

Lec 19 - PyMC3 + ArviZ

Statistical Computing and Computation

Sta 663 | Spring 2022

Dr. Colin Rundel

pymc3 + ArviZ

PyMC3 is a probabilistic programming package for Python that allows users to fit Bayesian models using a variety of numerical methods, most notably Markov chain Monte Carlo (MCMC) and variational inference (VI). Its flexibility and extensibility make it applicable to a large suite of problems. Along with core model specification and fitting functionality, PyMC3 includes functionality for summarizing output and for model diagnostics.

ArviZ is a Python package for exploratory analysis of Bayesian models. Includes functions for posterior analysis, data storage, sample diagnostics, model checking, and comparison. The goal is to provide backend-agnostic tools for diagnostics and visualizations of Bayesian inference in Python, by first converting inference data into xarray objects.

```
import pymc3 as pm  
import arviz as az
```

Model basics

All models are derived from the `Model()` class, unlike what we have seen previously PyMC makes heavy use of Python's context manager using the `with` statement to add model components to a model.

```
with pm.Model() as norm:  
    x = pm.Normal("x", mu=0, sigma=1)
```

```
x = pm.Normal("x", mu=0, sigma=1)
```

```
## TypeError: No model on context stack, which is needed to instantiate distributions. Add variable inside a 'w
```

Additional components can be added to an existing model via additional `with` statements (only the first needs `pm.Model()`)

```
with norm:  
    y = pm.Normal("y", mu=x, sigma=1, shape=3)
```

```
norm.vars
```

Random Variables

`pm.Normal()` is an example of a PyMC distribution, which are used to construct models, these are implemented using the `FreeRV` class which is used for all of the builtin distributions (and can be used to create custom distributions). Some useful methods and attributes,

```
norm.x.dshape
```

```
## ()
```

```
norm.x.dsize
```

```
## 1
```

```
norm.x.distribution
```

```
## <pymc3.distributions.continuous.Normal object at
```

```
norm.x.init_value
```

```
## array(0.)
```

```
norm.model
```

```
norm.x.random()
```

```
## array(0.94831)
```

```
norm.y.random()
```

```
## array([ 0.65532,  0.0627 , -0.94107])
```

```
norm.x.logp({"x": 0, "y": [0,0,0]})
```

```
## array(-0.91894)
```

```
norm.y.logp({"x": 0, "y": [0,0,0]})
```

```
## array(-2.75682)
```

```
norm.logp({"x": 0, "y": [0,0,0]})
```

Variable heirarchy

Note that we defined $y| x \sim N(x, 1)$, so what is happening when we use `norm.y.random()`?

```
norm.y.random()  
  
## array([-0.05382,  0.27083,  1.12145])  
  
obs = norm.y.random(size=1000)  
np.mean(obs)  
  
## 0.017603505100856152  
  
np.var(obs)  
  
## 2.0796380254179776  
  
np.std(obs)  
  
## 1.442095012618093
```

Each time we ask for a draw from `y`, PyMC is first drawing from `x` for us.

Beta-Binomial model

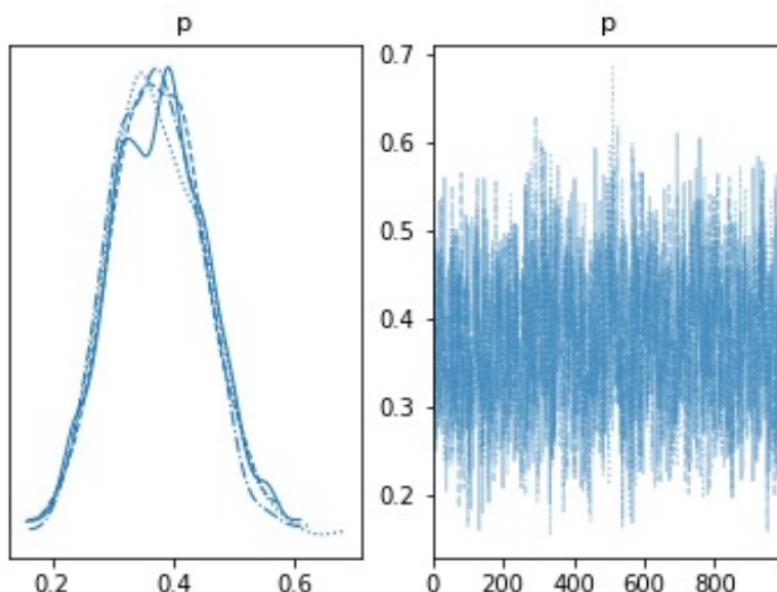
We will now build a basic model where we know what the solution should look like and compare the results.

```
with pm.Model() as beta_binom:  
    p = pm.Beta("p", alpha=10, beta=10)  
    x = pm.Binomial("x", n=20, p=p, observed=5)
```

