STAN, PYMC, PYRO, NUMPYRO

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Problem Overview

Cannot directly compute the posterior for most interesting models (intractable) and so need to approximate using a potentially expensive (slow) sampling algorithm. Want to identify best algorithm and implementation (software) to use for the AllocAI Mixed Marketing Model (MMM).

Takeaways

0. **Effective sample size per second**. To pick between sampling methodologies and software implementations, we can use "effective sample size per second" as a comparison metric (arviz package). This strikes the right balance between *samples per second* and *auto-correlation*.

1. **Try both HMC-NUTS & Variational Inference**. For a relatively complex model formulation (with difficult posterior to traverse), we should consider both HMC-NUTS and Variantional Inference methods. Variational Inference scales better to larger datasets (>50,000 rows) but converges to a more approximate posterior than HMC-NUTS, particularly for smaller datasets.

2. **NumPyro for HMC-NUTS**. NumPyro is built with Theano/Aesara's linear algebra and computational graph libraries. It's HMC-NUTS implementation is custom-built to maximize JAX optimizations (jit, grad, vmap) and considered best-in-class for both small and large datasets.

3. **Pyro for Variational Inference**. Pyro is built on PyTorch's deep learning framework and is considered best-in-class for large datasets (>50,000 rows) if gpu hardware available. This is particularly useful for Variational Inference and Bayesian Neural Network model types. For small to medium datasets, Pyro will be slower that NumPyro, Edward2 and Stan for all MCMC sampling routines.

4. **PyMC 4.0 includes NumPyro API**. In June 2022, PyMC released a major re-write of its probabilistic programming language. Two main items: (1) started actively maintaining and developing Theano/Aesara backend, and (2) introduced integrations for NumPyro and BlackJAX. Unclear if actually as good as NumPyro (no published benchmarks), but I would be surprised if the difference is substantial.

5. **Parallelization for Auto-Diff & Multiple Chains**. There are two ways we can parallelize computation for bayesian inference: (1) vectorization and multi-threading on a single core (JAX library is best); and (2) scheduling multiple sample chains across cores (all platforms support this for cpu and gpu hardware).

Sampling Methodologies (MCMC)

We typically evaluate sampling methods based on "effective sample size per second". This is really a combination of time per sample and auto-correlation.

As model formulations become more complex, the other relevant criterion is "feasibility". For example, we cannot always solve analytically for the conditional distributions wrt each parameter, which rules out Gibbs sampling.

	Metropolis Hastings	Gibbs Sampling	Hamiltonian Monte Carlo	No U-Turn Sampling	Variational Inference
time per step	Fast. Compute Hastings Ratio at each step	Lightening Fast! Direct sampling only	Very slow! Re-computes graident at each step	Slow! As good or better than HMC algorithm	Lightening Fast! Sample directly from approx distribution Q
auto-correlation	High! Often low number of "effective samples"	Moderate. Significant improvement on MH	Low! Gradient steps result in effective samples	Low. As good or better than HMC algorithm	None! We sample directly from an approximate posterior
acceptance ratio	Low. Problem if joint pdf is complex	Not required (= 100%)	High. Acceptance more likely with gradient steps	High. Similar to HMC algorithm	Not required (=100%)
complex posteriors	Low. Random walk if high-dim space	Moderate, need conditional pdfs	High. Leapfrog integrator adapts to complexity	Best! Minimal wasted computation	Low. Exacerbates inaccuracies of this method, no guarantees
other comments	Simple & fast, but crude for complex posterior	Best option if able to compute conditionals	Pre NUTS, best-in-class for complex models	Work horse of bayesian inference toolchains	Very useful for large datasets. To approximate for complex models, small dataset

Metropolis-Hastings (MH) was developed in 1950s, with many subsequent MCMC techniques derived from it. Each chain starts with initialization of an arbitrary parameter vector x, then propose a step of random direction (picked from a Gaussian random walk distribution), and accept or reject based on the ratio of log probability evaluated at the proposed position vs the current positioni (hastings ratio). This acceptance criteria ensures we tend to move towards higher probability density regions more than lower density regions.

