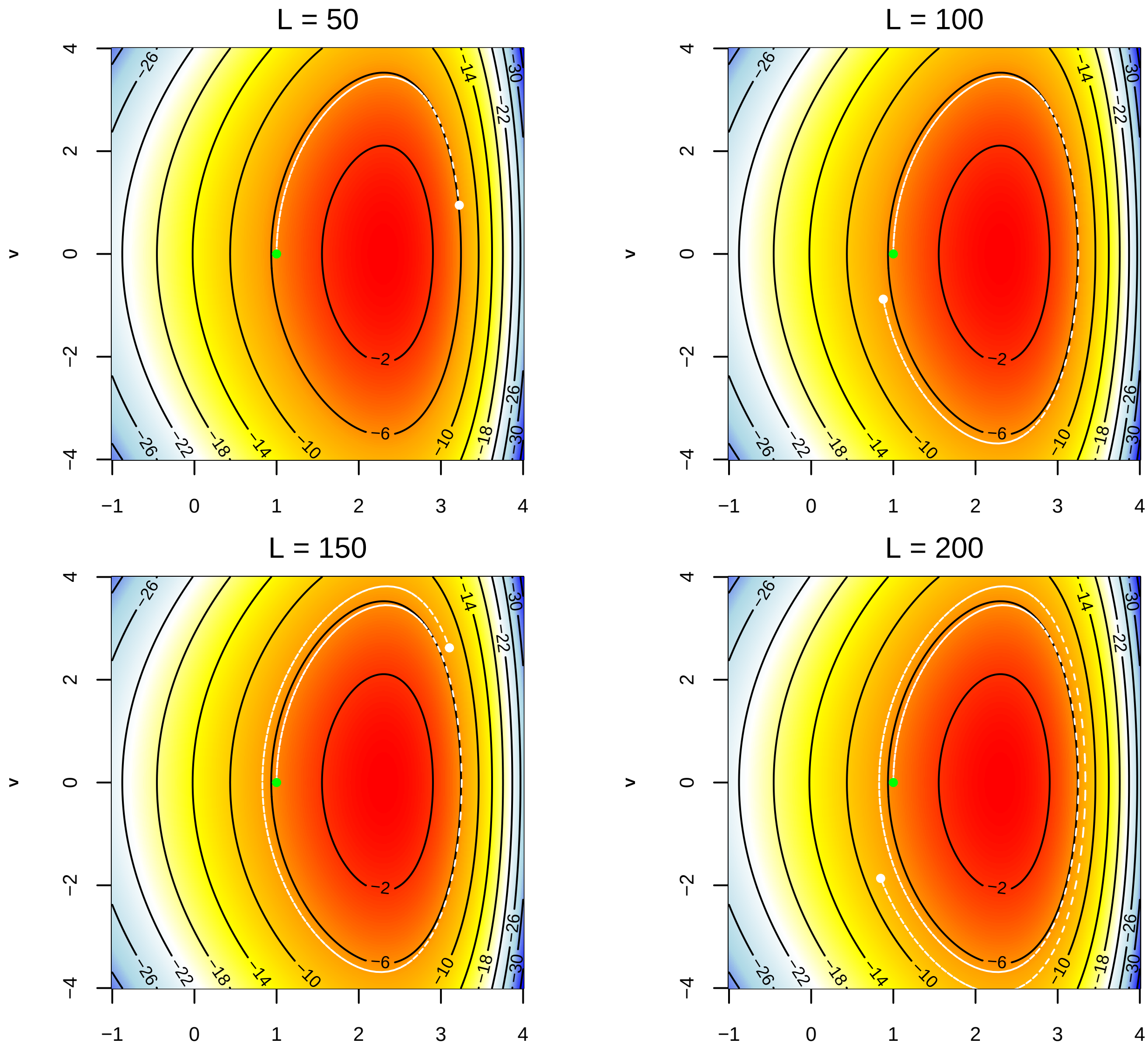


Now with $\delta = 0.02$.



These plots demonstrate that if moving quickly around the parameter space is a priority, then the choice of L

makes a big difference; in the next four plots we demonstrate where the proposal lands with $L = 50, 100, 150$ and 200.



The leapfrog proposal traverses the contours of $\pi_{X,V}(x, v)$: with $L = 50$ or 150, the landing point is distant from the starting point, whereas for $L = 100$ or 200 the landing point is quite close to the starting point.

Of course, this is starting point dependent: if we start from $(x, v) = (1.5, 1)$ then the leapfrog trajectory is different.