Yang Z, Rodríguez CE. 2013. Searching for efficient Markov chain Monte Carlo proposal kernels. *Proc Natl Acad Sci USA* 110:19307–19312

SI Text S3 (extended version). P_{jump} for uniform and Bactrian kernels on N(0, 1) target

Ziheng Yang, 12 November 2013

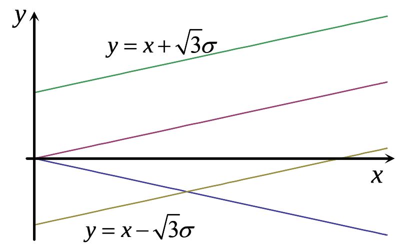
(The equation numbers here differ from those in the paper)

Note that both uniform and Bactrian kernels are symmetrical with $q(y|x) = q(x|y) = q(|y-x|)$. Thus

$$
\begin{aligned}
P_{\text{jump}} &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi(x)q(y\,|\,x)\,\mathrm{I}_{\phi(y)>\phi(x)}\,\mathrm{d}x\,\mathrm{d}y + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi(x)q(y\,|\,x)\,\mathrm{I}_{\phi(y)\le\phi(x)}\,\frac{\phi(y)}{\phi(x)}\,\mathrm{d}x\,\mathrm{d}y \\
&= 2\iint_{\phi(y)>\phi(x)} \phi(x)q(y\,|\,x)\,\mathrm{d}y\,\mathrm{d}x \qquad \leftarrow \text{detailed balance} \qquad (1)\\
&= 4\int_0^{\infty}\int_{-x}^{x} \phi(x)q(y\,|\,x)\,\mathrm{d}y\,\mathrm{d}x. \qquad \leftarrow \text{symmetry}
\end{aligned}
$$

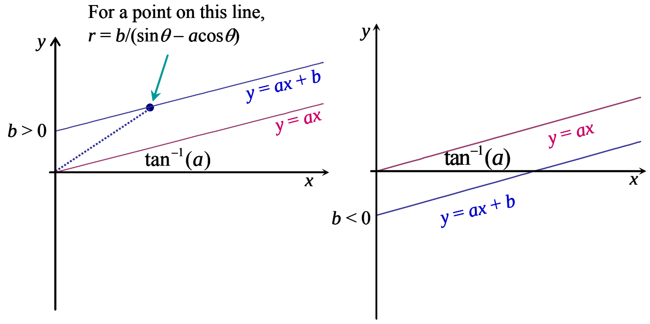
The mass of $\phi(x)q(y|x)$ left of the y axis is the same as right of the y axis. Also right of the y axis, $\phi(y) > \phi(x)$ iff $-x < y < x$.

For the uniform kernel, we have



$$
\begin{aligned}
P_{\text{jump}} &= \frac{2}{\sqrt{3}\sigma}\left[\int_0^{\frac{\sqrt{3}\sigma}{2}}\int_{-x}^{x} \phi(x)\,\mathrm{d}y\,\mathrm{d}x + \int_{\frac{\sqrt{3}\sigma}{2}}^{\infty}\int_{x-\sqrt{3}\sigma}^{x} \phi(x)\,\mathrm{d}y\,\mathrm{d}x\right] \\
&= \frac{2}{\sqrt{3}\sigma}\left[2\int_0^{\frac{\sqrt{3}\sigma}{2}} x\phi(x)\,\mathrm{d}x + \sqrt{3}\sigma\int_{\frac{\sqrt{3}\sigma}{2}}^{\infty} \phi(x)\,\mathrm{d}x\right] \\
&= \frac{2}{\sqrt{3}\sigma}\left[\sqrt{\frac{2}{\pi}}\left(1-\mathrm{e}^{-\frac{3\sigma^2}{8}}\right) + \sqrt{3}\sigma\left(1-\Phi(\tfrac{\sqrt{3}\sigma}{2})\right)\right] \\
&= \sqrt{\frac{8}{3\pi\sigma^2}}\left(1-\mathrm{e}^{-\frac{3\sigma^2}{8}}\right) + 2\left(1-\Phi(\tfrac{\sqrt{3}\sigma}{2})\right).
\end{aligned}
$$

Before we consider the Bactrian kernel, we give the following integral, which we need later.



