Bayesian modelling

Hamiltonian Monte Carlo and probabilistic programming

Léo Belzile

Last compiled Monday Feb 17, 2025

Curse of dimensionality

This material is drawn from

- Neal (2011),
- Betancourt (2017)

Check out these animations by Chi Feng

Motivation

We are interested in calculating expectations of some function g against the posterior.

$$\int_{\mathbb{R}^d} g(\boldsymbol{\theta})p(\boldsymbol{\theta} \mid \boldsymbol{y})\mathrm{d}\boldsymbol{\theta}.$$

The integral is determined by the product of the ``volume'' of $g(\cdot)$ and the density.

Curse of dimensionality

As the dimension of the posterior, d, grows, the mass concentrates in a small region, the so-called **typical set**. The number of regions/directions to consider increases exponentially in d.

If we start at the stationary distribution, most proposals from a random walk Metropolis will fall outside of the typical set and get rejected.

This phenomenon also explains the decrease in performance of numerical integration schemes (quadrature).

Better informed proposals

For differentiable targets, we saw that we can do better than random walk Metropolis–Hastings.

- Idea: use the gradient to make an informed proposal (e.g., in MALA)
- There are two remaining challenges.
  - it makes a single step from the current position. But why stop at one?
  - the gradient needs not be aligned with the typical set (Betancourt analogy with satellite in orbit).

Hamiltonian Monte Carlo

Hamitonian Monte Carlo borrows ideas from Hamiltonian dynamics.

Consider the evolution over time of a particle characterized by a

- position $\boldsymbol{\theta} \in \mathbb{R}^d$ along with potential energy $U(\boldsymbol{\theta}) = -\log p(\boldsymbol{\theta} \mid \boldsymbol{y})$
- an added auxiliary vector $\boldsymbol{s} \in \mathbb{R}^d$ of **momentum** (describing mass and velocity) with accompaying kinetic energy $K(\boldsymbol{s}) = -\log p(\boldsymbol{s})$.

Hamiltonian

Write the negative of the log of the joint density as

$$H(\boldsymbol{\theta}, \boldsymbol{s}) = -\log p(\boldsymbol{s}) - \log p(\boldsymbol{\theta}) = U(\boldsymbol{\theta}) + K(\boldsymbol{s}).$$

The partial derivatives of the Hamiltonian give the evolution over time of the system:

$$\begin{aligned}\frac{\mathrm{d}\theta_j}{\mathrm{d}t} &= \frac{\partial H}{\partial s_j} = \frac{\partial K}{\partial s_j} \\ \frac{\mathrm{d}s_j}{\mathrm{d}t} &= -\frac{\partial H}{\partial \theta_j} = -\frac{\partial U}{\partial \theta_j}, \qquad j = 1, \ldots, d.\end{aligned}$$

There is no explicit solution to these differential equations in most settings.

Kinetic energy

The most popular choice of kinetic energy is the Gaussian,

$$K(\boldsymbol{s}) = \frac{1}{2}\boldsymbol{s}^\top \mathbf{M}^{-1}\boldsymbol{s}$$

the negative of a mean zero log Gaussian density with positive-definite covariance matrix $\mathbf{M}$.

Typically, we take $\mathbf{M} = \mathrm{diag}\{m_1, \ldots, m_d\}$ diagonal, or else proportional $\mathbf{M} = m\mathbf{I}_d$.

Properties of Hamiltonian dynamics

The mapping T_s from time t at $(\boldsymbol{\theta}(t), \boldsymbol{s}(t))$ to time $t+\varepsilon$, $(\boldsymbol{\theta}(t+\varepsilon), \boldsymbol{s}(t+\varepsilon))$ satisfies the following properties:

- Reversible: MCMC will thus preserve the invariant target distribution
- Conservation of energy: proposals from Hamiltonian dynamics would lead to acceptance probability of 1.
- Symplecticness/volume preserving: the Jacobian of T_s is one — no need to calculate it.

