Zagatti HW04

May 18, 2022

1 Homework 03 - Sebastiano Zagatti

1.1 Exercise 1:

Let θ_1 and θ_2 be real valued parameters in [0,1] and consider the generative model

$$\begin{split} &\theta_1 \sim \theta_1\text{-prior} \\ &\theta_2 \sim \theta_2\text{-prior} \\ &\hat{y} = \frac{\theta_1 + x^2}{\theta_2 \cdot x} \\ &y \sim \mathcal{N}(\hat{y}, 1) \end{split}$$

- a. Use pyro to implement the model as a function model(theta1_prior, theta2_prior, x, obs), where theta1_prior and theta2_prior are pyro.distributions objects, x and obs are torch tensors, and draws from the normal distribution are conditioned on obs.
- b. Choose two suitable prior distributions for θ_1 and θ_2 (e.g. suitably rescaled Normal or Beta distributions) and use HMC or NUTS algorithm to find their posterior distributions given the observations

$$x = (47, 87, 20, 16, 38, 5)$$

 $y = (58.76, 108.75, 25.03, 20.03, 47.51, 6.37).$

c. Discuss how different prior distributions lead to different estimates of θ_1 and θ_2 . Comment on the convergence checks and plot the posterior distributions.

Solution

a. Pyro implementation of model:

[1]: |pip install pyro-ppl

Requirement already satisfied: pyro-ppl in /usr/local/lib/python3.7/dist-packages (1.8.1)

Requirement already satisfied: pyro-api>=0.1.1 in /usr/local/lib/python3.7/dist-packages (from pyro-ppl) (0.1.2)

Requirement already satisfied: torch>=1.11.0 in /usr/local/lib/python3.7/dist-packages (from pyro-ppl) (1.11.0+cu113)

Requirement already satisfied: numpy>=1.7 in /usr/local/lib/python3.7/dist-

```
packages (from pyro-ppl) (1.21.6)
Requirement already satisfied: tqdm>=4.36 in /usr/local/lib/python3.7/dist-packages (from pyro-ppl) (4.64.0)
Requirement already satisfied: opt-einsum>=2.3.2 in
/usr/local/lib/python3.7/dist-packages (from pyro-ppl) (3.3.0)
Requirement already satisfied: typing-extensions in
/usr/local/lib/python3.7/dist-packages (from torch>=1.11.0->pyro-ppl) (4.2.0)
```

```
[2]: import torch
import numpy as np
import random
import matplotlib.pyplot as plt
import seaborn as sns
import pyro
import pyro.distributions as dist
from pyro.infer.mcmc import MCMC, HMC, NUTS
pyro.set_rng_seed(0)
```

b. Let's first define the tensors for the observations:

```
[4]: x = torch.tensor([47.0, 87.0, 20.0, 16.0, 38.0, 5.0])
y = torch.tensor([58.76, 108.75, 25.03, 20.03, 47.51, 6.37])
```

