Pyro

Bayesian Data Analysis with PPLs: Bayesian Regression in Pyro

UBER AI Labs

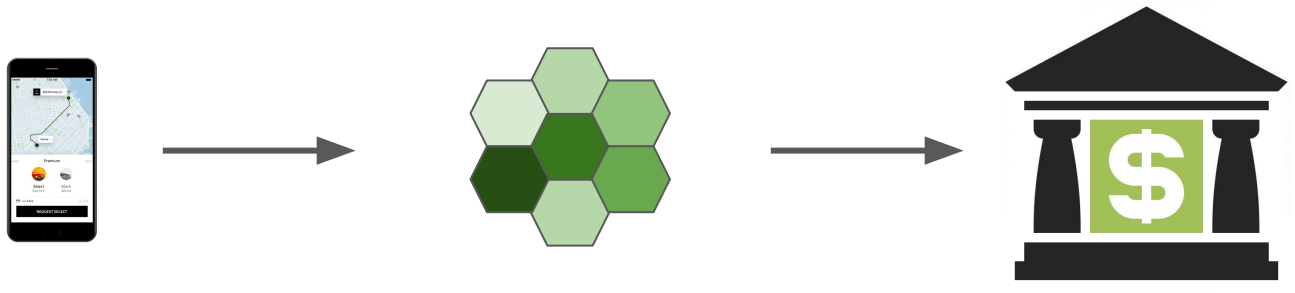
In this tutorial:

1. Why probabilistic machine learning?
2. Building a probabilistic regression model in Pyro
3. Approximate inference in Bayesian regression with SVI and MCMC
4. Pros and cons of SVI vs MCMC: subsampling, bias

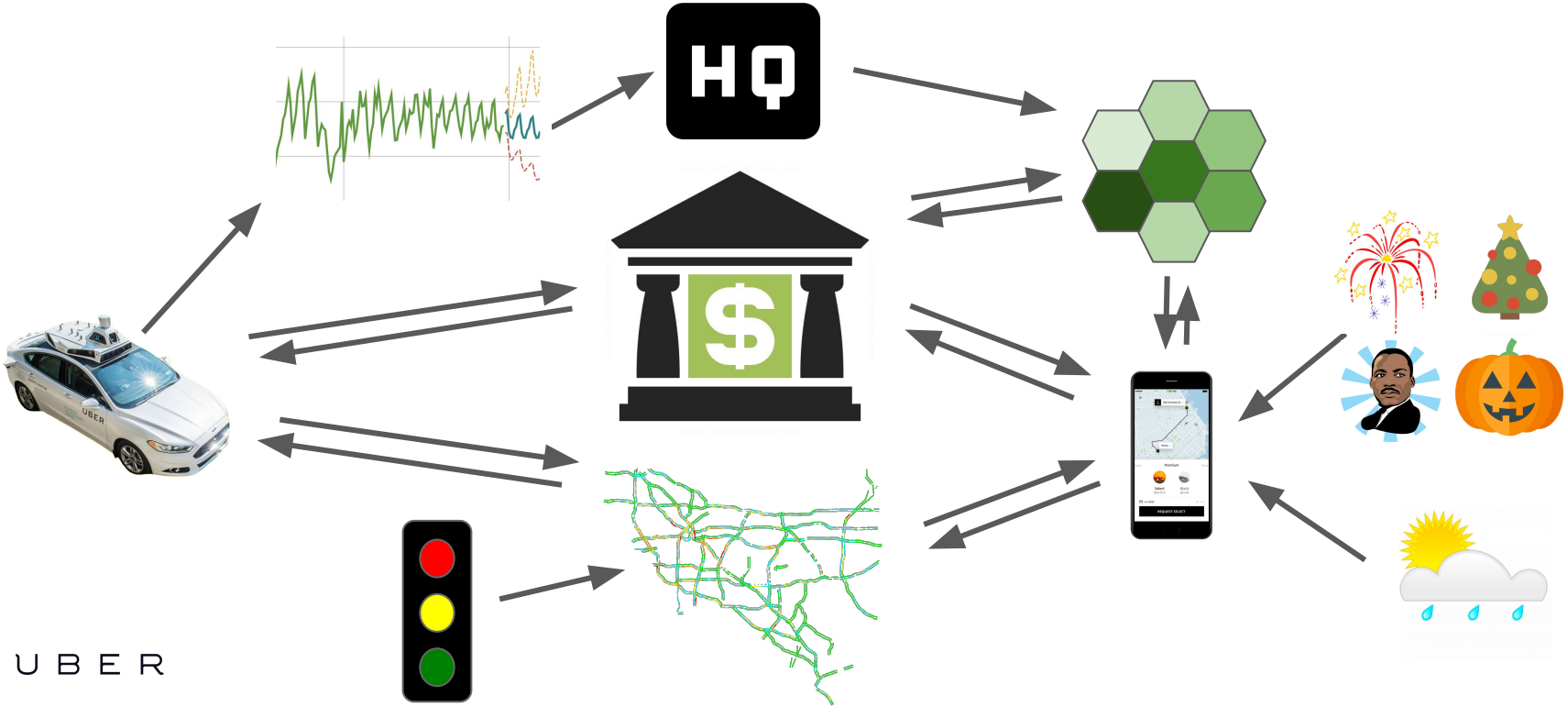
Based on the following Pyro tutorials:

- Bayesian regression 1: here
- Bayesian regression 2: http://pyro.ai/examples/bayesian_regression.html

Machine learning problems in theory



Machine learning problems in practice



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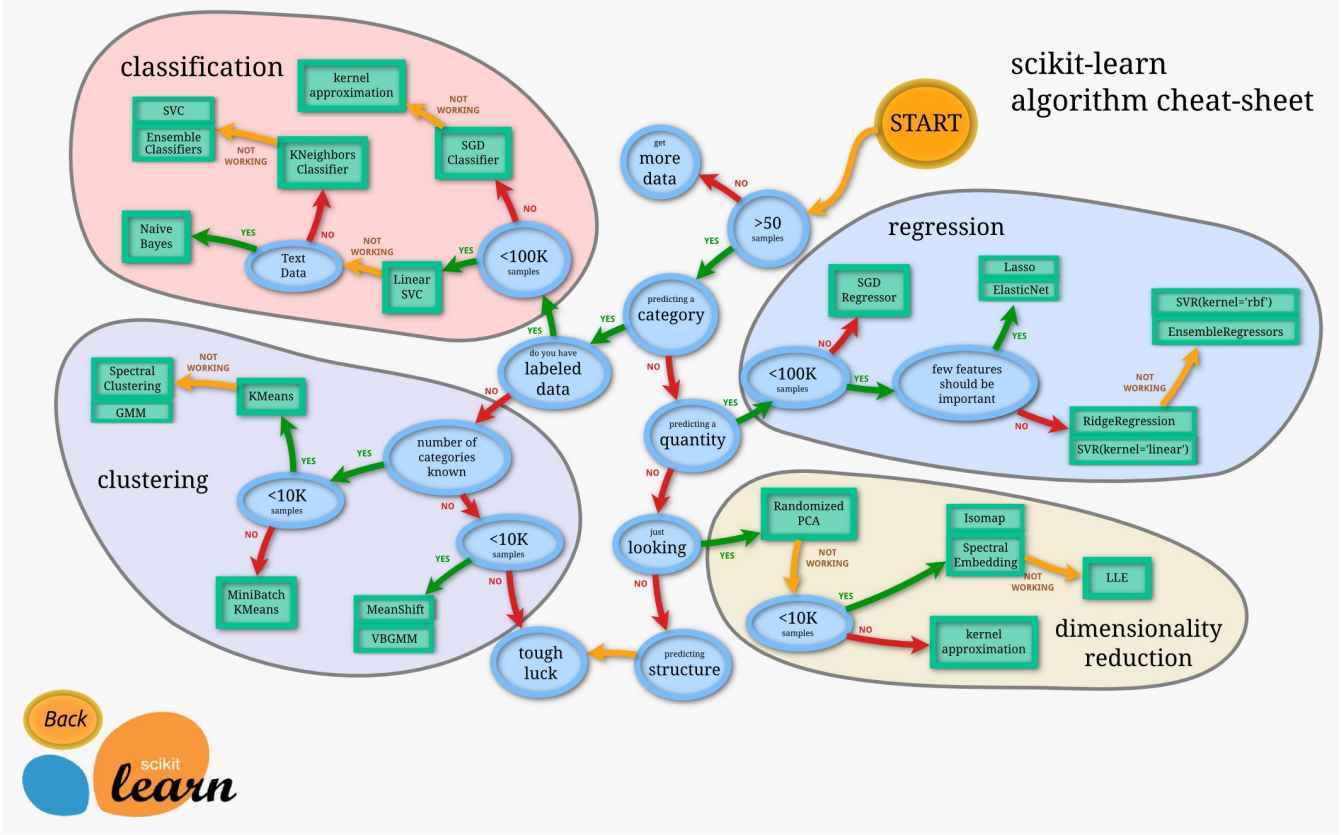
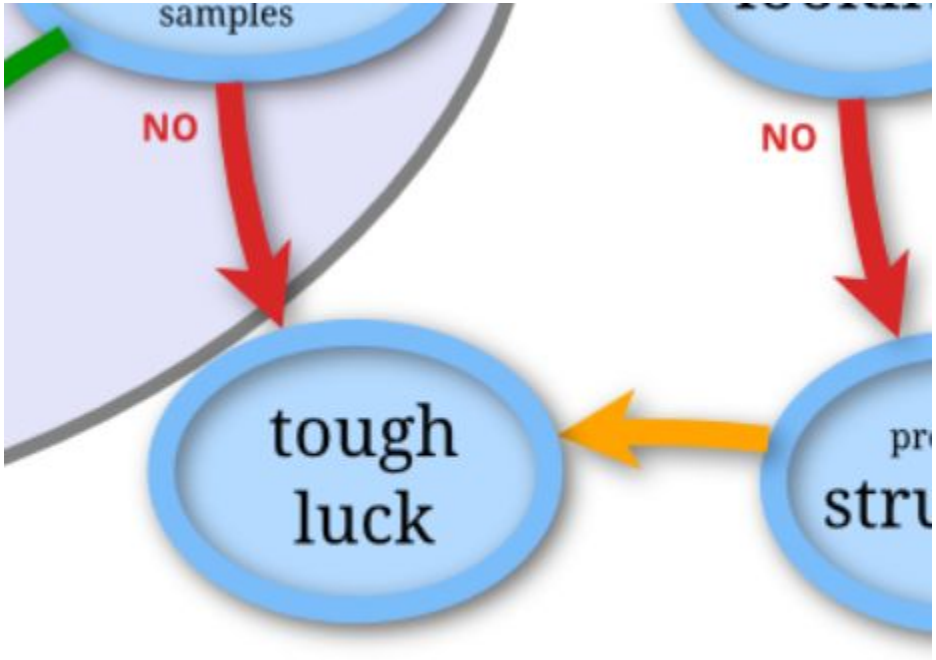
Machine learning solutions in practice



http://scikit-learn.org/stable/tutorial/machine_learning_map/index.html

Machine learning solutions in practice



Probabilistic Modeling and Inference

Unified account of generalization, regularization, unsupervised learning, calibrated uncertainty estimates, multitask/transfer learning, model composition, ...

