Supplementary Material for Slice Sampling on Hamiltonian Trajectories

1. Hamiltonian Dynamics for Non-Gaussian Distributions

Assume we have some prior π for $\mathbf{f}$, where

$$-\log \pi(\mathbf{f}|\boldsymbol{\alpha}) = \log Z - g(\mathbf{f}|\boldsymbol{\alpha}), \tag{1}$$

for some hyperparameters $\boldsymbol{\alpha}$ and where Z is the normalizing constant. Then we can again set up a Hamiltonian,

$$H(\mathbf{f}, \mathbf{p}) = g(\mathbf{f}|\boldsymbol{\alpha}) + \frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p}. \tag{2}$$

Hamilton's equations yield the system of differential equations

$$\nabla_t^2 \mathbf{f} = -M^{-1}\nabla_{\mathbf{f}} g(\mathbf{f}|\boldsymbol{\alpha}). \tag{3}$$

This can be solved exactly for some cases of $g(\mathbf{f}|\boldsymbol{\alpha})$; the Gaussian example above is one such case.

When $M = \text{diag}(m_1, \ldots, m_d)$ and $g(\mathbf{f}|\boldsymbol{\alpha}) = \sum_{i=1}^d h_i(f_i)$, the system is an uncoupled system and often has an analytic solution. In particular, $f_i(t)$ is the solution to

$$\frac{1}{2}\left(\int \left[c_1 - \frac{1}{m_i}h_i(f_i)\right]^{-1/2} df_i\right)^2 = (t + c_2)^2, \tag{4}$$

where c_2 is determined by $f_i(0)$ and

$$c_1 = \frac{1}{2}\left(\dot{f}_i(0)\right)^2 + \frac{1}{m_i}h_i(f_i(0)), \tag{5}$$

where $\dot{f}_i(t)$ denotes the time-derivative of f_i at time t. For certain distributions, (4) has an analytic solution.

1.1. Exp(λ) and Laplace(λ)

Working with the general form of the solution can be difficult, especially when the sample space is constrained. The exponential distribution is one such example, but it induces a potential for which solutions are easy to obtain directly. Let the prior be such that the components of $\mathbf{f}$ are mutually independent and $f_i \sim \text{Exp}(\lambda_i)$ so that

$$-\log \pi(f_i|\lambda_i) = -\log(\lambda_i) + \lambda_i \cdot f_i, \quad f_i > 0. \tag{6}$$

Hamilton's equations are particularly simple in this case, which describes one-dimensional projectile motion, e.g. a bouncing ball in a constant gravitational potential. The solution to Hamilton's equations is

$$f_t(t) = \frac{\lambda_i}{2m_i}t^2 + \dot{f}_i(0)t + f_i(0), \quad 0 \le t \le T_0. \tag{7}$$

An example of such a trajectory is shown in Figure 1a. $T_0 > 0$ is the time at which the particle has position coordinate equal to 0, at which point its momentum changes signs, i.e. it "bounces." For $t > T_0$, the particle repeatedly traces out the same trajectory. We find T_0 as

$$T_0 = \frac{m_i}{\lambda_i}\dot{f}_i(0) + \sqrt{\frac{m_i^2}{\lambda_i^2}\dot{f}_i(0)^2 + \frac{2m_i}{\lambda_i}f_i(0)}. \tag{8}$$

This yields the period of the trajectory,

$$T = 2\sqrt{\frac{m_i^2}{\lambda_i^2}\dot{f}_i(0)^2 + \frac{2m_i}{\lambda_i}f_i(0)}. \tag{9}$$

Every time at which the particle reaches zero is then $z_j = T_0 + (j-1)T$. Hamilton's equations also yield the momentum,

$$p_i(t) = -\lambda_i t + m_i \dot{f}_i(0), \tag{10}$$

which we can use to find the momentum at the reflection point T_0, but before reflection,

$$p_i(T_0^-) = -\sqrt{m_i^2 \dot{f}_i(0)^2 + 2m_i\lambda_i f_i(0)}. \tag{11}$$

After the first reflection, we have $p_i(T_0^+) = -p_i(T_0^-)$, and the dynamics proceed according to the equation

$$f_i(t) = -\frac{\lambda_i}{2m_i}(t - z_j)^2 + \frac{p_i(T_0^+)}{m_i}(t - z_j), \quad z_j \le t \le z_{j+1}. \tag{12}$$

We can use slightly different equations to describe the dynamics under a Laplace prior All that is required is some bookkeeping on the sign of the motion because the particle is not reflected at $f_i = 0$, but the sign on the potential switches. An example is shown in Figure 1b.

