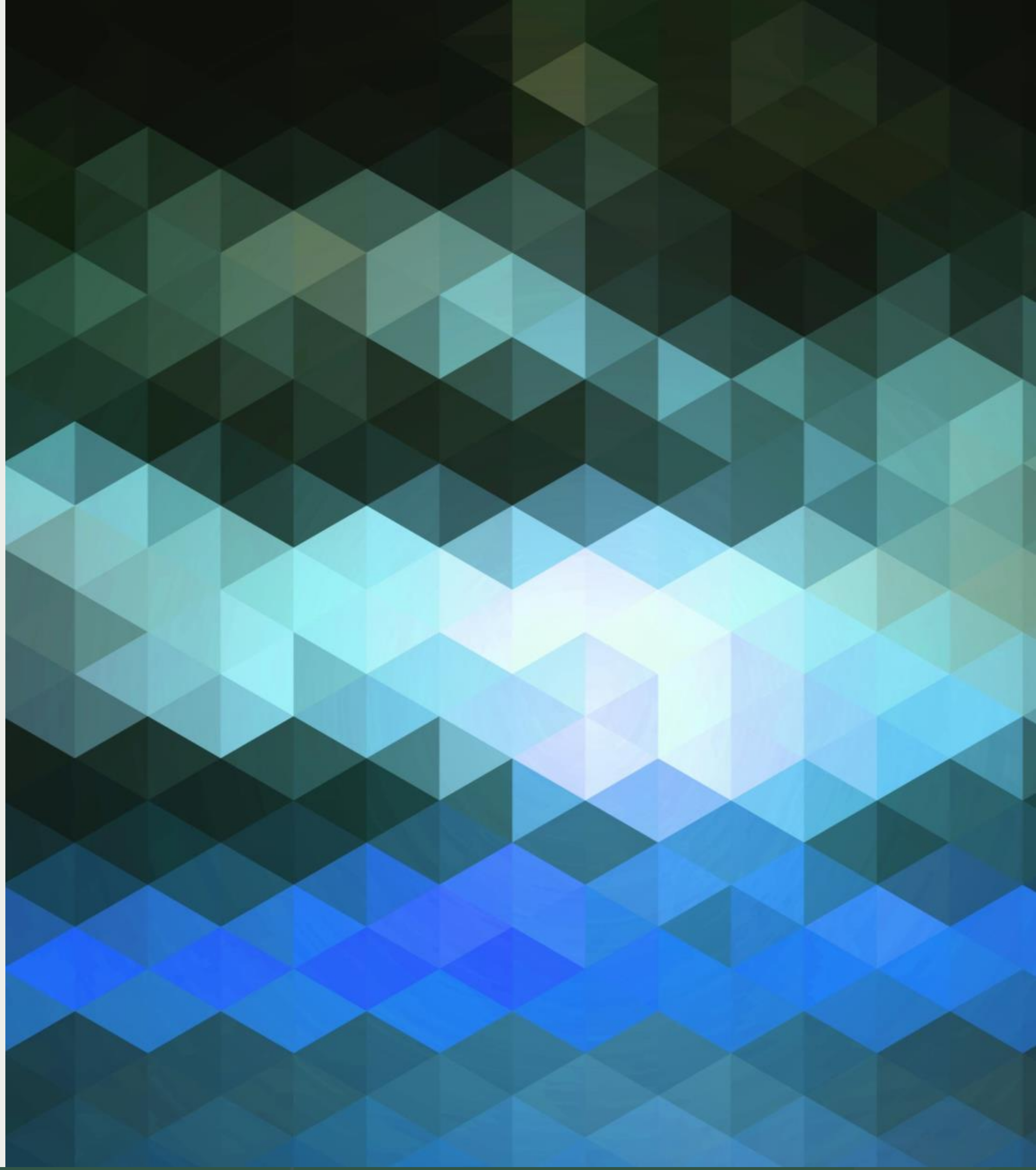
Bayesian Optimisation with a Probabilistic Model