Hastings Ratio: let $q(\theta_0, \theta_1)$ be our transition density (often assumed symmetric and cancels) and $\pi(y, \theta)$ be our join density. Then,

$$\text{accept prob.} = \min(1, \frac{q(\theta_0, \theta_1)\pi(y, \theta_1)}{q(\theta_1, \theta_0)\pi(y, \theta_0)})$$

Gibbs Sampling was developed in 1980s. The first fundamental departure from the Metropolis-Hasting algorithm. Main idea is to sample directly (without acceptance ratio) from conditional distributions for each parameter. This provides us a more principled way to navigate the posterior space than gaussian random walk and avoids the need to compute either graident or acceptance ratios for each step. Because of this, the algorithm is lightening fast and converges quickly! However, computing these condition distributions which can be tricky for larger problems.

Conditional distribution with respect to parameter x_i. Let $\{x_{-i}\} = \{x_1, x_2, ..., x_{i-1}, x_{i+1}, ..., x_n\}$,

$$p(x_i|y, x_{-i}) = \frac{p(y, x)}{\int p(x, y)dx_{-i}} = \frac{p(y, x_{-i}|x_i) \cdot p(x_i))}{\int p(x, y)dx_{-i}}$$

Hamiltonian Monte Carlo (HMC) is an evolution of Metropolis-Hastings developed in the 1980/90s. Instead of a gaussian random walk, HMC proposes choosing step direction based on the "gradient of negative log likelihood". This approach is based on Hamiltonian mechanics. The system is propagated numerically using a "leapfrog integrator" which is important for the algorithm's stability.

Implementation: Compute the Hamiltonian $H(\rho, \theta)$ given independently drawn momentum ρ and our current parameter values θ. Note, $V(\theta) = -l(\theta) = -\log p(\theta|y)$.

$$H(\theta, y) = -\log p(\rho, \theta) - \log p(\rho|\theta) - \log p(\theta) = V(\theta) + K(\rho, \theta)$$

We now evolve the system using the following equations from Hamiltonian mechanics.

$$\begin{aligned}\frac{d\theta}{dt} &= +\frac{\partial H}{\partial \rho} = +\frac{\partial K}{\partial \rho} + \frac{\partial V}{\partial \rho} = M^{-1}\rho \\ \frac{d\rho}{dt} &= -\frac{\partial H}{\partial \theta} = -\frac{\partial K}{\partial \theta} - \frac{\partial V}{\partial \theta} = -\frac{\partial V}{\partial \theta}\end{aligned}$$

Therefore, to implement the above system, we need only to calculate the gradient of our potential energy (negative log likelihood) with respect to our parameters θ.

No U-Turn Sampling (NUTS) is an extension from HMC developed in early 2010s (Hoffman and Gelman). The main idea is to adaptively set the number of leapfrog steps L. This refers the number of steps our numerical integrator takes with a given graident and is specified by the user as a hyperparameter in the HMC algorithm. If L is too small, the algorithm exhibits an undesirable random walk behaviour. If L is too large, the algorithm wastes computation. To find the golidlocks