We also introduce two auxiliary function in order to avoid code duplication:

```
fig, ax = plt.subplots(len(mcmc_samples), n_chains, figsize=(15,8))
for i, key in enumerate(mcmc_samples.keys()):
    for j, chain in enumerate(mcmc_samples[key]):
        sns.lineplot(x=range(n_samples), y=chain, ax=ax[i][j])
        ax[i][j].set_title(key + " chain "+str(i+1))

for key in mcmc_samples.keys():
    print("expected ", key, " = ", mcmc_samples[key].mean().item())

fig, ax = plt.subplots(1, 2, figsize=(15,8))
    for i, key in enumerate(mcmc_samples.keys()):
        sns.distplot(mcmc_samples[key], ax = ax[i])
        ax[i].set_title("P(" + key + " | y = obs)")
        ax[i].set_xlabel(xlabel = key)

def doing nuts(model, theta1 dist, theta2 dist, xx, yy, samples, warmup, warmu
```

```
[6]: def doing_nuts(model, theta1_dist, theta2_dist, xx, yy, samples, warmup,
      ⇔chains):
       kernel = NUTS(model)
      mcmc = MCMC(kernel, num_samples=samples, warmup_steps=warmup,_
      →num_chains=chains)
      posterior = mcmc.run(theta1_prior = theta1_dist, theta2_prior = theta2_dist,__
      \rightarrow x = xx, obs = yy)
      mcmc.summary()
       mcmc samples = mcmc.get samples(group by chain=True)
      n_chains = mcmc.num_chains
      n_samples = mcmc.num_samples
       print("chains = ", n_chains, "samples = ", n_samples)
       fig, ax = plt.subplots(len(mcmc_samples), n_chains, figsize=(15,8))
       for i, key in enumerate(mcmc_samples.keys()):
         for j, chain in enumerate(mcmc_samples[key]):
           sns.lineplot(x=range(n_samples), y=chain, ax=ax[i][j])
           ax[i][j].set_title(key + " chain "+str(i+1))
       for key in mcmc_samples.keys():
         print("expected ", key, " = ", mcmc_samples[key].mean().item())
       fig, ax = plt.subplots(1, 2, figsize=(15,8))
       for i, key in enumerate(mcmc_samples.keys()):
         sns.distplot(mcmc_samples[key], ax = ax[i])
         ax[i].set_title("P(" + key + " | y = obs)")
         ax[i].set_xlabel(xlabel = key)
```

We are now going to show different choices of prior distributions for θ_1 and θ_2 , using both MCMC and NUTS to find their posterior distribution given the observations.

• MCMC with BETA priors:

```
[8]: doing_mcmc(model = model, theta1_dist = dist.Beta(.5, .5), theta2_dist = dist.

Beta(5.0, 1.0), xx = x, yy = y, samples = 500, warmup=1000, chains=3)
```

/usr/local/lib/python3.7/dist-packages/pyro/infer/mcmc/api.py:500: UserWarning: num_chains=3 is more than available_cpu=1. Chains will be drawn sequentially. num_chains, available_cpu

	mean	std	median	5.0%	95.0%	${\tt n_eff}$	${ t r}_{ t hat}$
theta_1	0.54	0.36	0.57	0.03	1.00	525.53	1.01
theta_2	0.80	0.01	0.80	0.79	0.81	90.52	1.03

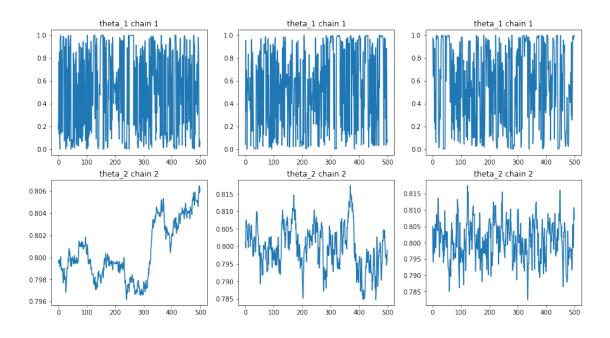
Number of divergences: 0 chains = 3 samples = 500 expected theta 1 = 0.53562

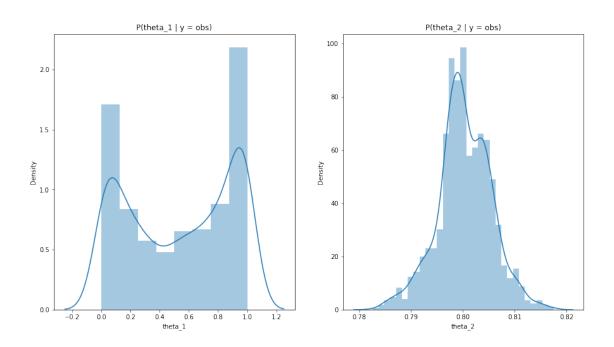
expected theta_1 = 0.5356252789497375 expected theta_2 = 0.8002839088439941

/usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).

warnings.warn(msg, FutureWarning)

/usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).





