Pragmatic Probabilistic Programming

Parameter Adaptation in PyMC3

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Introduction

I am an open source contributor on a number of libraries, notably PyMC3, which is a library for probabilistic programming in Python. One of the benefits of PyMC3 is the friendly, simple API that abstracts away the details of the inference, allowing domain experts to fit models without needing to be experts at inference:

```
import pymc3 as pm

with my_model:  # defined earlier
    trace = pm.sample()  # ✨✨magic✨✨
```

This essay has two goals:

1. Provide some intuition into the geometry of some of the algorithms and diagnostics that we use in probabilistic programming to give some appreciation to what happens in the ✨✨magic✨✨ step, and
2. Do a code tour to describe how PyMC3 tunes sampler parameters.

This talk is partly in reaction to a question I was recently asked:

"What does PyMC3 do that I cannot find in the Stan manual?"

While I love PyMC3's ease of use, extensibility, and community, we have a well-earned reputation for borrowing good ideas from other projects, particularly the wonderful Stan library.

Jake VanderPlas
@jakevdp

"There's an old saying... 'Python is the second-best language for everything'" - @callahad #PyCon2018

7:05 PM · May 11, 2018

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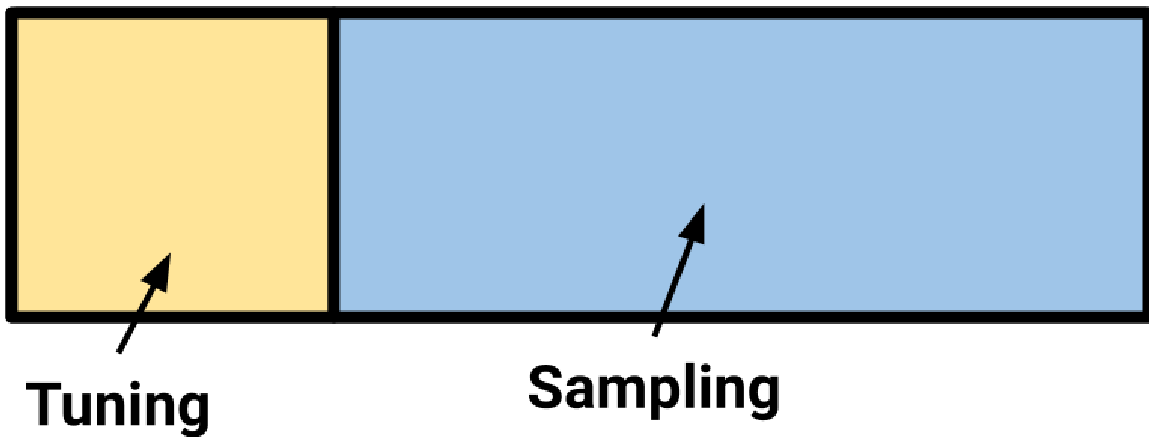
What is tuning?

"Tuning" broadly describes what happens before sampling. In Bayesian inference, our goal is to calculate expectations[1] over probability distributions. MCMC achieves that by producing samples that are *asymptotically guaranteed* to come from the distribution of interest: the "stationary distribution".

When we tune, we throw away these asymptotic guarantees, searching for parameters for our sampler that will speed up the calculation of these expectations. In the particular case of PyMC3, we default to having 500 tuning samples, after which we *fix* all the parameters so that the asymptotic guarantees are again in place, and draw 1,000 new samples. By default, the first 500 tuning samples are discarded, as it would be theoretically shaky ground to suggest they came from the stationary distribution at all.