Everything follows from two simple rules:

Sum rule: $P(x) = \sum_y P(x, y)$

Product rule: $P(x, y) = P(x)P(y|x)$

$$P(\theta|\mathcal{D}) = \frac{P(\mathcal{D}|\theta)P(\theta)}{P(\mathcal{D})}$$

$P(\mathcal{D}\|\theta)$	likelihood of θ
$P(\theta)$	prior probability of θ
$P(\theta\|\mathcal{D})$	posterior of θ given $\mathcal{D}$

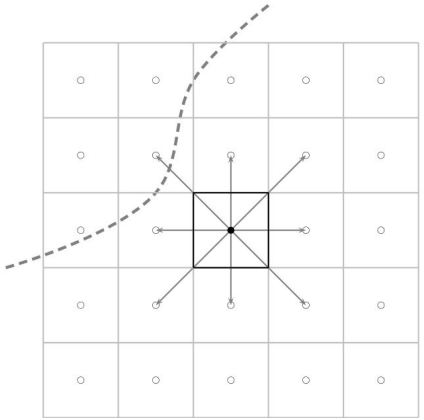
(h/t Zoubin)

Predicting GDP from terrain

Q: Did rugged terrain shield some African countries from the negative long-term economic effects of the slave trade?

We will attempt to estimate GDP in 2000 for African and non-African countries from a measure of terrain ruggedness

These predictions will necessarily have uncertainty, so we will use Bayesian linear regression



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McElreath, D., *Statistical Rethinking, Chapter 7*, 2016

Nunn, N. & Puga, D., *Ruggedness: The blessing of bad geography in Africa*

Probabilistic regression: model

We model expected log(GDP) as a linear function of terrain ruggedness and whether the country is in Africa or not:

```
def model(is_cont_africa, ruggedness):
    ...
    mu = a + b_a * is_cont_africa + b_r * ruggedness + \
        b_ar * is_cont_africa * ruggedness
    ...
```

Probabilistic regression: model

We model the data as drawn from a `Normal` around the predicted mean:

```
def model(is_cont_africa, ruggedness):
    ...
    mu = a + b_a * is_cont_africa + b_r * ruggedness + \
        b_ar * is_cont_africa * ruggedness
    return pyro.sample("obs", Normal(mu, sigma))
```

Probabilistic regression: model

We put simple, independent priors on all regression coefficients:

```
def model(is_cont_africa, ruggedness):
    a = pyro.sample("a", Normal(8., 1000.))
    b_a = pyro.sample("bA", Normal(0., 1.))
    b_r = pyro.sample("bR", Normal(0., 1.))
    b_ar = pyro.sample("bAR", Normal(0., 1.))
    sigma = pyro.sample("sigma", Uniform(0., 10.))

    mu = a + b_a * is_cont_africa + b_r * ruggedness + \
        b_ar * is_cont_africa * ruggedness

    ...
```

Probabilistic regression: “mean-field” guide

An especially simple guide: an independent `Normal` for each latent variable:

```
def guide(is_cont_africa, ruggedness, data):
    ...
    loc_a = pyro.param("loc_a", ...)
    scale_a = pyro.param("scale_a", ...)
    a = pyro.sample("a", Normal(loc_a, scale_a))
    ...
    sigma_dist = Normal(...)
    sigma = pyro.sample("sigma", sigma_dist)
```

Inference as optimization: understanding the ELBO

We want a loss function that is always non-negative and is zero when our guide q(**z**) is equal to the true posterior p(**z** | x):

$$\mathcal{L}(q_\phi(\mathbf{z}), p(\mathbf{z}|x)) \geq 0 \qquad \mathcal{L}(p(\mathbf{z}|x), p(\mathbf{z}|x)) = 0$$

One such loss function is the KL divergence:

$$\mathrm{KL}(q_\phi(\mathbf{z})||p(\mathbf{z}|x)) = \mathbb{E}_q[\log q_\phi(\mathbf{z}) - \log p(\mathbf{z}|x)]$$

Inference as optimization: understanding the ELBO

Evaluating the KL divergence requires knowing the true posterior p(**z** | x). Instead we use an approximation that only requires evaluating p(x, **z**):

$$\begin{aligned}\mathrm{ELBO} &= \mathbb{E}_q[\log p(x, \mathbf{z}) - \log q_\phi(\mathbf{z})] \\ &= C - \mathrm{KL}(q_\phi(\mathbf{z}) || p(\mathbf{z}|x))\end{aligned}$$