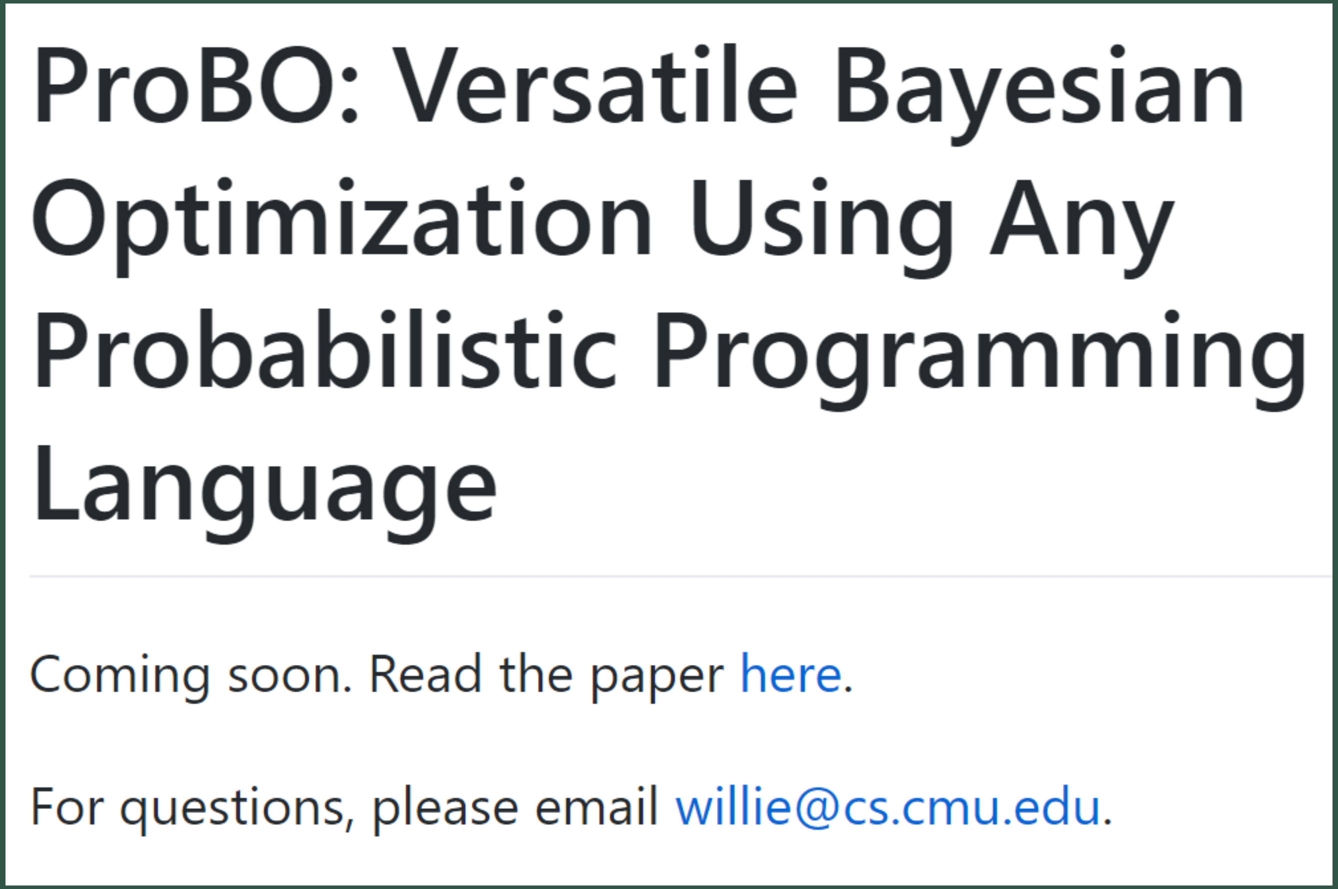
(in Python)