A necessary discretization step

There is no explicit solution to the Hamiltonian differential equation. We must move away from continuous time…

- For solving the differential equation numerically, Euler’s method doesn’t work because it does not preserve volume, and this leads to divergences.

Leapfrog integrator

The leapfrog integrator performs a half step for momentum, then does a full step for the position using the updated components, etc.

$$s_j(t+\varepsilon/2) = s_j(t) - \frac{\varepsilon}{2}\frac{\partial U(\boldsymbol{\theta})}{\partial \theta_j}\bigg|_{\boldsymbol{\theta}(t)}$$

$$\theta_j(t+\varepsilon) = \theta_j(t) + \varepsilon\frac{s_j(t+\varepsilon/2)}{m_j}$$

$$s_j(t+\varepsilon) = s_j(t+\varepsilon/2) - \frac{\varepsilon}{2}\frac{\partial U(\boldsymbol{\theta})}{\partial \theta_j}\bigg|_{\boldsymbol{\theta}(t+\varepsilon)}$$

Hamiltonian Monte Carlo algorithm

Consider the joint distribution with positions $\boldsymbol{\theta}$ and momentum variables $\boldsymbol{s}$, $p(\boldsymbol{\theta}, \boldsymbol{s}) \propto \exp\{-H(\boldsymbol{\theta}, \boldsymbol{s})\}$.

We start with a position vector $\boldsymbol{\theta}_{t-1}$ at step $t-1$:

1. Sample a new momentum vector $\boldsymbol{s}_{t-1} \sim$ Gauss$(\mathbf{0}_d, \mathbf{M})$.
2. Use Verlet's (leapfrog) integrator to evolve the state vector for $L = \lfloor \tau/\varepsilon \rfloor$ steps of size ε to get a proposal tuple $(\boldsymbol{\theta}_t^\star, \boldsymbol{s}_t^\star)$

Hamiltonian Monte Carlo algorithm

3. Flip the momentum variable, $\boldsymbol{s} \mapsto -\boldsymbol{s}$.
4. Metropolis step: if $U \sim \mathsf{unif}(0,1) < R$, where

$$\log R = -H(\boldsymbol{\theta}^{\star}, \boldsymbol{s}_t^{\star}) + H(\boldsymbol{\theta}_{t-1}, \boldsymbol{s}_{t-1}),$$

   set $\boldsymbol{\theta}_t = \boldsymbol{\theta}_t^{\star}$, else keep the previous value and set $\boldsymbol{\theta}_t = \boldsymbol{\theta}_{t-1}$.
5. Discard the momentum vector

Tuning

Hamiltonian Monte Carlo (HMC) has numerous tuning parameters

1. size of the leapfrog step ε.
2. length of the integration time τ (or equivalently the number of steps $L = \lfloor \tau/\varepsilon \rfloor$).
   - too small leads HMC to bear close resemblance to random walk,
   - too large leads to wasteful calculations.
3. choice of the mass matrix $\mathbf{M}$ (pre-conditioner obtained during warmup period).

Leapfrog and error

The Störmer–Verlet (leapfrog) integrator is a second order method, so for step size ε:

- local error $\mathrm{O}(\varepsilon^3)$ and
- global error of size $\mathrm{O}(\varepsilon^2)$ (accumulated error over L steps).

Leapfrog updates one variable at a time, a shear transformation.

Leapfrog step should be $\mathrm{O}(d^{-1/4})$ (Beskos et al., 2013)

Optimal acceptance rate

In practice, we use a Metropolis step to adjust for the discretization of the system.

- This leads to acceptance rates less than the theoretical value of 1.
- with optimal acceptance rate of 0.651 (Beskos et al., 2013); see Neal (2011) for heuristics.
- software like Stan tunes to around 0.8, but can be adjusted in settings.

It's nuts!