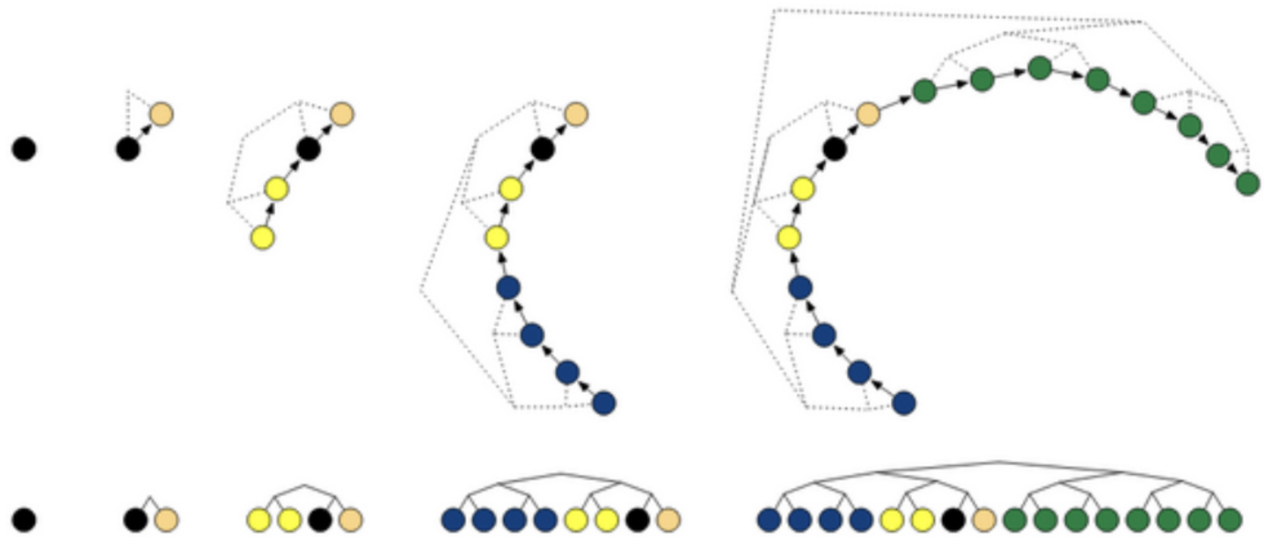


Figure 1: No-Turn Sampler

number of integration steps, we conitnue until a “U-Turn” condition is satisfied. This is particularly effective in high-dimensional parameter spaces that are difficult to explore.

Figure 1 shows an example of building a binary tree via repeated doubling. Each doubling proceeds by choosing a direction (forwards or backwards) uniformly at random, then simulating Hamiltonian dynamics for 2^j leapfrog steps in that direction, where j is the number of previous doublings (and the height of the binary tree).

Variational Inference (VI) was developed in mid 2010s and can be viewed as an extension of the Expectation-Maximisation (EM) algorithm. Unlike the previous algorithms, VI is not a Monte Carlo sampling method. The main idea is to iteratively maximize the likelihood of a proposal distribution Q such that it converges to the true posterior (i.e. minimizes KL divergence). We do this by choosing parameters for Q that maximize ELBO which is a tractable lower bound on the likelihood of our observed data and is a function of q. We can then sample directly from our distribution Q to approximate the posterior.

For many applications, variational inference produces comparable results to Gibbs Sampling at similarly lightening fast speeds, but do not need to derive the conditional distributions to sample from. Assuming we pick a simple proposal distribution Q, the update equations for VI should be straight forward.

Evidence Lower Bound (ELBO): Jensen’s inequality applied to the log probability of the observations. This produces a useful lower-bound on the log-likelihood of some observed data. By choosing a good approximation q of our posterior, we are maximizing the ELBO ($\mathbb{E}_q[l]$).

$$\log p(x) \geq \mathbb{E}_q[l] \approx \mathbb{E}_q[\log p(x, Z)] - \mathbb{E}_q[\log q(Z)]$$

KL divergence = negative ELBO + log marginal probability of x. Minimizing KL divergence is equivalent to maximizing the ELBO since the log marginal prob. ($\log p(x)$) does not depend on q.

$$\mathrm{KL}(q(z)||p(z|x)) = -(\mathbb{E}_q[\log p(x,Z)] - \mathbb{E}_q[\log q(Z)]) + \log p(x)$$