Ross Tooley



Motivation

Inspired by ProBO

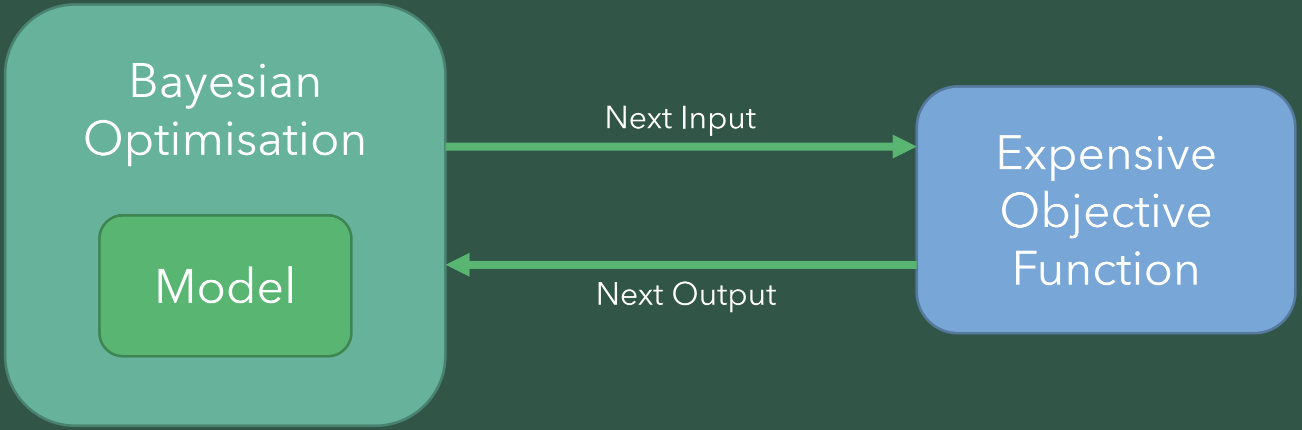


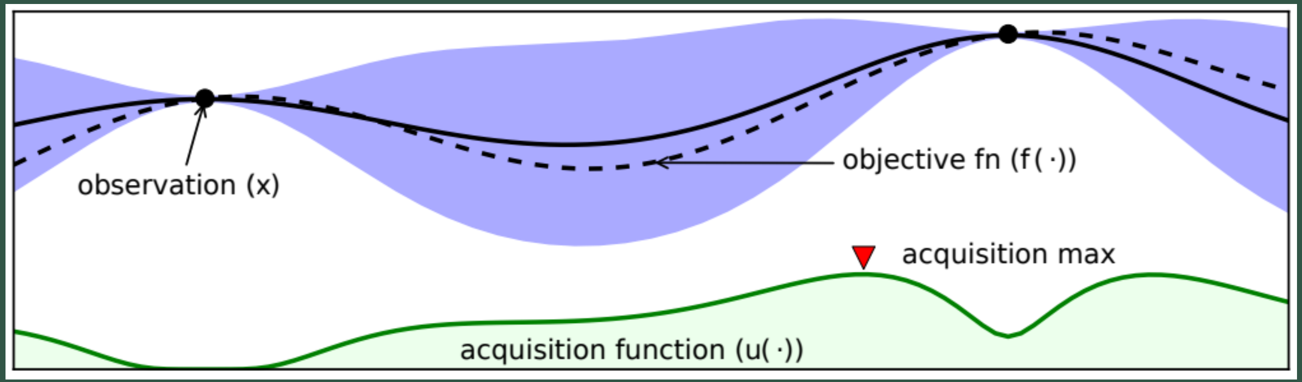
ProBO: Versatile Bayesian Optimization Using Any Probabilistic Programming Language

Coming soon. Read the paper here.