Tuning in Metropolis-Hastings

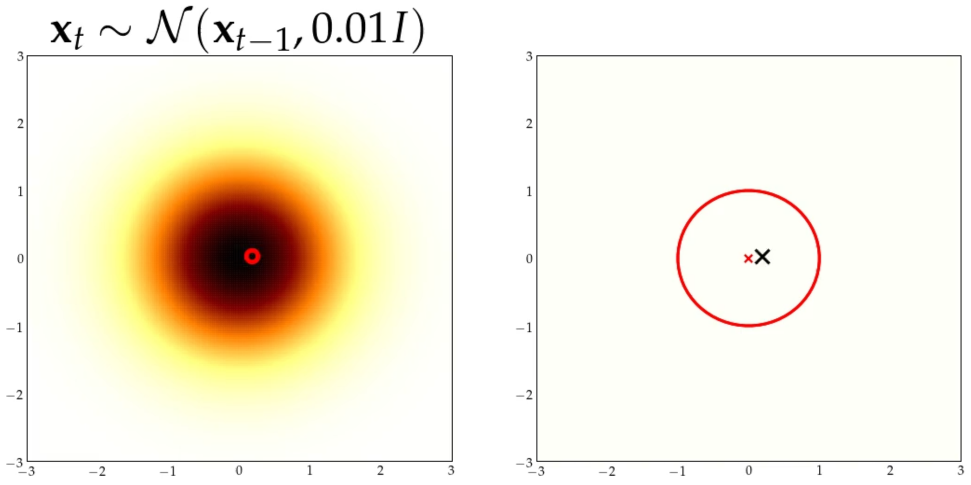
To warm up, consider a Metropolis-Hastings sampler. Recall that Metropolis-Hastings works by making a proposal, and accepting or rejecting based on the ratio of the density of the stationary distribution at the proposed point and at the current point: Always accept if the proposal has higher probability, and sometimes reject if the proposal has lower probability:

$$A(x_t) = \min\left\{1, \frac{\pi(x_t)}{\pi(x_{t-1})}\right\}$$

If we consider a proposal distribution that is a normal centered at the previous point with diagonal covariance, there is one parameter to tune, which is the step size.

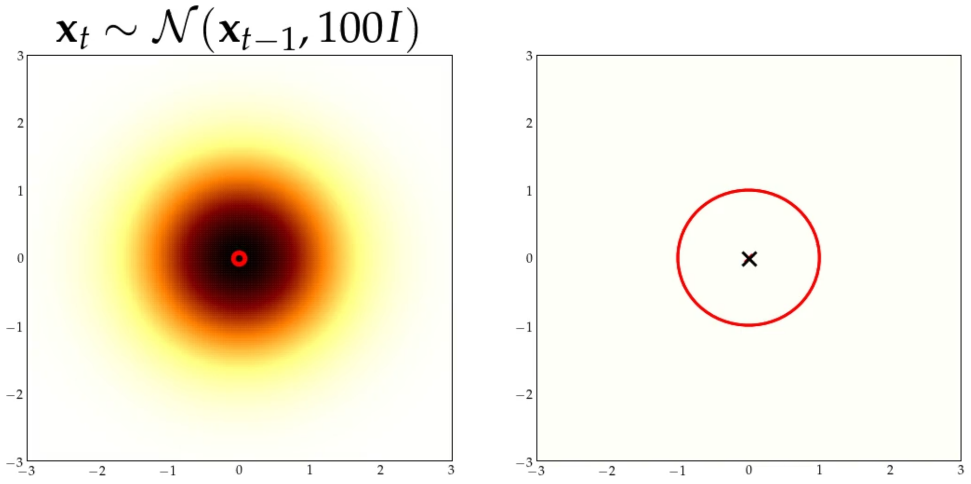
$$x_{t+1} \sim \mathcal{N}(x_t, sI)$$

What are our tradeoffs when choosing step size? Here is a very small step size, being used to sample from an isotropic Gaussian.