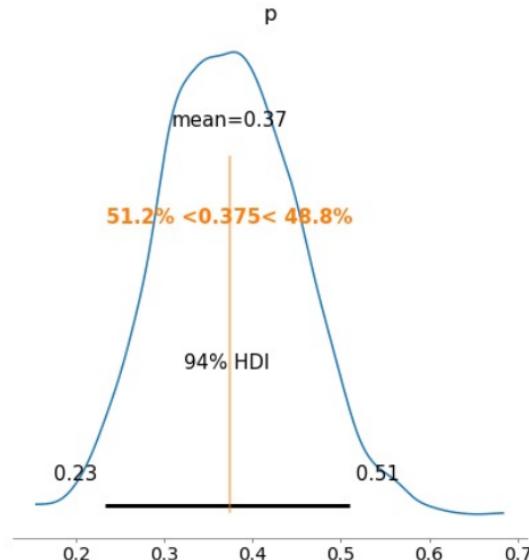
In order to sample from the posterior we add a call to `sample()` within the model context.

```
with beta_binom:  
    trace = pm.sample(return_inferencedata=True, random_seed=1234)  
  
## █  
## Auto-assigning NUTS sampler...  
## Initializing NUTS using jitter+adapt_diag...  
## Multiprocess sampling (4 chains in 4 jobs)  
## NUTS: [p]  
## Sampling 4 chains for 1_000 tune and 1_000 draw iterations (4_000 + 4_000 draws total) took 6 seconds.
```

```
ax = az.plot_trace(trace, figsize=(6,4))  
plt.show()
```



```
ax = az.plot_posterior(trace, ref_val=[15/40])  
plt.show()
```



```
p = np.linspace(0, 1, 100)
post_beta = scipy.stats.beta.pdf(p,15,25)

ax = az.plot_posterior(trace, hdi_prob="hide", point_estimate=None)
plt.plot(p,post_beta, "-k", alpha=0.5, label="Theoretical")
plt.legend(['PyMC NUTS', 'Theoretical'])
plt.show()
```



InferenceData results

```
print(trace)

## Inference data with groups:
##   > posterior
##   > log_likelihood
##   > sample_stats
##   > observed_data

print(type(trace))

## <class 'arviz.data.inference_data.InferenceData'>
```

xarray: N-D labeled arrays and datasets in Python

xarray (formerly xray) is an open source project and Python package that makes working with labelled multi-dimensional arrays simple, efficient, and fun!

Xarray introduces labels in the form of dimensions, coordinates and attributes on top of raw NumPy-like arrays, which allows for a more intuitive, more concise, and less error-prone developer experience. The package includes a large and growing library of domain-agnostic functions for advanced analytics and visualization with these data structures.

Xarray is inspired by and borrows heavily from pandas, the popular data analysis package focused on labelled tabular

```
print(trace.posterior)

## <xarray.Dataset>
## Dimensions: (chain: 4, draw: 1000)
## Coordinates:
##   * chain      (chain) int64 0 1 2 3
##   * draw       (draw) int64 0 1 2 3 4 5 6 7 8 ... 992 993 994 995 996 997 998 999
## Data variables:
##   p          (chain, draw) float64 0.4051 0.4491 0.4985 ... 0.353 0.3691 0.3691
## Attributes:
##   created_at:           2022-03-18T17:47:37.298366
##   arviz_version:        0.11.4
##   inference_library:    pymc3
##   inference_library_version: 3.11.5
##   sampling_time:        5.83094596862793
##   tuning_steps:         1000

print(trace.posterior["p"].shape)

## (4, 1000)

print(trace.sel(chain=0).posterior["p"].shape)

## (1000,)

print(trace.sel(draw=slice(500, None, 10)).posterior["p"].shape)
```

As DataFrame

Posterior values, or subsets, can be converted to DataFrames via the `to_dataframe()` method

```
trace.posterior.to_dataframe()
```

```
##                  p
## chain draw
## 0      0    0.405115
## 1      0    0.449149
## 2      0    0.498481
## 3      0    0.522682
## 4      0    0.346336
## ...
## 3     995   0.380507
## 996   0.404883
## 997   0.353017
## 998   0.369109
## 999   0.369109
##
## [4000 rows x 1 columns]
```

```
trace.posterior["p"][:, :].to_dataframe()
```

```
##      chain      p
## draw
## 0      0    0.405115
## 1      0    0.449149
## 2      0    0.498481
## 3      0    0.522682
## 4      0    0.346336
## ...
## 995   0    0.463122
## 996   0    0.437503
## 997   0    0.437503
## 998   0    0.339669
## 999   0    0.393476
##
## [1000 rows x 2 columns]
```