Because the constant C does not depend on the guide, maximizing the ELBO minimizes the KL between guide q(**z**) and true posterior p(**z** | x)

Inference as optimization: training the guide with SVI

```
svi = SVI(conditioned_model,
          guide,
          Adam({"lr": .005}),
          loss=Trace_ELBO())


...
for i in range(10000):
    svi.step(is_cont_africa, ruggedness, log_gdp)
```

MCMC in Pyro: Hamiltonian Monte Carlo (HMC)

Pyro provides a No U-Turn Sampler MCMC kernel (as in Stan, PyMC3) for scalable, asymptotically unbiased inference:

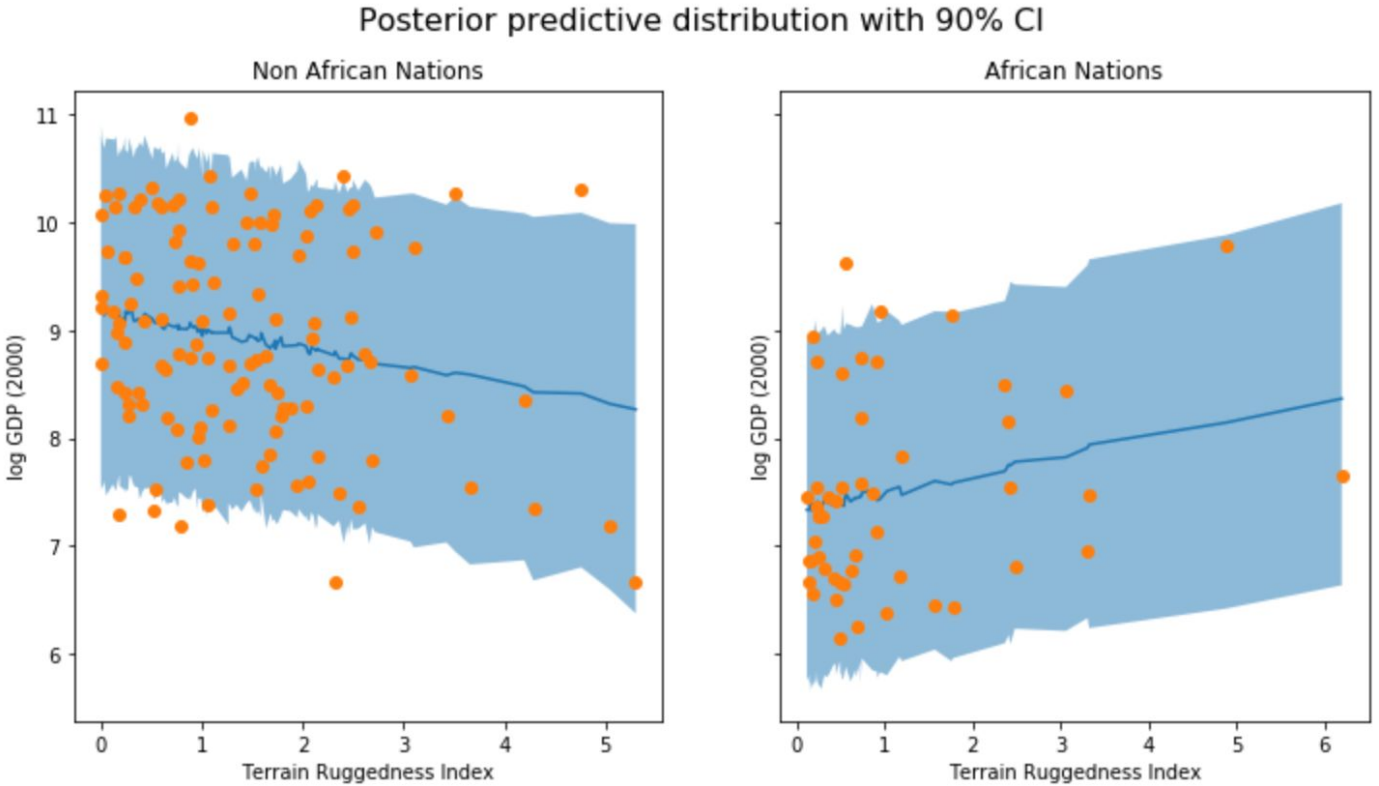
```
nuts_kernel = pyro.infer.NUTS(conditioned_model, adapt_step_size=True)
```