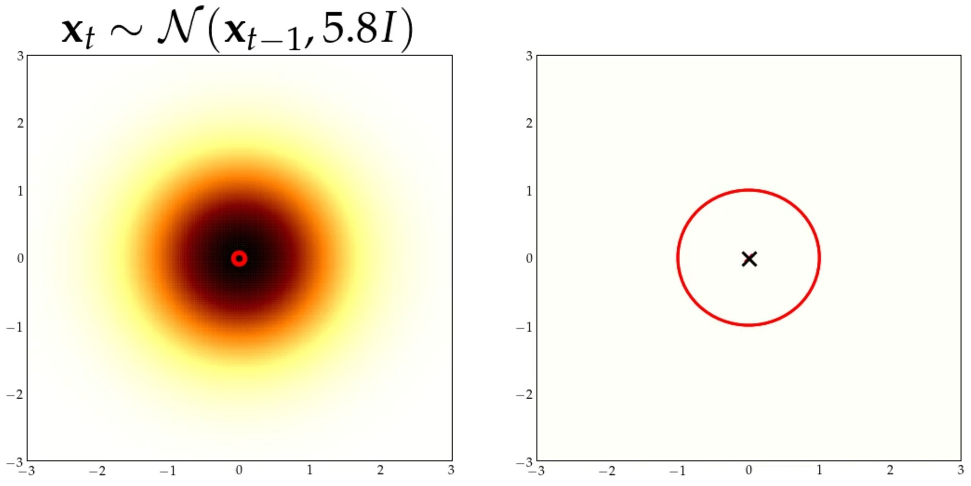
Notice that nearly every proposal is being accepted, because the steps are small enough that the underlying stationary distribution does not change very much. On the right-hand side is an empirical estimate of the mean and 1 standard deviation ellipse, compared with the true mean and standard deviation.

Going in the other direction, these are very large steps for the proposal - 10,000 times as large as the previous figure - and notice that most proposals are rejected.



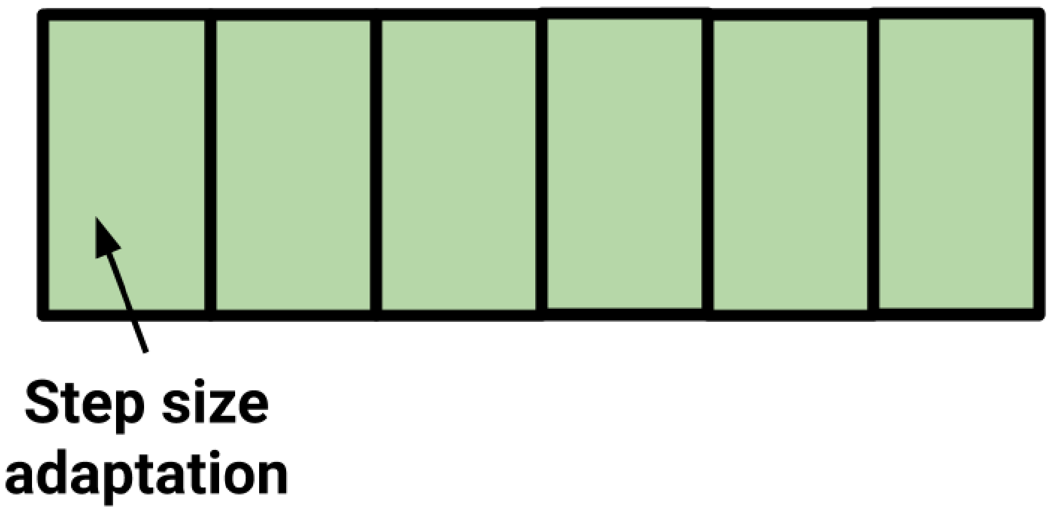
You can see the empirical mean and standard deviation keep updating as the current position is resampled. There is some evidence that says an acceptance probability of 23.4% is optimal in terms of these expectations converging[2] . In practice, PyMC3 tries to get the acceptance probability between 20% and 50% through tuning.

Here we have a tuned diagonal proposal distribution. There is a mix of acceptances and rejections, and it looks like the mean and covariance are converging to the true values more quickly.