Reference documentation

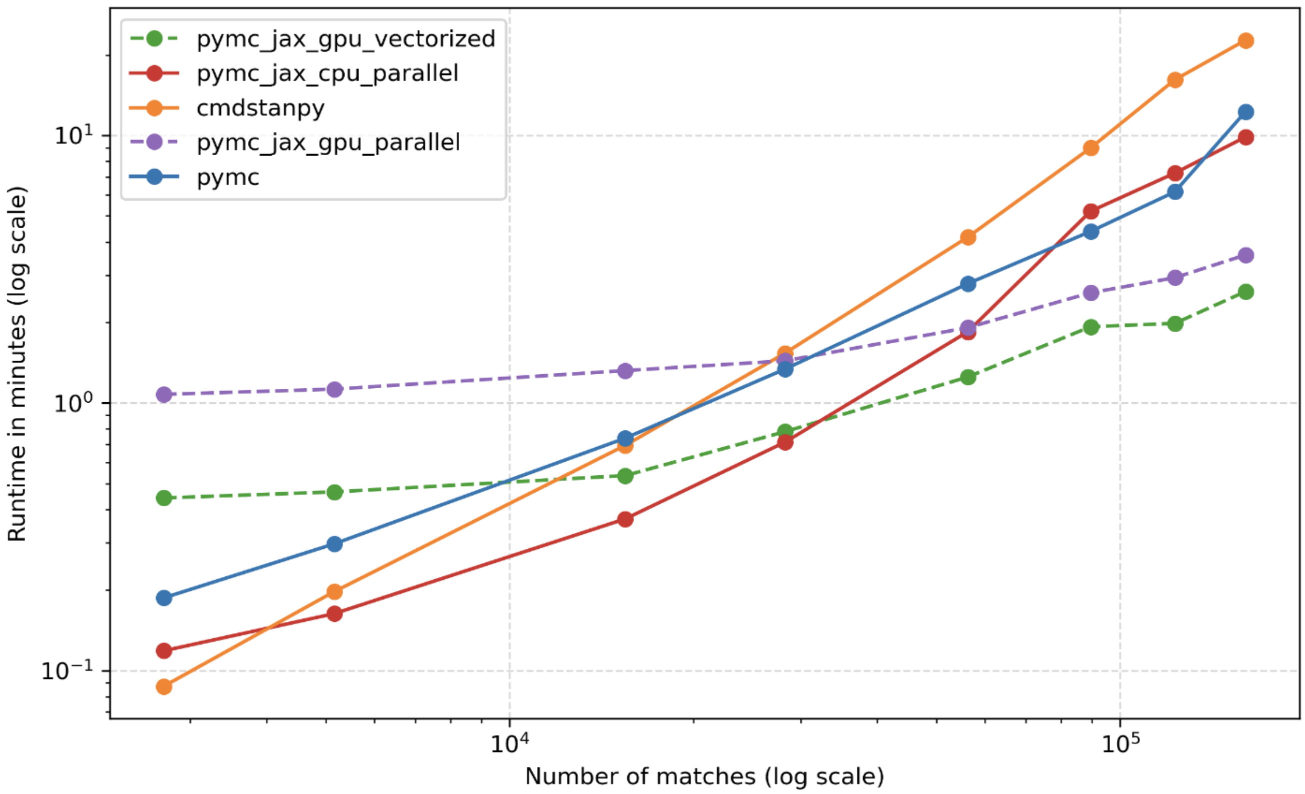
- The No-U-Turn Sampler: Adaptively Setting Path Lengths in Hamiltonian Monte Carlo (Gelman & Hoffman, 2011) [1]
- Variational Inference: A Review for Statisticians (Blei, Kucukelbir & McAuliffe, 2018) [2]
- Overview of MCMC Sampling Metholodies (Julian Cooper, 2022) [3]