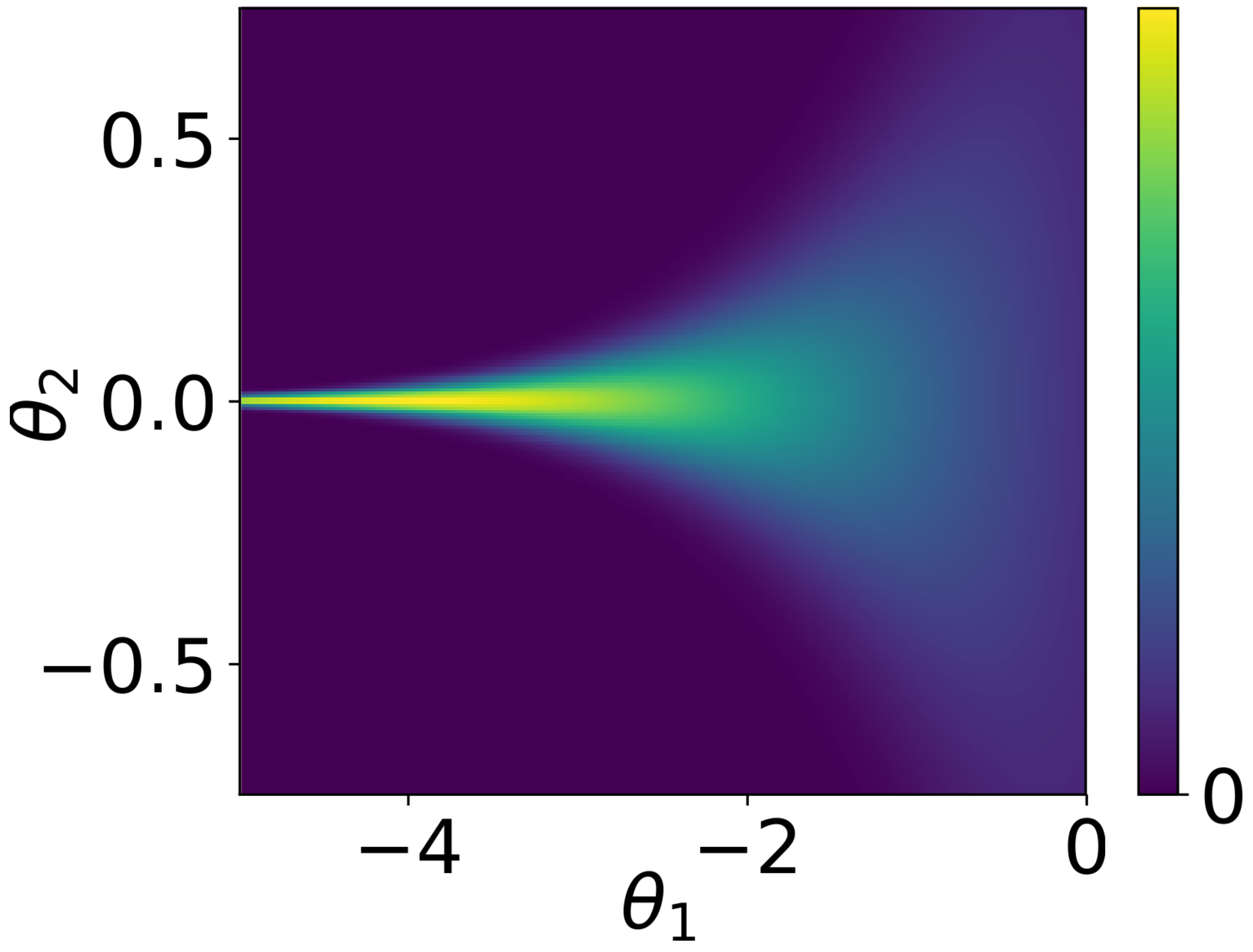
- Homan & Gelman (2014) propose the no U-turn sampler (NUTS), which continues the trajectory until the sampler turns back, to determine the number of steps L, along with tuning of ε.
- Stan uses an adaptation of NUTS due to Betancourt (2016)

HMC and divergences

In theory, the energy of the Hamiltonian should stay constant, but the numerical scheme leads to small perturbations (hence the rejection step).