Remember: **all three of these examples have theoretical convergence guarantees, but we are interested in fast convergence of these expectations.**

In any rate, this tuning is implemented in a windowed fashion in PyMC3, which will also be the strategy for tuning in our gradient-based samplers.



During each of these windows, we make an estimate of a quantity – here the acceptance rate – and then update parameters based on that estimate. This is actual source code, and by default, every 100 samples, this switch statement runs.

```
def tune(scale, acc_rate):
  """Tunes the scaling parameter for the proposal
```

```
    distribution according to the acceptance rate over the
    last tune_interval:

    Rate    Variance adaptation
    ----    -------------------
    <0.001        x 0.1
    <0.05         x 0.5
    <0.2          x 0.9
    >0.5          x 1.1
    >0.75         x 2
    >0.95         x 10
    """
    if acc_rate < 0.001:
      # reduce by 90 percent
      scale *=0.1
    elif acc_rate < 0.05:
      # reduce by 50 percent
      ...
    elif acc_rate > 0.95:
      # increase by one thousand percent
      scale *= 10

    return scale
```

Aside: Effective Sample Size

It is worth noting here that the animations above are asking you to judge convergence heuristically. In reality, *effective sample size* is the diagnostic that we are trying to intuit. The number comes from the observation that for independent, identically distributed random variables, the variance of the empirical mean, $\hat{\mu}$, is the true variance divided by the number of samples:

$$\hat{\mu} = \frac{1}{n}\sum_{j=1}^{n} x_j$$

$$\text{Var}(\hat{\mu}) = \frac{\sigma^2}{n},$$

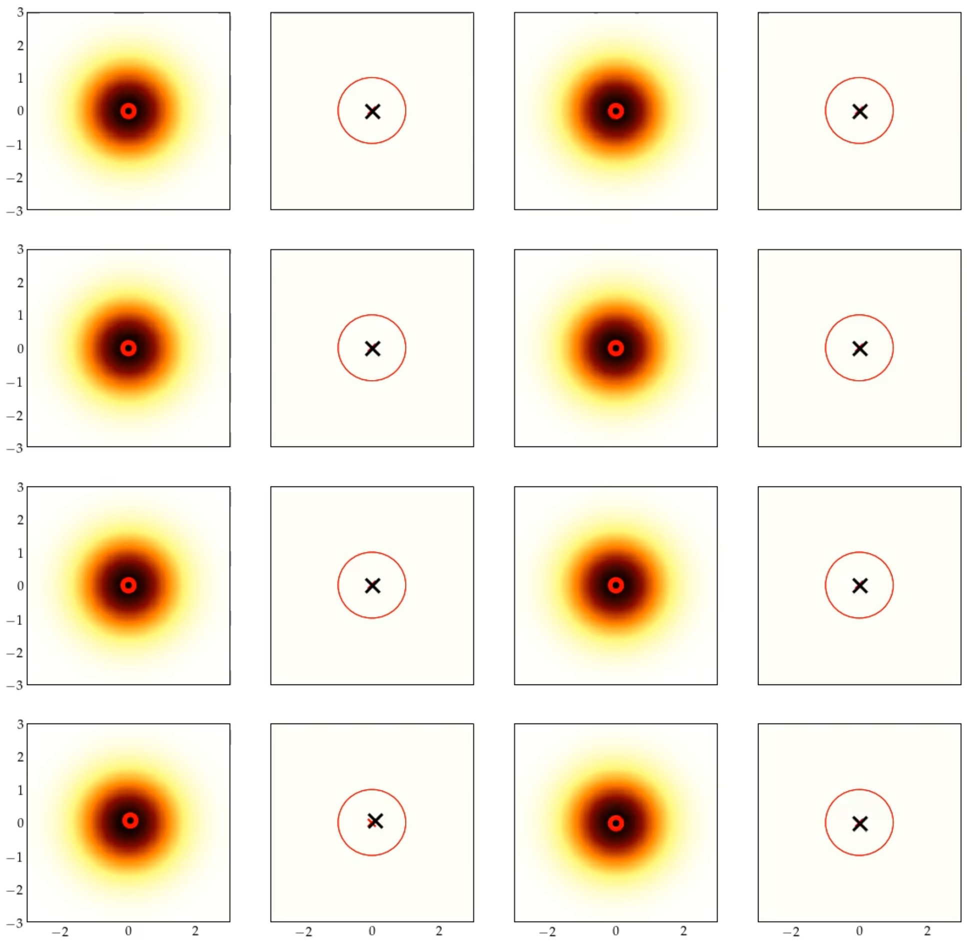
where σ is the true standard deviation of the underlying distribution.