MultiTrace results

```
with beta_binom:  
    mt = pm.sample(random_seed=1234)  
  
## [1]   
## FutureWarning: In v4.0, pm.sample will return an `arviz.InferenceData` object instead of a `MultiTrace` by default.  
# You can pass return_inferencedata=True or return_inferencedata=False to be safe and silence this warning.  
##     return wrapped_(*args_, **kwargs_)  
## Auto-assigning NUTS sampler...  
## Initializing NUTS using jitter+adapt_diag...  
## Multiprocess sampling (4 chains in 4 jobs)  
## NUTS: [p]  
## Sampling 4 chains for 1_000 tune and 1_000 draw iterations (4_000 + 4_000 draws total) took 5 seconds.  
  
mt  
  
## <MultiTrace: 4 chains, 1000 iterations, 2 variables>  
  
type(mt)  
  
## <class 'pymc3.backends.base.MultiTrace'>
```

```
ax = az.plot_trace(mt, figsize=(6,4))

## Got error No model on context stack. trying to find log_likelihood in translation.
## FutureWarning: Using `from_pymc3` without the model will be deprecated in a future release. Not using the model argument will return less accurate and less useful results. Make sure you use the model argument or call from_pymc3 within the context.
##     warnings.warn(
## Got error No model on context stack. trying to find log_likelihood in translation.

plt.show()
```

```
with beta_binom:  
    ax = az.plot_trace(mt, figsize=(6,4))  
plt.show()
```



Working with MultiTrace

```
mt['p']
```

```
## array([0.40512, 0.44915, 0.49848, 0.52268, 0.34634, 0.33228, 0.2552 , 0.34267, 0.24986, 0.38481, 0.39414, 0.4012 , 0.42459, 0.3994 , 0.38614, 0.49096, 0.4057 , 0.40255, 0.43986, 0.40974, ## 0.53249, 0.44479, 0.29335, 0.48019, 0.41937, 0.38748, 0.37968, 0.26982, 0.27831, ..., 0.46317, 0.50399, 0.37687, 0.25664, 0.34679, 0.53207, 0.56233, 0.39998, 0.39998, 0.35253, 0.22216, ## 0.54898, 0.44927, 0.48805, 0.27699, 0.27699, 0.27699, 0.30037, 0.23423, 0.27166, 0.31804, 0.24879, 0.36096, 0.367 , 0.38051, 0.40488, 0.35302, 0.36911, 0.36911])
```

```
mt['p'].shape
```

```
## (4000,)
```

```
mt['p', 500: ].shape
```

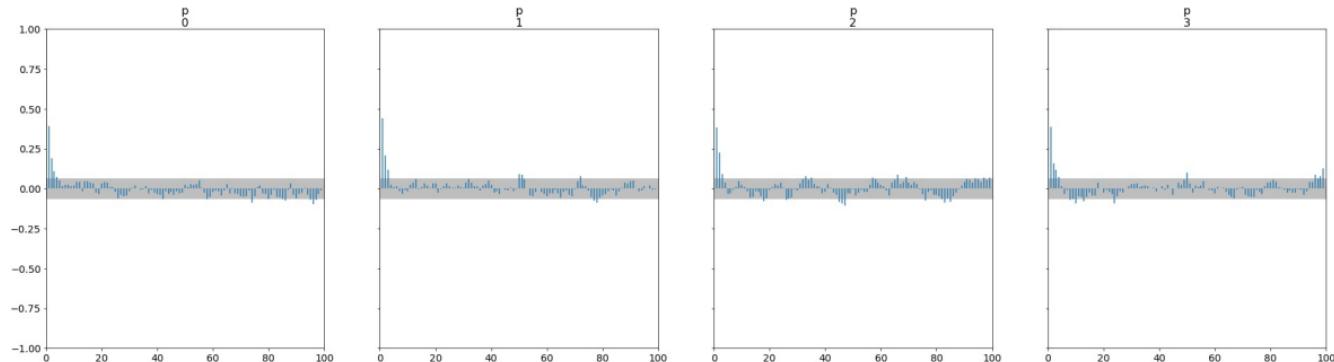
```
## (2000,)
```

```
mt.get_values(varname="p", burn=500, thin=10, chains=[0,1]).shape
```

```
## (100,)
```