- If the value of the Hamiltonian changes too much, this is identified as a **divergence**. These occur when the geometry of the posterior is heavily constrained (funnel shaped).
- Reparametrization of the model can help improve this: see the Stan manual.

Neal's funnel



Achieving independence

We have seen that for differentiable posterior $p(\boldsymbol{\theta} \mid \boldsymbol{y})$, using the gradient information can improve convergence by informing about the direction of the mode.

- Neal (2011) discusses how informally, random walk Metropolis requires $\mathrm{O}(d^2)$ steps to get an independent draw, compared to $\mathrm{O}(d^{4/3})$ for MALA.
- HMC scales like $\mathrm{O}(d^{5/4})$, a notable improvement in performance.
- It however comes at the cost of repeated gradient evaluations (L by update).

Take-home

- HMC is more efficient than what we have seen, but not a silver bullet: it works very well for not overly complicated models and moderate sample sizes.
- HMC works better than many MCMC, but requires special tuning best left to specialized implementations already available in software.
- Most implementations don't cover the case of discrete random variables (Nishimura et al., 2020).

Probabilistic programming

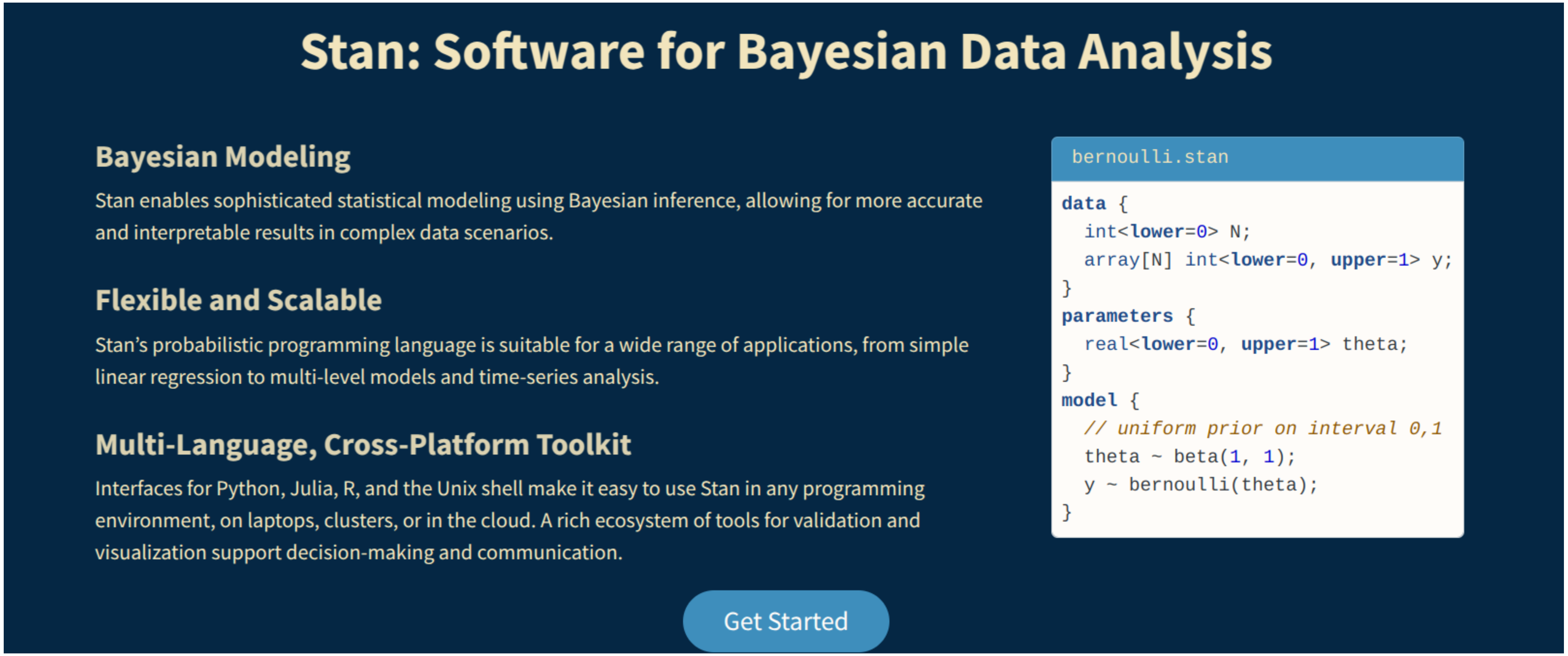
There are several languages and interfaces that implement probabilistic programming where the user has only to specify the likelihood and prior.