Then the effective sample size is defined as the denominator that makes this relationship still be true:

$$\text{Var}(\hat{\mu}) = \frac{\sigma^2}{n_{\text{eff}}}.$$

This quantity is difficult to compute: you might use multiple chains to estimate $\mathrm{Var}(\hat{\mu})$, and estimating σ^2. There is a great recent paper[3] giving better up to date details.

We might visualize this relationship by running our previous experiment many times, to estimate the variance of the empirical mean over all our samples.



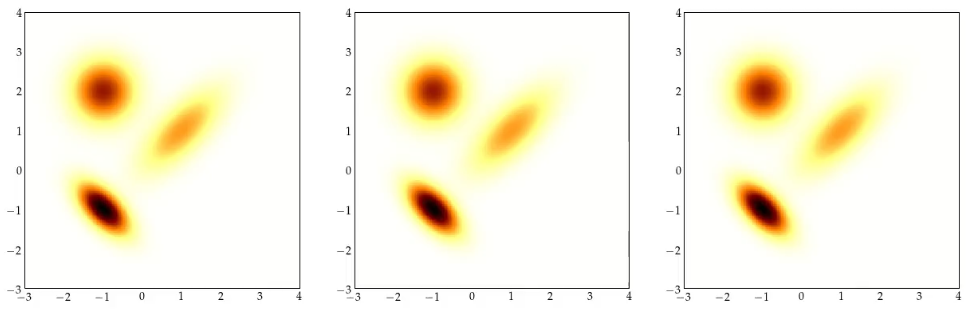
Tuning in Hamiltonian Monte Carlo

Next we talk about the real interesting bit here: adaptation in gradient-based samplers, specifically Hamiltonian Monte Carlo. As a warning, the story is importantly different for the No-U-Turn sampler[4] , mainly because of the dynamic tree building, compared to a fixed path length in HMC.

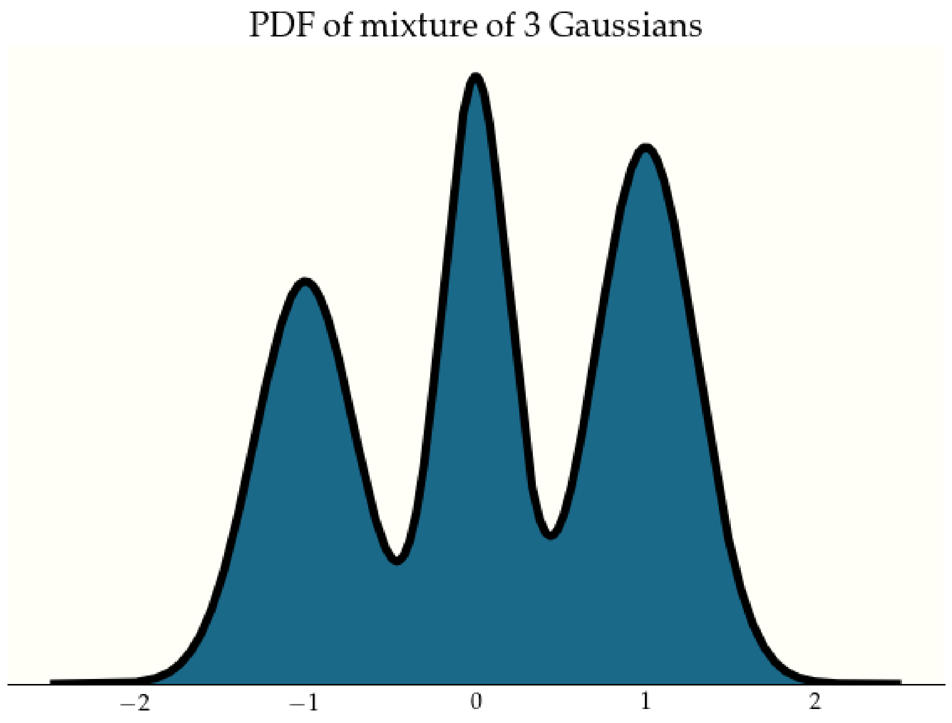
Recall that in Hamiltonian Monte Carlo, there is a system of differential equations we solve, integrating a position, $\mathbf{q}$, and momentum, $\mathbf{p}$, for some fixed amount of time[5] .