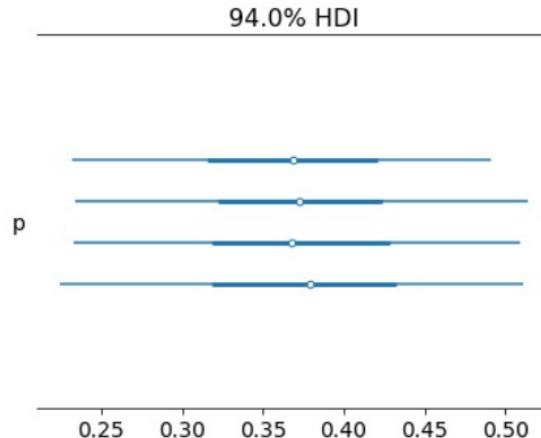
Autocorrelation plots

```
ax = az.plot_autocorr(trace)
plt.show()
```



Forrst plots

```
ax = az.plot_forest(trace)
plt.show()
```



Other useful diagnostics

Standard MCMC diagnostic statistics are available via `summary()` from ArviZ

```
az.summary(trace)
```

```
##      mean      sd hdi_3% hdi_97% mcse_mean mcse_sd ess_bulk ess_tail r_hat
## p  0.374  0.076  0.232   0.509     0.002    0.001   1596.0   2654.0   1.0
```

individual methods are available for each statistics,

```
print(az.ess(trace, method="bulk"))
```

```
## <xarray.Dataset>
## Dimensions: ()
## Data variables:
##     p      float64 1.596e+03
```

```
print(az.ess(trace, method="tail"))
```

```
## <xarray.Dataset>
## Dimensions: ()
## Data variables:
##     p      float64 2.654e+03
```

```
print(az.rhat(trace))
```

```
## <xarray.Dataset>
## Dimensions: ()
## Data variables:
##     p      float64 1.001
```

```
print(az.mcse(trace))
```

```
## <xarray.Dataset>
## Dimensions: ()
## Data variables:
##     p      float64 0.001905
```

Demo 1 - Linear regression

Given the below data, we will fit a linear regression model to the following synthetic data,

```
np.random.seed(1234)
n = 11
m = 6
b = 2
x = np.linspace(0, 1, n)
y = m*x + b + np.random.randn(n)
```

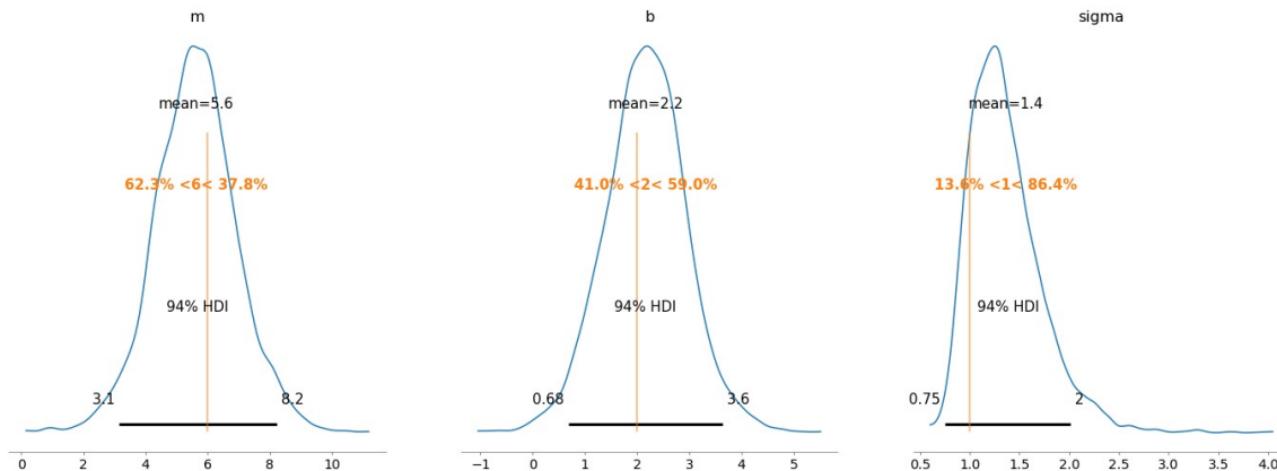
Model

```
with pm.Model() as lm:  
    m = pm.Normal('m', mu=0, sd=50)  
    b = pm.Normal('b', mu=0, sd=50)  
    sigma = pm.HalfNormal('sigma', sd=5)  
  
    likelihood = pm.Normal('y', mu=m*x + b, sd=sigma, observed=y)  
  
    trace = pm.sample(return_inferencedata=True, random_seed=1234)  
  
## █  
## Auto-assigning NUTS sampler...  
## Initializing NUTS using jitter+adapt_diag...  
## Multiprocess sampling (4 chains in 4 jobs)  
## NUTS: [sigma, b, m]  
## Sampling 4 chains for 1_000 tune and 1_000 draw iterations (4_000 + 4_000 draws total) took 6 seconds.  
## There was 1 divergence after tuning. Increase `target_accept` or reparameterize.  
  
az.summary(trace)  
  
##          mean      sd  hdi_3%  hdi_97%  mcse_mean  mcse_sd  ess_bulk  ess_tail  r_hat  
## m      5.620  1.327  3.145   8.235     0.037    0.026   1325.0   1519.0   1.0  
## b      2.157  0.783  0.682   3.638     0.022    0.016   1268.0   1392.0   1.0  
## sigma  1.363  0.369  0.754   2.013     0.009    0.007   1440.0   1461.0   1.0
```

```
ax = az.plot_trace(trace)
plt.show()
```



```
ax = az.plot_posterior(trace, ref_val=[6,2,1])  
plt.show()
```



```
plt.scatter(x, y, s=30, label='data')

post_m = trace.posterior['m'][0, -500:]
post_b = trace.posterior['b'][0, -500:]

plt.figure(layout="constrained")
plt.scatter(x, y, s=30, label='data')
for m, b in zip(post_m.values, post_b.values):
    plt.plot(x, m*x + b, c='gray', alpha=0.1)
plt.plot(x, 6*x + 2, label='true regression line', lw=3., c='red')
plt.legend(loc='best')
plt.show()
```