We apply the kernel and save the results with `pyro.infer.MCMC`

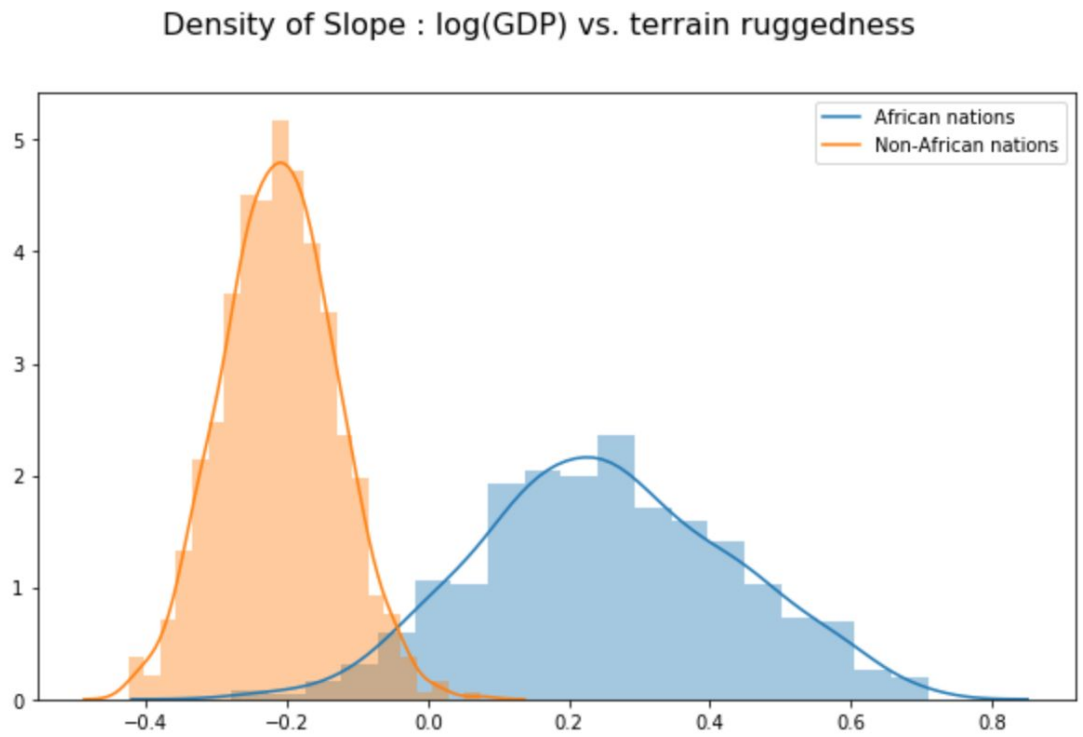
```
hmc_posterior = pyro.infer.MCMC(nuts_kernel,
                                num_samples=1000,
                                warmup_steps=200)

hmc_posterior = hmc_posterior.run(is_cont_africa, ruggedness, log_gdp)
```