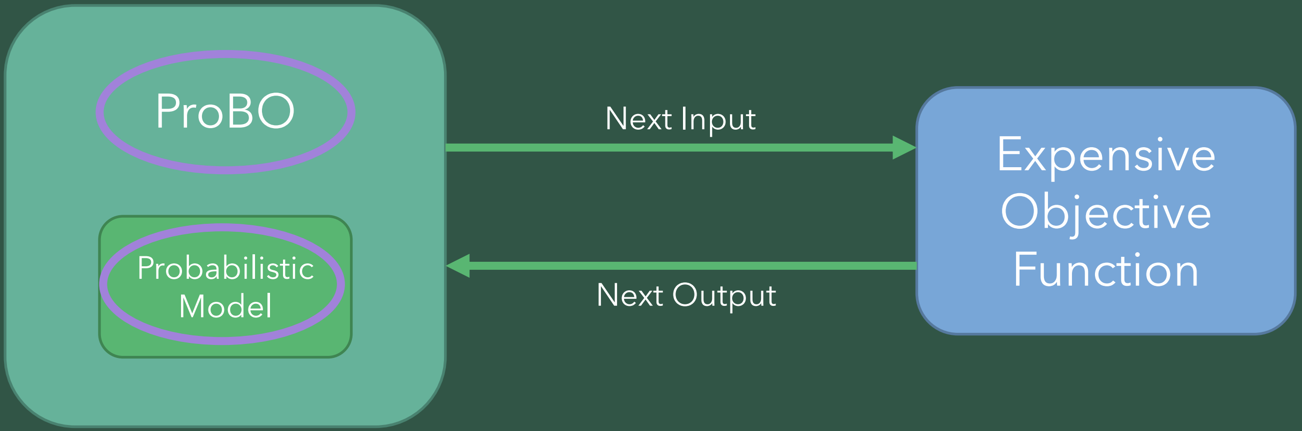
For questions, please email willie@cs.cmu.edu.

BO Recap


Bayesian Optimisation
Model
Next Input
Next Output
Expensive Objective Function


observation (x)
objective fn (f(·))
acquisition max
acquisition function (u(·))