Historically, Bugs paved the way to practitioners.

It relies on Gibbs sampling (updating one parameter at the time), but is not actively developed. Still the source of many exercises and inspiration for the syntax of other implementations (e.g., Nimble, JAGS).

Stan

The programming language Stan is written in C++ and offers cross-platform interfaces.



Stan: Software for Bayesian Data Analysis

Bayesian Modeling

Stan enables sophisticated statistical modeling using Bayesian inference, allowing for more accurate and interpretable results in complex data scenarios.

Flexible and Scalable

Stan's probabilistic programming language is suitable for a wide range of applications, from simple linear regression to multi-level models and time-series analysis.

Multi-Language, Cross-Platform Toolkit

Interfaces for Python, Julia, R, and the Unix shell make it easy to use Stan in any programming environment, on laptops, clusters, or in the cloud. A rich ecosystem of tools for validation and visualization support decision-making and communication.

bernoulli.stan

```
data {
  int<lower=0> N;
  array[N] int<lower=0, upper=1> y;
}
parameters {
  real<lower=0, upper=1> theta;
}
model {
  // uniform prior on interval 0,1
  theta ~ beta(1, 1);
  y ~ bernoulli(theta);
}
```

Other MCMC software

- Nimble, C++ with **R** interface
- Turing.jl, Julia
- PyMC, Python
- Pigeons, Julia

Stochastic volatility model

Financial returns Y_t typically exhibit time-varying variability. The **stochastic volatility** model is a parameter-driven model that specifies

$$\begin{aligned} Y_t &= \exp(h_t/2)Z_t \\ h_t &= \gamma + \phi(h_{t-1} - \gamma) + \sigma U_t \end{aligned}$$

where $U_t \overset{\text{iid}}{\sim}$ Gauss$(0, 1)$ and $Z_t \sim\overset{\text{iid}}{\sim}$ Gauss$(0, 1)$.

It is possible to introduce leverage by adding Cor$(Z_t, U_t) = \rho$.

References

Beskos, A., Pillai, N., Roberts, G., Sanz-Serna, J.-M., & Stuart, A. (2013). Optimal tuning of the hybrid Monte Carlo algorithm. *Bernoulli*, *19*(5A), 1501–1534. https://doi.org/10.3150/12-BEJ414

Betancourt, M. (2016). Identifying the optimal integration time in Hamiltonian Monte Carlo. *arXiv*. https://doi.org/10.48550/arXiv.1601.00225

Betancourt, M. (2017). A conceptual introduction to Hamiltonian Monte Carlo. *arXiv Preprint*. https://doi.org/10.48550/arXiv.1701.02434

Homan, M. D., & Gelman, A. (2014). The no-U-turn sampler: Adaptively setting path lengths in Hamiltonian Monte Carlo. *Journal of Machine Learning Research*, *15*(1), 1593–1623.

Neal, R. M. (2011). MCMC using Hamiltonian dynamics. In S. Brooks, A. Gelman, G. Jones, & X. L. Meng (Eds.), *Handbook of Markov chain Monte Carlo* (pp. 113–162). CRC Press. https://doi.org/10.1201/b10905-5

Nishimura, A., Dunson, D. B., & Lu, J. (2020). Discontinuous Hamiltonian Monte Carlo for discrete parameters and discontinuous likelihoods. *Biometrika*, *107*(2), 365–380. https://doi.org/10.1093/biomet/asz083