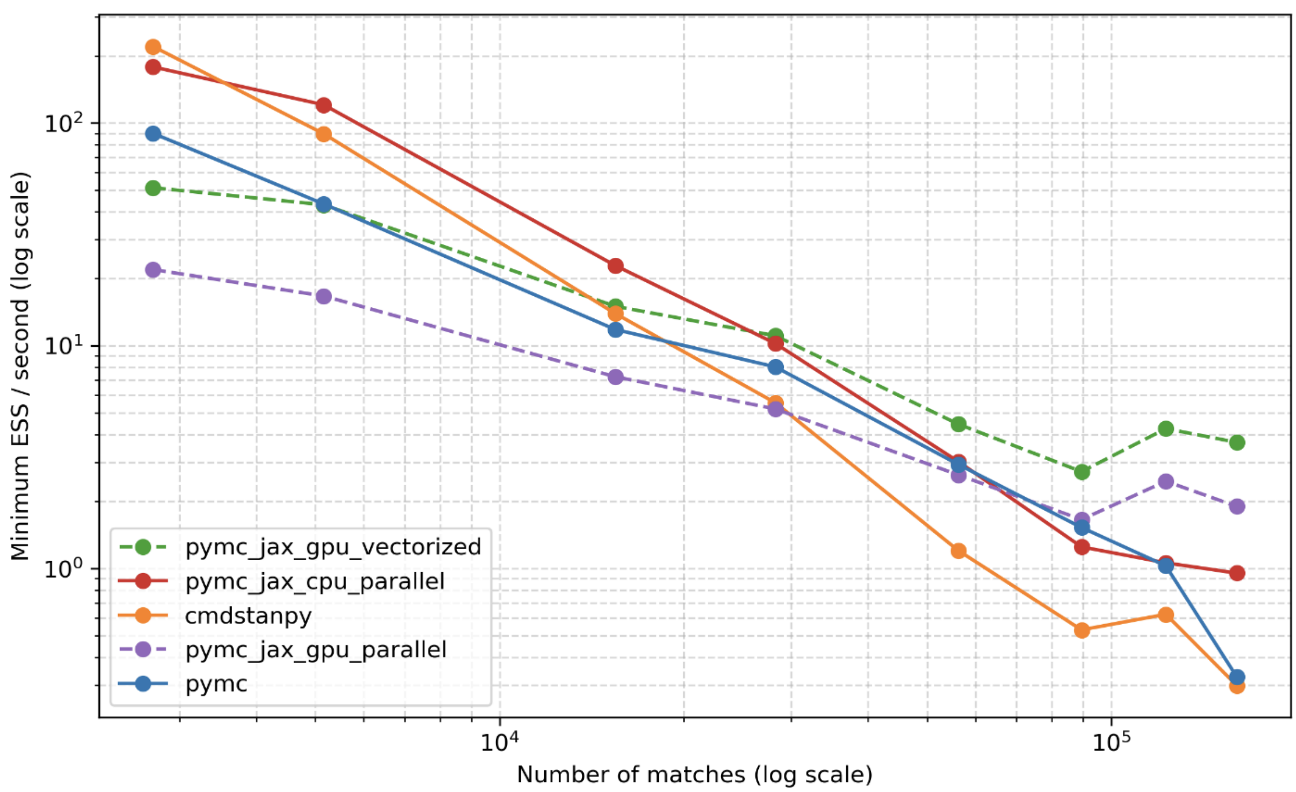
Probabilistic Programming Languages

We consider the Probabilistic Programming Languages (PPLs) that offer a python development interface, including Stan, PyMC, Pyro, Edward2 and NumPyro.

While most of these languages offer the full range of MCMC sampling and model evaluation methods for bayesian inference, they differ substantially in their choice of backend (= host language they are compiled to). This produces differences in stability and speed of auto-differentiation, vectorization and hardware acceleration (multiple cpu or gpu cores).