Posterior Predictive

```
with lm:  
    pp = pm.sample_posterior_predictive(trace, samples=200)  
  
## █  
## UserWarning: samples parameter is smaller than nchains times ndraws, some draws and/or chains may not be rep  
    in the returned posterior predictive sample  
##     warnings.warn(  
  
pp['y'].shape  
  
## (200, 11)
```

```
plt.figure(layout="constrained")
plt.plot(x, pp['y'].T, c="grey", alpha=0.1)
plt.scatter(x, y, s=30, label='data')
plt.show()
```

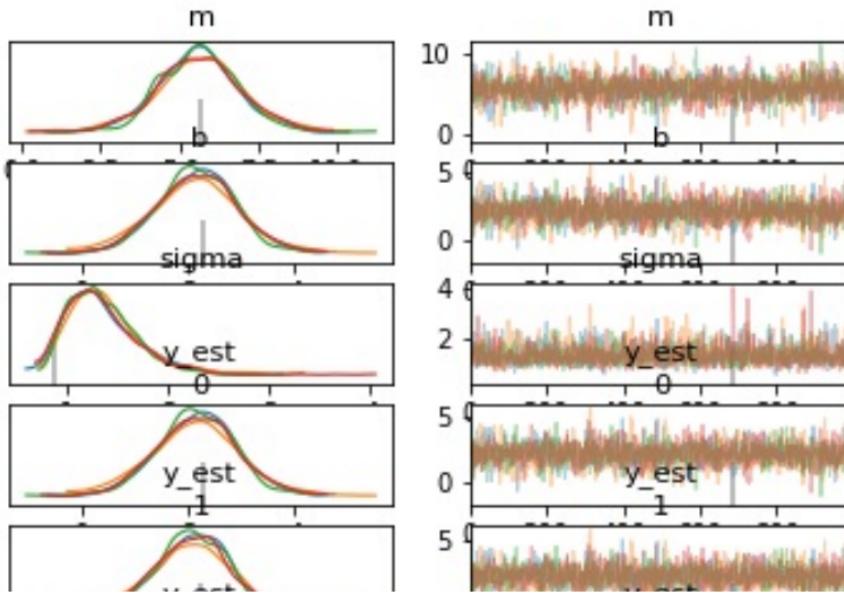


Model revision

```
with pm.Model() as lm2:  
    m = pm.Normal('m', mu=0, sd=50)  
    b = pm.Normal('b', mu=0, sd=50)  
    sigma = pm.HalfNormal('sigma', sd=5)  
  
    y_est = pm.Deterministic("y_est", m*x + b)  
  
    likelihood = pm.Normal('y', mu=y_est, sd=sigma, observed=y)  
  
    trace = pm.sample(return_inferencedata=True, random_seed=1234)  
    pp = pm.sample_posterior_predictive(trace, var_names=["y_est"], samples=200)
```

```
## [REDACTED]  
## Auto-assigning NUTS sampler...  
## Initializing NUTS using jitter+adapt_diag...  
## Multiprocess sampling (4 chains in 4 jobs)  
## NUTS: [sigma, b, m]  
## Sampling 4 chains for 1_000 tune and 1_000 draw iterations (4_000 + 4_000 draws total) took 6 seconds.  
## There was 1 divergence after tuning. Increase `target_accept` or reparameterize.  
## UserWarning: samples parameter is smaller than nchains times ndraws, some draws and/or chains may not be rep  
    in the returned posterior predictive sample  
##     warnings.warn(
```