$I(a, b) =$

$$\int_0^{\infty} \phi(x)\Phi(ax+b)\,\mathrm{d}x = \int_0^{\infty}\int_{-\infty}^{ax+b} \tfrac{1}{2\pi}\exp\{-\tfrac{x^2+y^2}{2}\}\,\mathrm{d}y\,\mathrm{d}x,$$

$-\infty < a, b < \infty$. As $I(-a, b) = \frac{1}{2} - I(a, -b)$, we consider the case of $a > 0$ only. We change to the polar system. If $b \ge 0$,

$$
\begin{aligned}
I_+(a,b) &= \frac{1}{2\pi}\int_{-\frac{\pi}{2}}^{\tan^{-1}(a)}\int_0^{\infty} \mathrm{e}^{-\frac{r^2}{2}}\,r\,\mathrm{d}r\,\mathrm{d}\theta + \frac{1}{2\pi}\int_{\tan^{-1}(a)}^{\frac{\pi}{2}}\int_0^{\frac{b}{\sin\theta - a\cos\theta}} \mathrm{e}^{-\frac{r^2}{2}}\,r\,\mathrm{d}r\,\mathrm{d}\theta \\
&= \frac{1}{2\pi}\int_{-\frac{\pi}{2}}^{\tan^{-1}(a)} 1\,\mathrm{d}\theta + \frac{1}{2\pi}\int_{\tan^{-1}(a)}^{\frac{\pi}{2}}\left[1-\exp\left\{-\tfrac{b^2}{2(\sin\theta - a\cos\theta)^2}\right\}\right]\mathrm{d}\theta \\
&= \frac{1}{2\pi}\left[\tan^{-1}(a) + \tfrac{\pi}{2}\right] + \frac{1}{2\pi}\left[\tfrac{\pi}{2} - \tan^{-1}(a) - \int_{\tan^{-1}(a)}^{\frac{\pi}{2}}\exp\left\{-\tfrac{b^2}{2(\sin\theta - a\cos\theta)^2}\right\}\mathrm{d}\theta\right] \qquad (4)\\
&= \frac{1}{2} - \frac{1}{2\pi}\int_{\tan^{-1}(a)}^{\frac{\pi}{2}}\exp\left\{-\tfrac{b^2}{2(\sin\theta - a\cos\theta)^2}\right\}\mathrm{d}\theta.
\end{aligned}
$$

Similarly if $b \le 0$,

$$I_{-}(a, b) = \frac{1}{2\pi}\int_{-\frac{\pi}{2}}^{\tan^{-1}(a)}\int_{\frac{b}{\sin\theta - a\cos\theta}}^{\infty} \mathrm{e}^{-\frac{r^2}{2}}\, r\,\mathrm{d}r\,\mathrm{d}\theta = \frac{1}{2\pi}\int_{-\frac{\pi}{2}}^{\tan^{-1}(a)} \exp\left\{-\frac{b^2}{2(\sin\theta - a\cos\theta)^2}\right\}\mathrm{d}\theta\,. \quad (5)$$

If $b = 0$, both $I_{+}(a, b)$ and $I_{-}(a, b)$ reduce to

$$\int_0^{\infty} \phi(x)\Phi(ax)\,\mathrm{d}x = \frac{1}{4} + \frac{1}{2\pi}\tan^{-1}(a)\,, \text{ with } a > 0. \quad (6)$$

Note that the proposal density for the Bactrian kernel (eq. 7 in the paper) can be written as

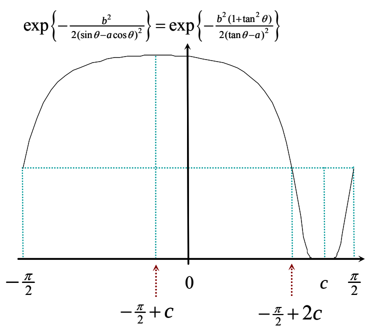
$$q(y|x) = \tfrac{1}{2}\,\phi(y;\, x + m\sigma^2,\, (1 - m^2)\sigma^2) + \tfrac{1}{2}\,\phi(y;\, x - m\sigma^2,\, (1 - m^2)\sigma^2). \quad (7)$$