ProBO Recap



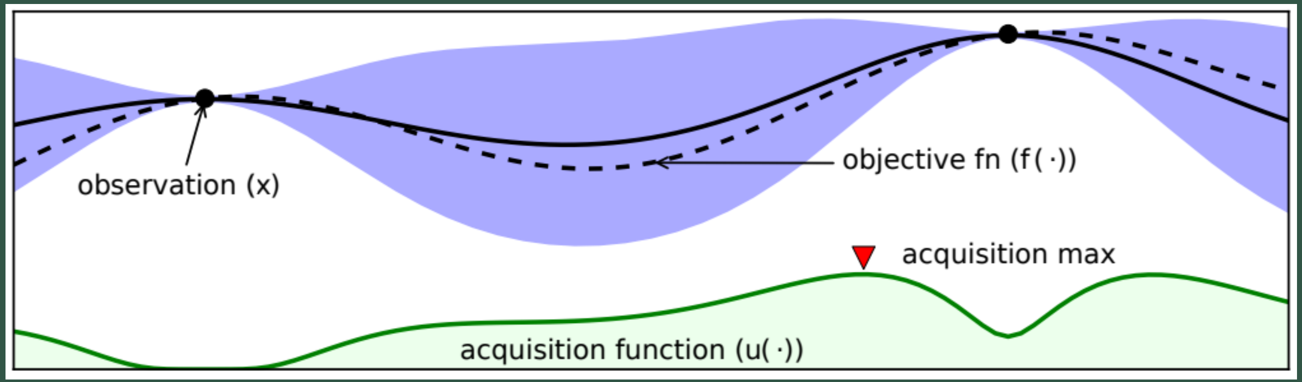
ProBO

Probabilistic Model

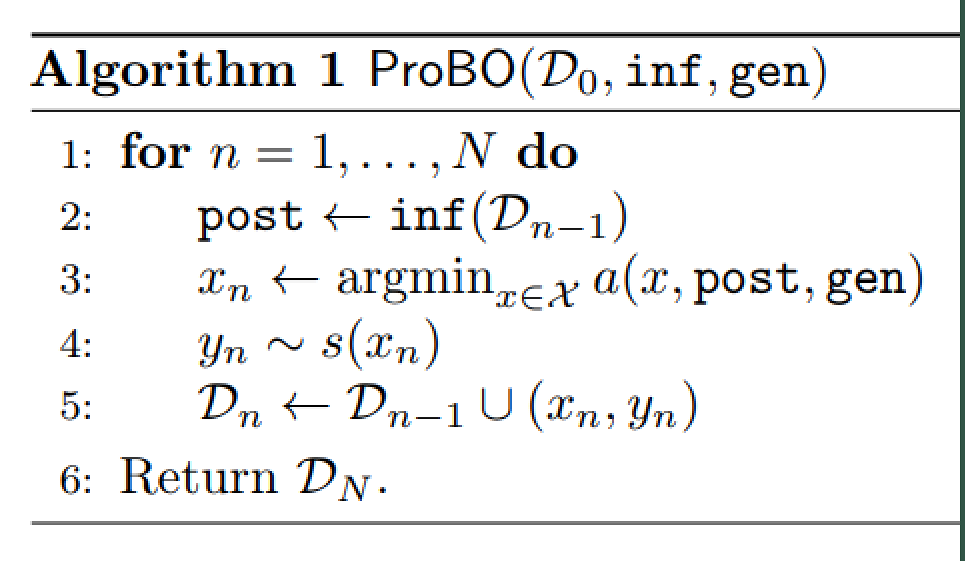
Next Input

Next Output

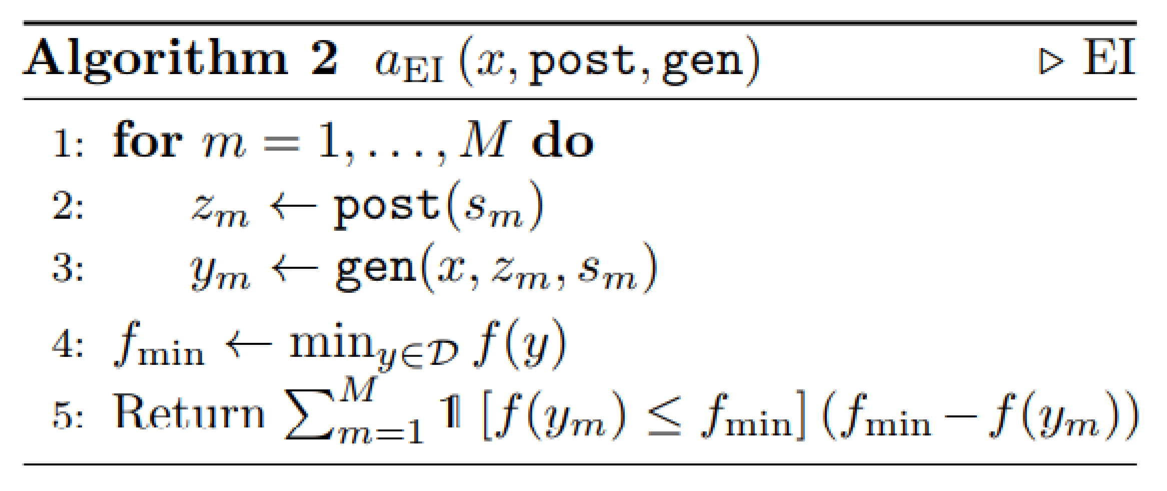
Expensive Objective Function



ProBO Recap

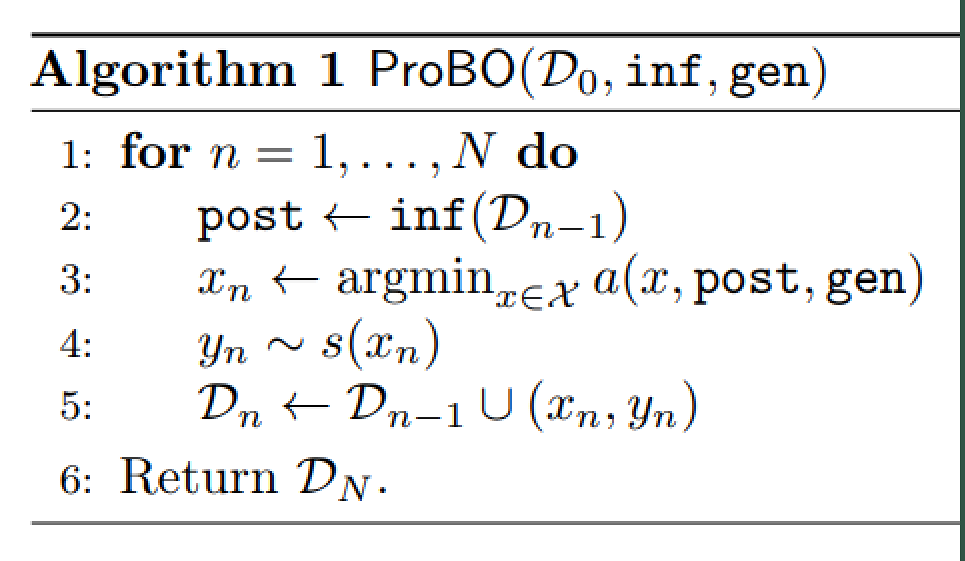


```
Algorithm 1 ProBO($\mathcal{D}_0, \texttt{inf}, \texttt{gen}$)
for $n = 1, \ldots, N$ do
    $\texttt{post} \leftarrow \texttt{inf}(\mathcal{D}_{n-1})$
    $x_n \leftarrow \text{argmin}_{x \in \mathcal{X}}\, a(x, \texttt{post}, \texttt{gen})$