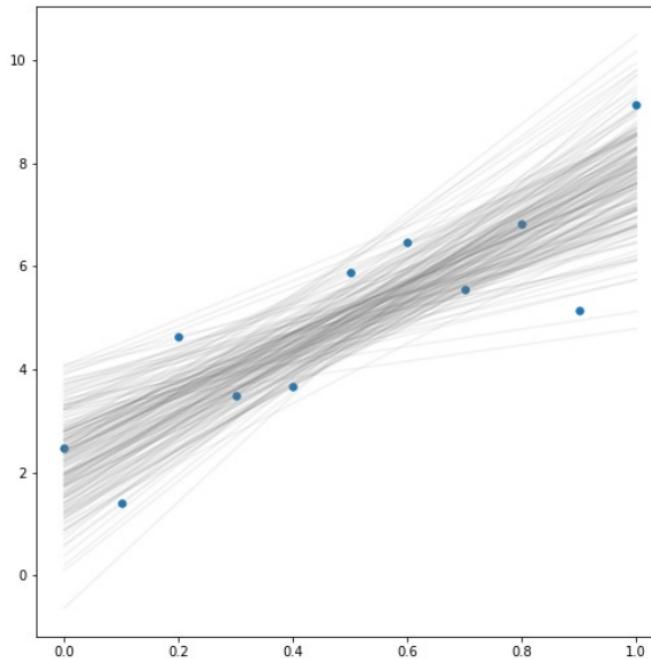
```
plt.figure(layout="constrained")
ax = az.plot_trace(trace, compact=False, figsize=(6,12))
plt.show()
```



```
pp['y_est'].shape
```

```
## (200, 11)
```

```
plt.figure(layout="constrained")
plt.plot(x, pp['y_est'].T, c="grey", alpha=0.1)
plt.scatter(x, y, s=30, label='data')
plt.show()
```



Demo 2 - Bayesian Lasso

```
n = 50
k = 100

np.random.seed(1234)
X = np.random.normal(size=(n, k))

beta = np.zeros(shape=k)
beta[[10, 30, 50, 70]] = 10
beta[[20, 40, 60, 80]] = -10

y = X @ beta + np.random.normal(size=n)
```

Naive Model

```
with pm.Model() as bayes_lasso:  
    b = pm.Laplace("beta", 0, 1, shape=k)#lam*tau, shape=k)  
    y_est = X @ b  
    s = pm.HalfNormal('sigma', sd=1)  
  
    likelihood = pm.Normal("y", mu=y_est, sigma=s, observed=y)  
  
    trace = pm.sample(return_inferencedata=True, random_seed=1234)  
  
## █  
## Auto-assigning NUTS sampler...  
## Initializing NUTS using jitter+adapt_diag...  
## Multiprocess sampling (4 chains in 4 jobs)  
## NUTS: [sigma, beta]  
## Sampling 4 chains for 1_000 tune and 1_000 draw iterations (4_000 + 4_000 draws total) took 18 seconds.  
## There were 2 divergences after tuning. Increase `target_accept` or reparameterize.  
## The acceptance probability does not match the target. It is 0.878942077718847, but should be close to 0.8. T  
increase the number of tuning steps.  
## The estimated number of effective samples is smaller than 200 for some parameters.
```

```
az.summary(trace)
```

```
##          mean      sd hdi_3% hdi_97% mcse_mean mcse_sd ess_bulk ess_tail r_hat
## beta[0]  0.067  0.861 -1.650   1.681    0.015   0.015  3234.0  1938.0  1.00
## beta[1]  0.215  0.729 -1.133   1.693    0.012   0.013  3632.0  2284.0  1.00
## beta[2] -0.080  0.852 -1.789   1.501    0.014   0.015  3866.0  2652.0  1.00
## beta[3] -0.290  0.814 -1.926   1.193    0.016   0.015  2870.0  1729.0  1.00
## beta[4]  0.079  0.809 -1.479   1.691    0.014   0.014  3577.0  2158.0  1.00
## ...
## ...
## ...
## ...
## beta[96]  0.106  0.726 -1.271   1.542    0.013   0.013  3471.0  2487.0  1.00
## beta[97] -0.156  0.716 -1.591   1.160    0.013   0.013  3188.0  1798.0  1.00
## beta[98]  0.289  0.763 -1.076   1.827    0.014   0.015  3107.0  2408.0  1.00
## beta[99] -0.278  0.768 -1.747   1.205    0.013   0.013  3575.0  2568.0  1.00
## sigma    0.980  0.478  0.275   1.859    0.046   0.032  102.0   211.0  1.05
##
## [101 rows x 9 columns]
```

```
az.summary(trace).iloc[[0, 10, 20, 30, 40, 50, 60, 70, 80, 100]]
```

```
##          mean      sd hdi_3% hdi_97% mcse_mean mcse_sd ess_bulk ess_tail r_hat
## beta[0]  0.067  0.861 -1.650   1.681    0.015   0.015  3234.0  1938.0  1.00
## beta[10]  8.327 1.242   5.945  10.622    0.027   0.019  2075.0  2710.0  1.00
## beta[20] -8.288 1.335 -10.697  -5.733    0.030   0.021  2003.0  1746.0  1.00
## beta[30]  8.610 1.023   6.678  10.447    0.023   0.017  2011.0  1702.0  1.00
## beta[40] -8.765 1.507 -11.485  -5.929    0.030   0.022  2461.0  2531.0  1.00
## beta[50]  8.966 1.016   6.995  10.860    0.023   0.016  2035.0  1842.0  1.00
## beta[60] -9.248 1.121 -11.381  -7.162    0.022   0.015  2708.0  2371.0  1.00
```

```
ax = az.plot_forest(trace)
plt.tight_layout()
plt.show()
```