	Stan	PyMC	Pyro	Edward2	NumPyro
sampling methods	HMC, NUTS, ADVI	M-H, Gibbs, HMC, NUTS, ADVI	HMC, NUTS, SVI	Gibbs, HMC, VI	Gibbs, HMC, NUTS, VI
backend libraries	Home-built, compiled in C++	Theano/Aesara with JAX integration	Facebook's PyTorch framework (2016)	Google's TensorFlow framework (2015)	Google's JAX framework (2018)
ease of use	Beautiful declarative language	Great support community, very pythonic	Need familiarity with PyTorch	Requires familiarity with TensorFlow	Pyro interface but with access to JAX libraries
hardware acceleration	C++ multi-thread & MPI support	JAX vectorization & CPU/GPU parallel support	CPU/GPU parallel support	CPU/GPU parallel support	JAX vectorization & CPU/GPU parallel support
other comments	Best documentation, good for small data	Since 4.0 upgrade, best MCMC option	Best for SVI and BNNets, large datasets	Some integration for JAX, not well adopted yet	Leightweight and fastest HMC-NUTS implementation





Stan (2012) compiles into C++ with built-from-scratch auto-differentiation using Boost and Eigen libraries. First widespread implementation of HMC-NUTS. Still preferred by statisticians for small data problems due to declarative language and great documentation.

PyMC (PyMC3 2015 / v4.0 2022) built on top of Theano -> Aesara. Stores a lightweight static computational graph which is more appropriate for bayesian inference. Version 4.0 introduced integration for JAX jit, vmap and grad libraries resulting it significant speed improvements.

Pyro (Uber, 2017) built on top of PyTorch (Facebook). Stores a memory-intensive dynamic computational graph. Really amazing for deep learning, especially RNNs or any generative models with variable input and output lengths, but generally slower for bayesian inference tasks.

Edward2 (2018) built on top of TensorFlow (Google). Similar to Theano/Aesara, TensorFlow stores a static computational graph which is appropriate for bayesian inference models and provides the most opportunities for speed-ups.

NumPyro (2019) extends Pyro's modeling API to a different JAX-based backend. This enables better hardware acceleration (multiple cpu or gpu cores), auto-differentiation and vectorization. Custom-built HMC-NUTS end-to-end JAX implementation which is considered best in class.

Reference documentation

- NumPyro: Composable Effects for Flexible and Accelerated Probabilistic Programming (UberAI: Phan, Pradhan & Jankowiak, 2019) [4]
- Pyro: Deep Universal Probabilistiv Programming (UberAI: Bingham et al., 2018) [5]
- PyMC 4.0 Release Announcement (Willard, Vieira & Chaudhari, 2022) [6]
- Comparative analysis of CmdStanPy, PyMC 4.0 and NumPyro (Ingram, 2021) [7]
- Deep Learning Libraries: Aesara, TensorFlow, PyTorch and JAX (Wang, 2022) [8]

NumPyro: Pyro with NumPy and JAX

NumPyro is a lightweight probabilistic programming library that provides a NumPy backend for Pyro. We rely on JAX for automatic differentiation and JIT compilation to GPU / CPU.

Interacting with NumPyro's API: It's not so bad! While Pyro's backend is written in PyTorch, its user API is very similar to PyMC (example). NumPyro adopts an identical user API. See code comparaison below for a simple linear regression model formulation. (Note, I've included a non-standard line parameterization to illustrate "transformed parameters".)

PyMC —>

```
import pymc as pm
import numpy as np

with Model() as model:
    # specify our parameter priors
    theta = pm.Uniform("theta", -0.5*np.pi, 0.5*np.pi)
    b_perp = pm.Normal("b_perp", 0, sigma=1)

    # transformed parameters we want to keep track of during sampling
```

```python
    m = pm.Deterministic("m", np.tan(theta))
    b = pm.Deterministic("b", b_perp / np.cos(theta))

    # likelihood function
    likelihood = pm.Normal("y", mu=m*x+b, sigma=yerr, observed=y)

    # sample from posterior (inference)
    %time inf_data = sampling_jax.sample_numpyro_nuts(2000, chains=2)
```