    $y_n \sim s(x_n)$
    $\mathcal{D}_n \leftarrow \mathcal{D}_{n-1} \cup (x_n, y_n)$
Return $\mathcal{D}_N$.
```

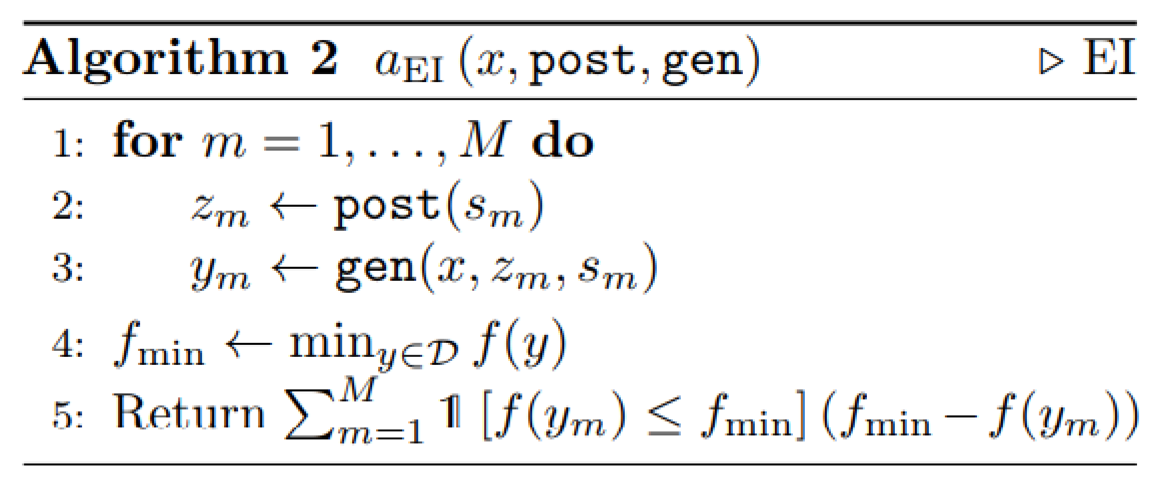


```
Algorithm 2 $a_{\text{EI}}\,(x, \texttt{post}, \texttt{gen})$                ▷ EI
for $m = 1, \ldots, M$ do
    $z_m \leftarrow \texttt{post}(s_m)$
    $y_m \leftarrow \texttt{gen}(x, z_m, s_m)$
$f_{\min} \leftarrow \min_{y \in \mathcal{D}} f(y)$
Return $\sum_{m=1}^{M} \mathbb{1}\left[f(y_m) \leq f_{\min}\right] (f_{\min} - f(y_m))$
```