Bayesian regression: results with HMC



Bayesian regression: results with HMC



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SVI vs MCMC: subsampling

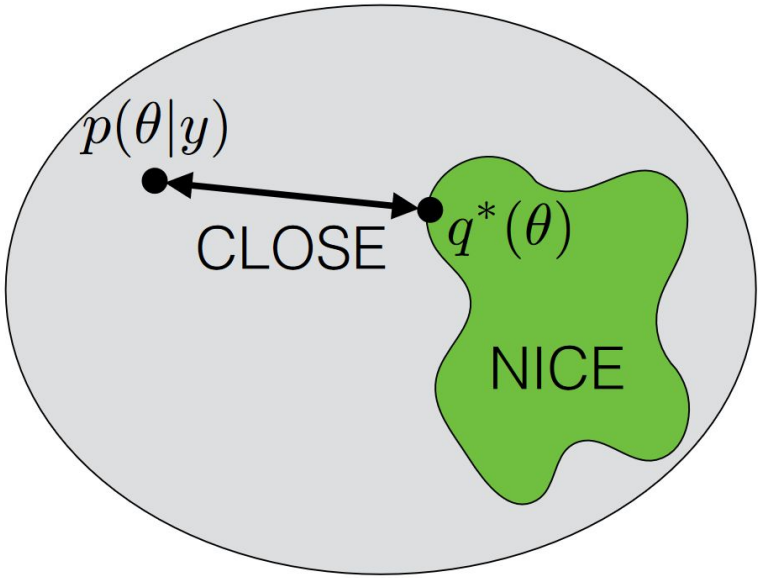
In SVI, we can subsample latent and observed variables with `pyro.iarange` which randomly samples a set of indices and rescales probabilities:

```
def subsample_model(is_cont_africa, ruggedness, data):
    a = pyro.sample("a", dist.Normal(8., 1000.))
    ...
    with pyro.iarange("data", len(ruggedness), subsample_size=1) as ix:
        pyro.sample("obs", dist.Normal(mu, sigma), obs=data[ix])
```

With subsampling, we can apply SVI to much larger models and data

SVI vs MCMC: biased approximation

Our parameterized family of guides may not include the true posterior:



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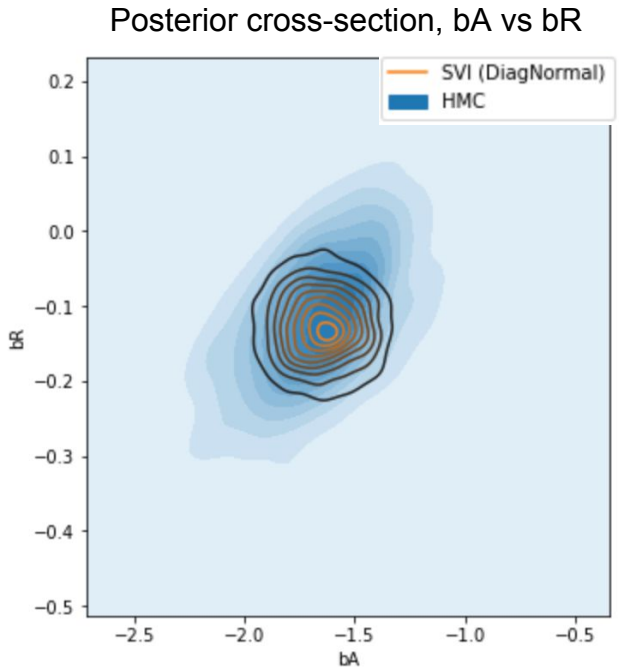
Variational Bayes and Beyond: Bayesian Inference for Big Data, Broderick, T.

SVI vs MCMC: biased approximation and underdispersion

Variational inference with simple guides underestimates posterior uncertainty...