Thus from eq. (1),

$$\begin{aligned}
P_{\text{jump}} &= 2\int_0^{\infty}\int_{-x}^{x} \phi(x)\times\left[\phi(y; x + m\sigma, (1-m^2)\sigma^2) + \phi(y; x - m\sigma, (1-m^2)\sigma^2)\right]\mathrm{d}y\,\mathrm{d}x \\
&= 2\int_0^{\infty} \phi(x)\times\left[\Phi\left(\tfrac{-m}{\sqrt{1-m^2}}\right) - \Phi\left(\tfrac{-2x-m\sigma}{\sqrt{1-m^2}\,\sigma}\right) + \Phi\left(\tfrac{m}{\sqrt{1-m^2}}\right) - \Phi\left(\tfrac{-2x+m\sigma}{\sqrt{1-m^2}\,\sigma}\right)\right]\mathrm{d}x \\
&= 1 - 2\int_0^{\infty} \phi(x)\times\left[\Phi\left(\tfrac{-2x-m\sigma}{\sqrt{1-m^2}\,\sigma}\right) + \Phi\left(\tfrac{-2x+m\sigma}{\sqrt{1-m^2}\,\sigma}\right)\right]\mathrm{d}x \\
&= -1 + 2\int_0^{\infty} \phi(x)\left[\Phi\left(\tfrac{2x+m\sigma}{\sqrt{1-m^2}\,\sigma}\right) + \Phi\left(\tfrac{2x-m\sigma}{\sqrt{1-m^2}\,\sigma}\right)\right]\mathrm{d}x.
\end{aligned} \quad (8)$$

Now define $a = \frac{2}{\sigma\sqrt{1-m^2}} > 0$, $b = \frac{m}{\sqrt{1-m^2}} > 0$. Eq. (8) then becomes

$$\begin{aligned}
P_{\text{jump}} &= -1 + 2[I_{+}(a, b) + I_{-}(a, -b)] \\
&= \frac{1}{\pi}\left[\int_{-\frac{\pi}{2}}^{\tan^{-1}(a)} \exp\left\{-\frac{b^2}{2(\sin\theta - a\cos\theta)^2}\right\}\mathrm{d}\theta - \int_{\tan^{-1}(a)}^{\frac{\pi}{2}} \exp\left\{-\frac{b^2}{2(\sin\theta - a\cos\theta)^2}\right\}\mathrm{d}\theta\right].
\end{aligned} \quad (9)$$



The integrand is the same in the two integrals and is 0 at $\theta = c = \tan^{-1}(a)$, and symmetrical around c; in other words it is the same at $c - d$ and at $c + d$, for $0 < d < \pi/2 - c$. Thus

$$P_{\text{jump}} = \frac{1}{\pi}\int_{-\frac{\pi}{2}}^{-\frac{\pi}{2}+2\tan^{-1}(a)} \exp\left\{-\frac{b^2}{2(\sin\theta - a\cos\theta)^2}\right\}\mathrm{d}\theta\,. \quad (10)$$

Now the integral is over an interval of length $2c$, and the integrand is symmetrical around the center: it is the same at $(-\pi/2 + c) - d'$ and at $(-\pi/2 + c) + d'$ for $0 < d' < c$. Thus

$$P_{\text{jump}} = \frac{2}{\pi}\int_{-\frac{\pi}{2}}^{-\frac{\pi}{2}+\tan^{-1}(a)} \exp\left\{-\frac{b^2}{2(\sin\theta - a\cos\theta)^2}\right\}\mathrm{d}\theta = \frac{2}{\pi}\int_0^{\tan^{-1}(a)} \exp\left\{-\frac{b^2}{2(\cos\theta + a\sin\theta)^2}\right\}\mathrm{d}\theta \quad (11)$$

Let $t = \tan\theta$, with $\mathrm{d}\theta = 1/(1 + t^2)\,\mathrm{d}t$. Then

$$P_{\text{jump}} = \frac{2}{\pi}\int_0^{a} \frac{1}{1+t^2}\exp\left\{-\frac{b^2(1+t^2)}{2(1+at)^2}\right\}\mathrm{d}t\,. \quad (12)$$

This reduces to eq. (11) in the paper if $b = 0$ (if $m = 0$).