$$\frac{d\mathbf{q}}{dt} = \mathbf{p}, \quad \frac{d\mathbf{p}}{dt} = -\frac{\partial V}{\partial \mathbf{q}}$$

This is a 2D mixture of 3 Gaussians, and I am just simulating Hamiltonian dynamics here, not taking any samples. The Hamiltonian equations conserve energy, so in this physical simulation, a trajectory far away from the probability mass will move slowly: it has traded velocity for potential energy. Conversely, when trajectories pass near regions of high probability, they will move fast, but have very little potential energy.



To look deeper into tuning parameters, let's drop down a dimension, and consider this one dimensional mixture of three Gaussians.



To perform HMC, we double the number of dimensions by adding a momentum parameter. We evolve the system for a fixed path length, and then the new position becomes our new sample, we discard the momentum, and resample a new one.

So the marginal x-axis samples are from our stationary distribution, and the marginal y-axis samples are from the momentum distribution, which we pick. In this case, I chose a normal distribution. One parameter we will work on tuning is the covariance of this momentum distribution. There is research that suggests a covariance that matches the stationary distribution is optimal.[6]

We also care about step size.

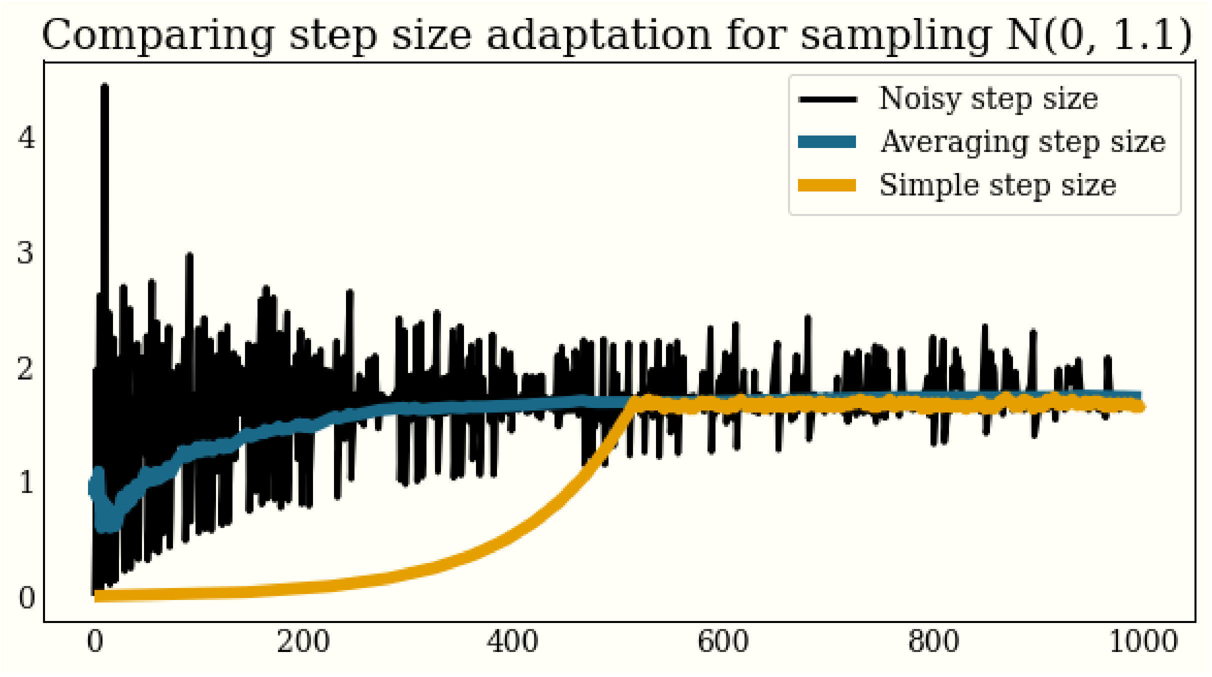
Each of these simulations are sampling 100 points from our stationary distribution, and is displayed with the same frame rate, so this is how the computer feels running your sampling. There *is* a tradeoff between large steps and integration error, and so you can not just take arbitrarily large steps. We actually have to do a Metropolis acceptance step at the end of each trajectory. By default, PyMC3 tries to get an acceptance rate of 65% for HMC, and 85% for NUTS.