ProBO Recap



```
Algorithm 1 ProBO($\mathcal{D}_0$, inf, gen)
for $n = 1, \ldots, N$ do
    post ← inf($\mathcal{D}_{n-1}$)
    $x_n \leftarrow \text{argmin}_{x \in \mathcal{X}}\, a(x, \text{post}, \text{gen})$
    $y_n \sim s(x_n)$
    $\mathcal{D}_n \leftarrow \mathcal{D}_{n-1} \cup (x_n, y_n)$
Return $\mathcal{D}_N$.
```



```
Algorithm 2 $a_{\text{EI}}(x, \text{post}, \text{gen})$    ▷ EI
for $m = 1, \ldots, M$ do
    $z_m \leftarrow \text{post}(s_m)$
    $y_m \leftarrow \text{gen}(x, z_m, s_m)$
$f_{\text{min}} \leftarrow \min_{y \in \mathcal{D}} f(y)$
Return $\sum_{m=1}^{M} \mathbb{1}\left[f(y_m) \leq f_{\text{min}}\right] \left(f_{\text{min}} - f(y_m)\right)$
```

Plan: implement pseudocode in Python

Enter BoTorch

BoTorch

BAYESIAN OPTIMIZATION IN PYTORCH

Enter BoTorch

Bayesian Optimization in PyTorch

Enter BoTorch… and Pyro

Enter BoTorch… and Pyro

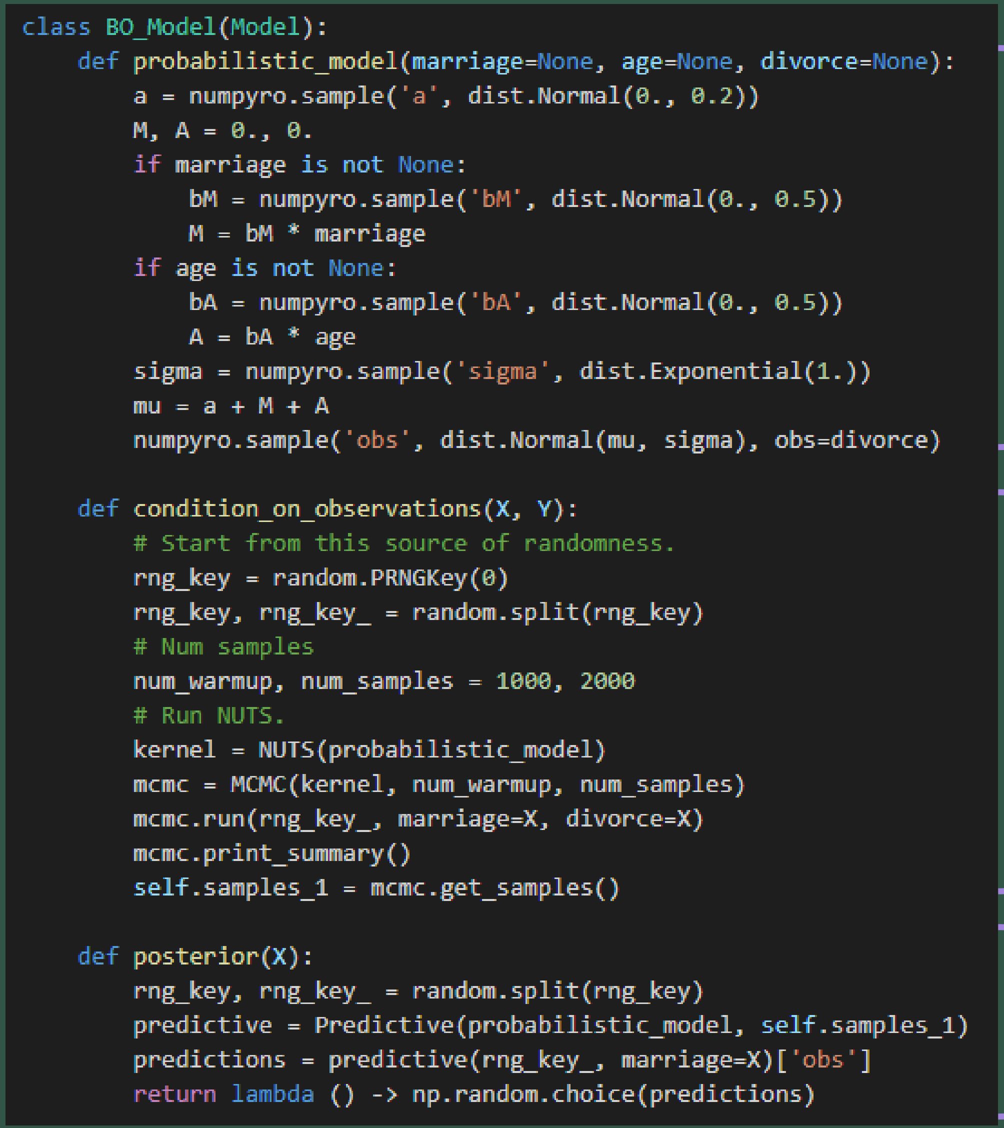
New Plan:

1. Implement ProBO in Python
2. Implement in BoTorch + Pyro
3. Compare

Work so far

(very little)

Some BoTorch + Pyro code



```
class BO_Model(Model):
    def probabilistic_model(marriage=None, age=None, divorce=None):
        a = numpyro.sample('a', dist.Normal(0., 0.2))
        M, A = 0., 0.