NumPyro —>

```python
import jax
import numpyro

import arviz as az
import numpy as np
import jax.numpy as jnp

from numpyro import distributions as dist, infer

def linear_model(x, yerr, y=None):
    # specify our parameter priors
    theta = numpyro.sample("theta", dist.Uniform(-0.5 * jnp.pi, 0.5 * jnp.pi))
    b_perp = numpyro.sample("b_perp", dist.Normal(0, 1))

    # transformed parameters we want to keep track of during sampling
    m = numpyro.deterministic("m", jnp.tan(theta))
    b = numpyro.deterministic("b", b_perp / jnp.cos(theta))

    # likelihood function
    with numpyro.plate("data", len(x)):
        numpyro.sample("y", dist.Normal(m * x + b, yerr), obs=y)

# sample from posterior (inference)
sampler = infer.MCMC(
    infer.NUTS(linear_model),
    num_warmup=2000,
    num_samples=2000,
    num_chains=2,
    progress_bar=True,
)
%time sampler.run(jax.random.PRNGKey(0), x, yerr, y=y)

# extract inference data table fron sampler object
inf_data = az.from_numpyro(sampler)
```

If one wanted to interrogate or make changes to the backend codebase for either Pyro or NumPyro, you would need to work in PyTorch or NumPy / JAX, but assuming we just want to specify and run models, the interfaces should not be considered an obstacle.

Components of the JAX python library: Deepmind built JAX in 2018 to replace Tensorflow and compete with Meta's PyTorch. Similarly to PyTorch, Aesara and Tensorflow, JAX is a python library purpose-built to speed up numeric computations. All of these libraries are primarily used for deep learning applications, but are also useful for PPLs due to their respective high-performance implementations for `autograd`.

- *Just-In-Time Compilation* (`jit`): Python is an interpreted language which means that statements are executed (sent to the compiler) one at a time. With JIT-compiled languages or functions, the compiler is sent a batch of statements are is allowed to optimize how it computes them.

  ```
  import jax
  import jax.numpy as jnp

  def selu(x, alpha=1.67, lambda_=1.05):
    return lambda_ * jnp.where(x > 0, x, alpha * jnp.exp(x) - alpha)

  x = jnp.arange(1000000)

  selu(x)

  # selu_jit = jax.jit(selu)
  # selu_jit(x)
  ```

  The above `selu` function includes six `jax.numpy` operations: `jnp.exp`, `jnp.multiply`, `jnp.subtract`, `jnp.gt`, `jnp.where`, and another `jnp.multiply`. Both x86 and RISC instruction sets have a "fused instruction" for $a * \exp b$ and so by passing these two to the compiler at once it can execute with a single instruction to the processing unit. Beyond fused instructions, the other most common speed up comes from sibling instructions (same instruction on multiple data inputs). More on that in parallel processing section.

  JAX uses Google's old (but amazing) XLA library from the TensorFlow framework. The `jit` wrapper is what allows JAX to maximize the speed benefits of XLA for linear algebra operations. In particular, when we use `jit`, JAX is replaces "NumPy arrays" with "JAX tracers" under-the-hood. Like PyTorch's "tensors", a tracer is really just an array that records its own computational graph. This incurs some memory overhead but enables JAX to pass more operations at once to XLA for compilation.

- *Automatic differentiation* (`grad`): For gradient-based sampling methods like HMC and NUTS, one can either derive and provide the hamiltonian gradient directly to the sampler or pass the computational graph used to produce the hamiltonian to JAX's `grad` function.

  Passing a computational graph is made simple by using JAX's array types (tracers) which automatically store everything needed for `grad` to perform automatic differentiation. In NumPyro's HMC-NUTS implementation, `grad` is used with `jit` wrapper to maximize the speed-up available with XLA compiler for the expensive gradient compute at each sampler step. This is were most of the JAX magic comes from!

```python
def sum_logistic(x):
  return jnp.sum(1.0 / (1.0 + jnp.exp(-x)))

x_small = jnp.arange(3.)
derivative_fn = grad(sum_logistic)
print(derivative_fn(x_small))
# [0.25, 0.19661197, 0.10499357]
```

The core developers of `autograd`(Maclaurin, Duvenaud, Johnson and Townsend) have moved to the JAX core dev team and were responsible for writing `grad`.