Tuning HMC

Step size adaptation is fairly quick. These are stochastic optimization problems. You can use a variant of what we used for Metropolis-Hastings earlier, but PyMC3 uses the dual averaging algorithm from the NUTS paper:

```
def dual_averaging_adapt(self, p_accept):
  self.error_sum += self.target_accept - p_accept
  log_step = (self.mu -
              t ** -0.5 * self.error_sum / self.gamma)
  eta = self.t ** -self.kappa
  self.log_averaged_step *= (1 - eta)
  self.log_averaged_step += eta * log_step
  self.t += 1
  return np.exp(log_step), np.exp(self.log_averaged_step)
```

It is a pretty dense algorithm, and the goal of putting it here is just to show that we can write it down in a few lines. The parts to call out are that there is a `log_step` that does some noisy exploration, and a stateful `log_averaged_step` that smooths out the exploratory steps. While tuning, we use the exploring step size, and after tuning we switch to the averaged step size.



Here is what the exploring step size, smoothed step size, and simple algorithm look like on a toy problem. You can see convergence is somewhat faster for the dual averaging algorithm. I initialized the simple step size adaptation (which we used in the Metropolis tuning earlier) at a pretty unfair spot. I do not think it is as bad as that.

Covariance estimation is also done in an online fashion:

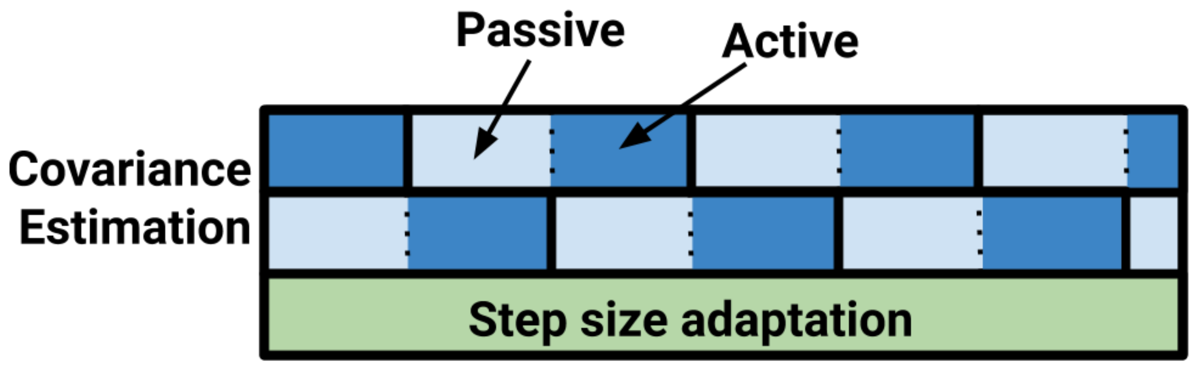
```
class _WeightedVariance:

  def add_sample(self, x):
    self.w_sum += 1
    old_diff = x - self.mean
    self.mean[:] += old_diff / self.w_sum
    new_diff = x - self.mean
    self.raw_var[:] += old_diff * new_diff
```