        if marriage is not None:
            bM = numpyro.sample('bM', dist.Normal(0., 0.5))
            M = bM * marriage
        if age is not None:
            bA = numpyro.sample('bA', dist.Normal(0., 0.5))
            A = bA * age
        sigma = numpyro.sample('sigma', dist.Exponential(1.))
        mu = a + M + A
        numpyro.sample('obs', dist.Normal(mu, sigma), obs=divorce)

    def condition_on_observations(X, Y):
        # Start from this source of randomness.
        rng_key = random.PRNGKey(0)
        rng_key, rng_key_ = random.split(rng_key)
        # Num samples
        num_warmup, num_samples = 1000, 2000
        # Run NUTS.
        kernel = NUTS(probabilistic_model)
        mcmc = MCMC(kernel, num_warmup, num_samples)
        mcmc.run(rng_key_, marriage=X, divorce=X)
        mcmc.print_summary()
        self.samples_1 = mcmc.get_samples()

    def posterior(X):
        rng_key, rng_key_ = random.split(rng_key)
        predictive = Predictive(probabilistic_model, self.samples_1)
        predictions = predictive(rng_key_, marriage=X)['obs']
        return lambda () -> np.random.choice(predictions)
```

Pyro model

Updating model

Sampling from model

BoTorch model

Work to do

(everything else)

Q&A

Thanks for listening!