- *Custom-built HMC-NUTS algorithm* (`nuts`): The original HMC-NUTS algorithm implements a `BuildTree` subroutine which recursively builds a binary tree to efficiently find the number of leapfrog steps L we should take along a given trajectory (ie. test for u-turn condition). Unfortunately recursive conditions like this limit batching of operations for the compiler (cannot use `jit`)!

  The NumPyro team proposed an alternate "iterative" method for building a subtree with some specified depth d. `jit` wrapper can now be applied to the entire `BuildTree` subroutine.

Algorithm 1 BUILDTREE

```
Input initial node z, tree depth d
if d = 0 then
    z' ← LEAPFROG(z)
    return TREE(z', z', False)
else
    T_L ← BUILDTREE(z, d − 1)
    if T_L.turning then
        return T_L
    else
        z ← T_L.right
        T_R ← BUILDTREE(z, d − 1)
        z_L ← T_L.left
        z_R ← T_R.right
        if T_R.turning then
            turning ← True
        else
            turning ← ISUTURN(z_L, z_R)
        return TREE(z_L, z_R, turning)
```

Algorithm 2 ITERATIVEBUILDTREE

```
Input initial node z, tree depth d
Initialize storage S[0], S[1], ..., S[d − 1]
for n ← 0 to 2^d − 1 do
    z ← LEAPFROG(z)
    if n is even then
        i ← BITCOUNT(n)
        S[i] ← z
    else
        // gets the number of candidate nodes
        l ← TRAILINGBIT(n)
        i_max ← BITCOUNT(n − 1)
        i_min ← i_max − l + 1
        for k ← i_max to i_min do
            turning ← ISUTURN(S[k], z)
            if turning then
                return TREE(S[0], z, True)
return TREE(S[0], z, False)
```

Figure 2: BuildTree Subroutine

- *Parallel Processing* (`pmap` & `vmap`): In general, there are two ways to parallelize the HMC-NUTS algorithm:
  - `pmap` (hardware acceleration): Single Program Multiple Device (SPMD). Idea is to run each chain as a separate program on a different device. A device in this case can just mean separate CPU cores or entirely separate processor units (CPU / GPU / TPU).

– `vmap` (vectorizaton): Single Instruction Multiple Data (SIMD). Idea is to parallelize computation at the instruction level on the same processor. We do this whenever we work with NumPy vector rather than for loops and lists. The speed-up comes from both (a) loading data as a block rather than repeated cache / memory / storage requests, and (b) applying single instruction to multiple data instances in register. For HMC-NUTS, this is used within the sampler itself for any transform or gradient vector operations.

Note, the opportunity for parallelization is much greater for non-gradient based MCMC sampling methods (M-H, Gibbs, etc.) since each subsequent sample is not dependent on the previous sample (step) taken.

PyMC's NumPyro API speed test: Using a model formulation and synthetic dataset taken from Foreman-Mackey's blog I ran a short experiment to see if PyMC's API would incur meaningful overhead costs when running NumPyro's NUTS implementation (jupyter nb).

	PyMC API	NumPyro	Speed-up
simple	1.87	1.87	0%
complex	3.75	3.01	20%

Note, we do not consider gpu acceleration since our Marketing Mix problem does not involve a large enough dataset for this to be worthwhile (message passing overhead outweigh benefit of parallel processing).

Takeaway: potential (likely small) speed up available for sufficiently complex model formulations. Since easy enough to migrate model, this is surely worth a try!

Reference Documentation

- NumPyro: Composable Effects for Flexible and Accelerated Probabilistic Programming (UberAI: Phan, Pradhan & Jankowiak, 2019) [4]
- JAX Official Documentation: How to Think in JAX (Deepmind, 2023) [9]
- Operator Fusion in XLA: Analysis and Evaluation (Snider & Liang, 2023) [10]
- Astronomer's Guide to Programming with NumPyro (Foreman-Mackey, 2022) [11]
- StackOverflow: Why is JAX's `jit` needed for `jax.numpy` operations [12]