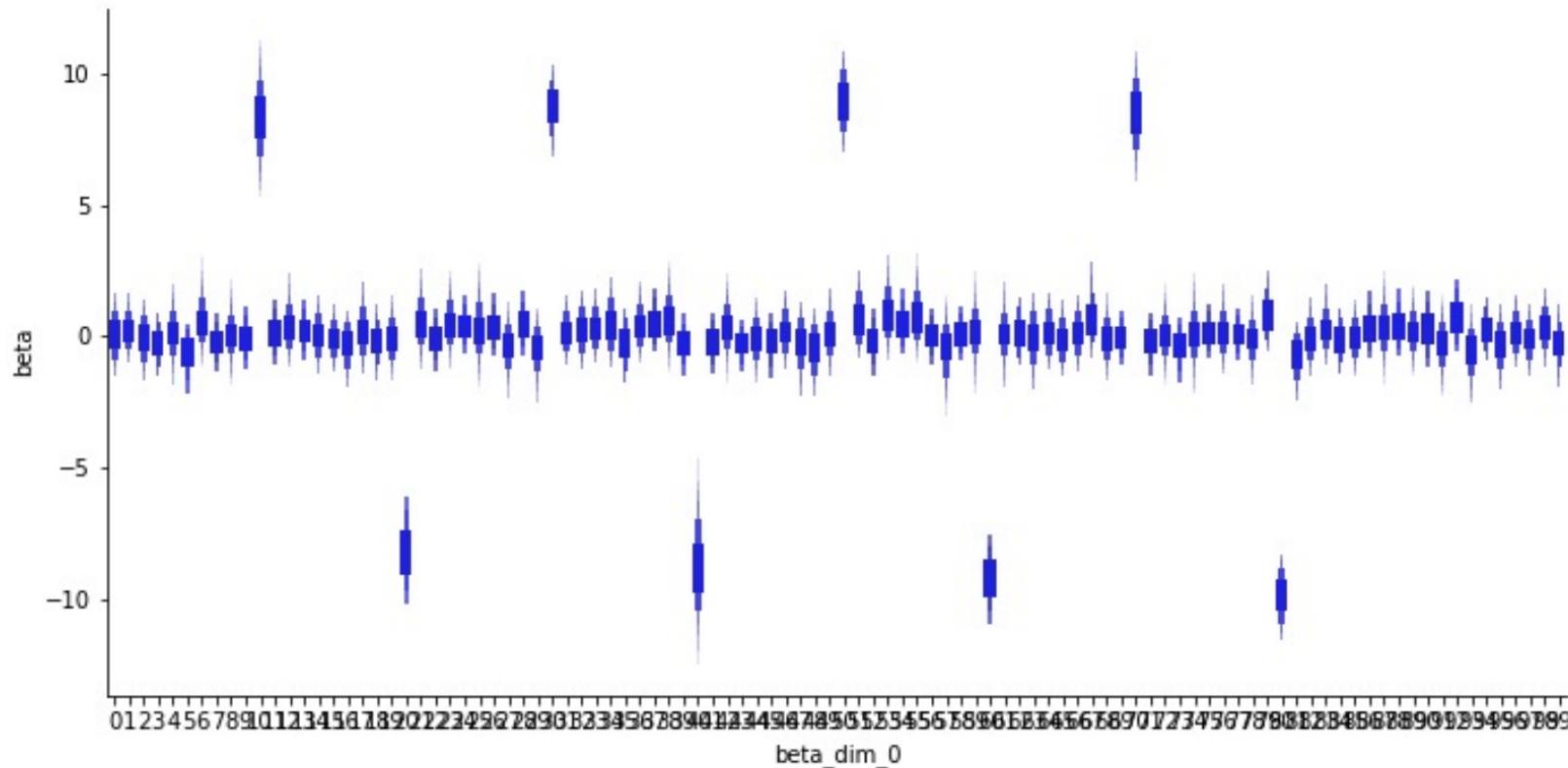
Plot helper

```
def plot_slope(trace, prior="beta", chain=0):
    post = (trace.posterior[prior]
            .to_dataframe()
            .reset_index()
            .query("chain == 0")
            )

    sns.catplot(x="beta_dim_0", y="beta", data=post, kind="boxen", linewidth=0, color='blue', aspect=2, show
    plt.tight_layout()
    plt.show()
```



```
plot_slope(trace)
```