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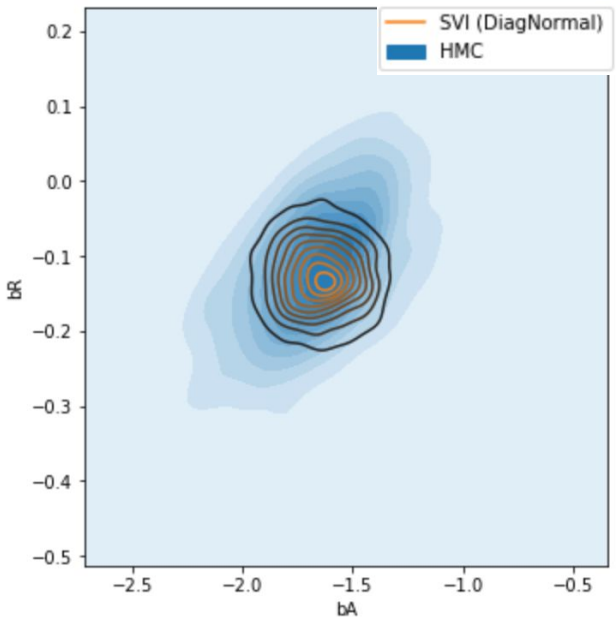
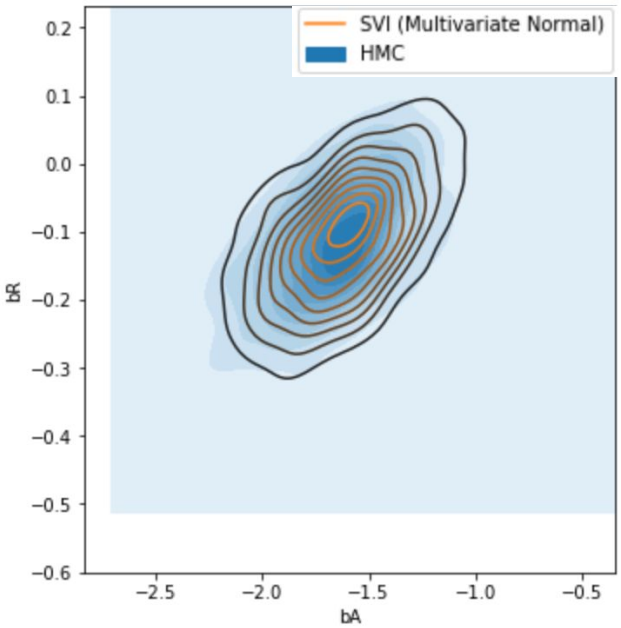
SVI vs MCMC: mitigating underdispersion

...but more expressive guides may do a better job of reducing this bias:

Posterior cross-section, bA vs bR



Posterior cross-section, bA vs bR



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Recap

1. A case for probabilistic machine learning
2. Built a probabilistic regression model in Pyro
3. Approximate inference in Bayesian regression with SVI and MCMC
4. Pros and cons of SVI vs MCMC: subsampling, bias

Coming up: using Pyro to build and learn powerful black-box generative models based on deep neural networks

pyro.ai

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Du Phan

Would you like to know more?

Pyro tutorials web page: http://pyro.ai/examples/index.html

Another walkthrough of Bayesian regression with SVI using advanced Pyro features:

http://pyro.ai/examples/bayesian_regression.html

A more complicated regression example demonstrating both SVI and MCMC:

https://github.com/uber/pyro/tree/dev/examples/eight_schools

Pyro MCMC, HMC, and NUTS documentation:

http://docs.pyro.ai/en/0.2.1-release/mcmc.html

Constraining parameters and guides in SVI

In SVI, we must ensure that all ELBO terms are finite:

$$\mathrm{ELBO} \equiv \mathbb{E}_{q_\phi(\mathbf{z})}\left[\log p_\theta(\mathbf{x}, \mathbf{z}) - \log q_\phi(\mathbf{z})\right]$$

Constraining parameter values in SVI

Parameters of distributions must be in the right range, assisted by `torch.distributions.constraints`

```
def guide(is_cont_africa, ruggedness, data):
    ...
    loc_a = pyro.param("loc_a")
    scale_a = pyro.param("scale_a", constraint=constraints.positive)
    a = pyro.sample("a", Normal(loc_a, scale_a))
    ...
```

Matching random variable supports in SVI

Distribution pairs in models and guides must have the same support, assisted by `torch.distributions.biject_to` and `TransformedDistribution`

```
def guide(is_cont_africa, ruggedness, data):
    ...
    sigma_transform = torch.distributions.biject_to(constraints.positive)
    sigma_dist = TransformedDistribution(Normal(...), sigma_transform)
    sigma = pyro.sample("sigma", sigma_dist)
```