1.2. Pareto(x_m, α) and GPD(μ, σ, ξ) via transformation

The Pareto and Generalized Pareto (denoted GPD) distributions are typically used to model processes with heavy tails. The density of the Pareto distribution is

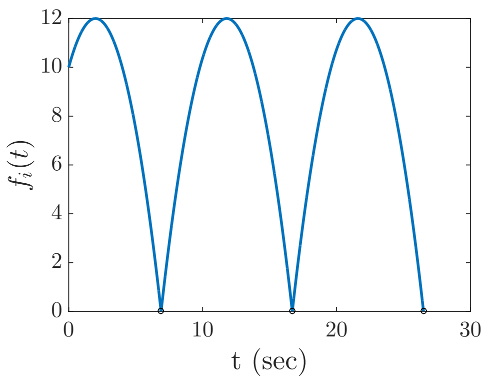
$$\pi(f_i|x_m, \alpha) = \alpha x_m^{\alpha} f_i^{-(\alpha+1)}, \\ f_i \geq x_m, \quad x_m > 0, \quad \alpha > 0. \tag{13}$$

We can show that the random variable $y_i := \log f_i - \log x_m$ is distributed as Exp(α), for $y_i > 0$. Using this fact, we can generate analytic trajectories as in subsection 1.1 for y_i and slice sample from the resulting curves $f_i(t) = x_m e^{y_i(t)}$. An example is shown in Figure 1c.

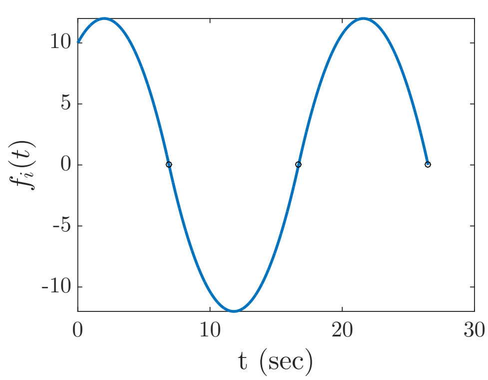
The GPD has the density

$$\pi(f_i|\mu,\sigma,\xi) = \frac{1}{\sigma}\left(1 + \xi \cdot \frac{f_i - \mu}{\sigma}\right)^{-(1+\xi^{-1})}, \\ f_i \geq \mu, \quad \xi \geq 0. \tag{14}$$

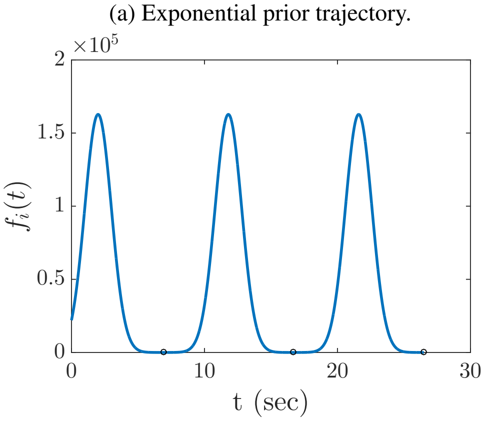
(The GPD is also defined for $\xi < 0$, in which case $\mu \leq f_i \leq \mu - \sigma/\xi$. We focus on the $\xi \geq 0$ case for now.) The random variable $y_i := \log\left(1 + \xi \frac{f_i - \mu}{\sigma}\right)$ is distributed as Exp(ξ^{-1}) for $y_i > 0$, and we can again use the calculations from subsection 1.1 to slice sample from the curve $f_i(t) = \mu + \frac{\sigma}{\xi}(e^{y_i(t)} - 1)$. An example is shown in Figure 1d.



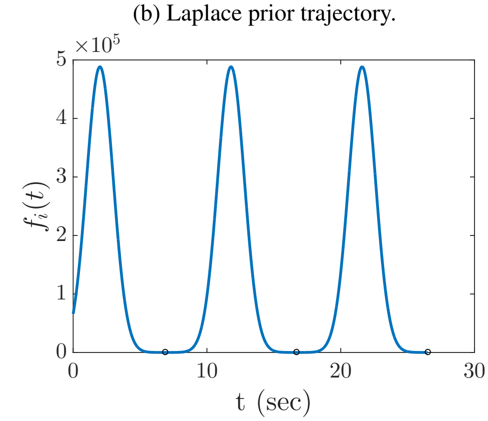
(a) Exponential prior trajectory.



(b) Laplace prior trajectory.



(c) Pareto prior from transformed exponential trajectory.



(d) GPD prior from transformed exponential trajectory.

Figure 1. Example trajectories under different priors.