There is some math going on here you can check, but it runs during tuning, on two different estimator objects, every step:

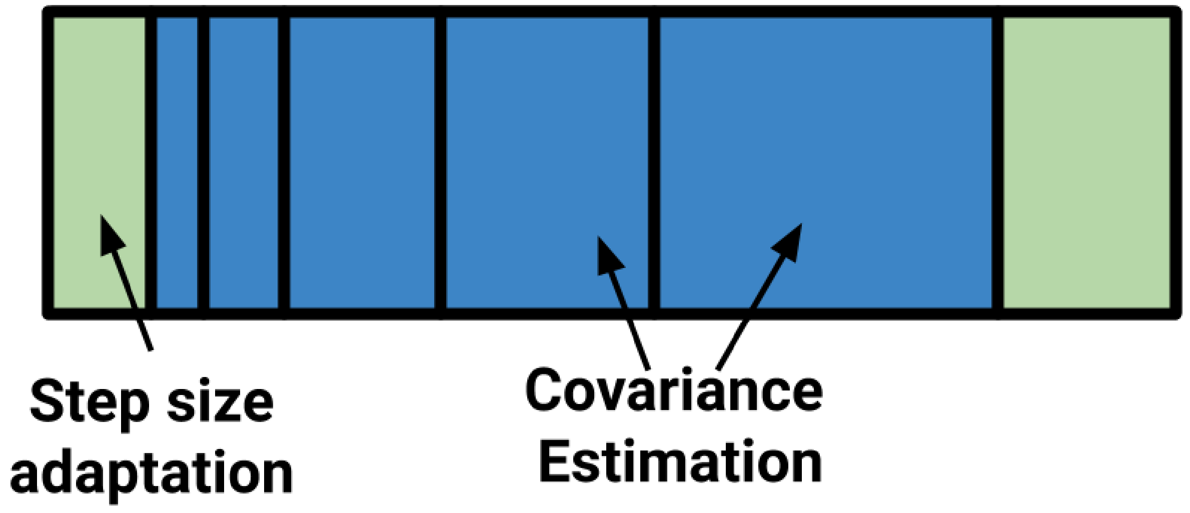
```
class QuadPotentialDiagAdapt:

  def update(self, sample):
        self._foreground_var.add_sample(sample)
        self._background_var.add_sample(sample)
        self._update_from_weightvar(self._foreground_var)

        n_samples = self._n_samples
        if n_samples > 0 and n_samples % self.window == 0:
                self._foreground_var = self._background_var
                self._background_var = _WeightedVariance()
        self._n_samples += 1
```

The foreground and background covariance estimators swap out every `window` steps, which is 100 by default.

So what does this look like?



PyMC3 has two covariance matrices updating constantly, and the exploratory step size is running the whole time as well. Compare this to this sketch of the Stan warmup routine:



The fast tuning of step size is done first, then expanding windows to estimate the covariance matrix, before a final step size adaptation.

Takeaways

- Automate what you can: a simple API that sets sensible defaults has worked well for us.

- Consider effective sample size: samples per second is not a good benchmark to optimize[7] .
- Windowed adaptation: it provides a few orders of magnitude of improvement to effective samples per second.