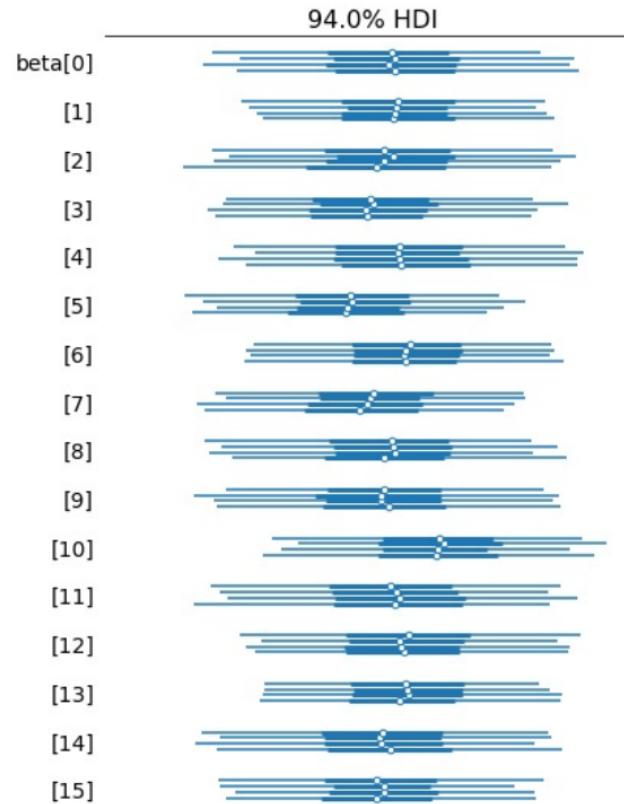


Weakly Informative Prior

```
with pm.Model() as bayes_weak:  
    b = pm.Normal("beta", 0, 10, shape=k)  
    y_est = X @ b  
  
    s = pm.HalfNormal('sigma', sd=2)  
  
    likelihood = pm.Normal("y", mu=y_est, sigma=s, observed=y)  
  
    trace = pm.sample(return_inferencedata=True, random_seed=12345)
```

```
##  
## Auto-assigning NUTS sampler...  
## Initializing NUTS using jitter+adapt_diag...  
## Multiprocess sampling (4 chains in 4 jobs)  
## NUTS: [sigma, beta]  
## Sampling 4 chains for 1_000 tune and 1_000 draw iterations (4_000 + 4_000 draws total) took 55 seconds.  
## The acceptance probability does not match the target. It is 0.9760397075294559, but should be close to 0.8.  
## increase the number of tuning steps.  
## The chain reached the maximum tree depth. Increase max_treedepth, increase target_accept or reparameterize.  
## There was 1 divergence after tuning. Increase 'target_accept' or reparameterize.  
## There were 15 divergences after tuning. Increase 'target_accept' or reparameterize.  
## The acceptance probability does not match the target. It is 0.7066410867916934, but should be close to 0.8.  
## increase the number of tuning steps.  
## There was 1 divergence after tuning. Increase 'target_accept' or reparameterize.
```

```
ax = az.plot_forest(trace)
plt.tight_layout()
plt.show()
```



```
plot_slope(trace)
```