• NUTS with BETA priors:

[9]: doing_nuts(model = model, theta1_dist = dist.Beta(.5, .5), theta2_dist = dist.

Beta(5.0, 1.0), xx = x, yy = y, samples = 500, warmup=1000, chains=3)

/usr/local/lib/python3.7/dist-packages/pyro/infer/mcmc/api.py:500: UserWarning: num_chains=3 is more than available_cpu=1. Chains will be drawn sequentially. num_chains, available_cpu

```
Sample [0]: 100%|
                       | 1500/1500 [00:24, 62.02it/s, step size=7.57e-01,
acc. prob=0.921]
Sample [1]: 100%|
                       | 1500/1500 [00:25, 59.50it/s, step size=8.57e-01,
acc. prob=0.881]
                       | 1500/1500 [00:20, 73.32it/s, step size=6.96e-01,
Sample [2]: 100%|
acc. prob=0.915]
                                  median
                                               5.0%
                                                        95.0%
                           std
                                                                   n_eff
                                                                             r_hat
                mean
```

theta 1 0.50 0.36 0.50 0.00 0.97 911.15 1.00 $theta_2$ 0.80 0.01 0.80 0.79 0.81 1044.51 1.00

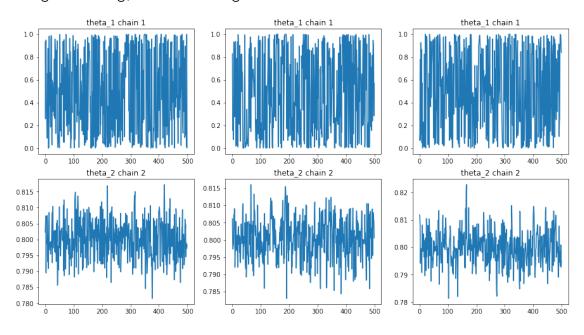
Number of divergences: 0 chains = 3 samples = 500

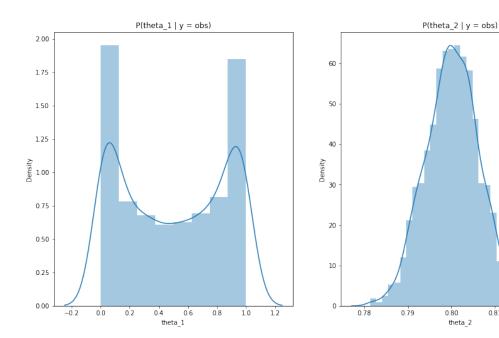
expected theta_1 = 0.49588146805763245expected theta_2 = 0.8002444505691528

/usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619:
FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).

warnings.warn(msg, FutureWarning)

/usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619:
FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).





• MCMC with Uniform priors:

```
[15]: doing_mcmc(model = model, theta1_dist = dist.Uniform(0.,1.), theta2_dist = dist.

Uniform(0.,1.), xx = x, yy = y, samples = 500, warmup=1000, chains=3)
```

/usr/local/lib/python3.7/dist-packages/pyro/infer/mcmc/api.py:500: UserWarning: num_chains=3 is more than available_cpu=1. Chains will be drawn sequentially. num_chains, available_cpu

Sample [0]: 100%| | 1500/1500 [00:37, 39.66it/s, step size=8.29e-01,

acc. prob=0.927]

Sample [1]: 100% | 1500/1500 [00:31, 47.67it/s, step size=8.83e-01,

acc. prob=0.873]

Sample [2]: 100% | 1500/1500 [00:42, 35.49it/s, step size=9.10e-01,

acc. prob=0.903]

Warmup [2]: 7% | 106/1500 [05:48, 3.29s/it, step size=1.83e-05,

acc. prob=0.778]

	mean	std	median	5.0%	95.0%	${\tt n_eff}$	r_hat
theta_1	0.49	0.29	0.47	0.00	0.89	246.65	1.01
theta_2	0.80	0.01	0.80	0.79	0.81	149.17	1.01

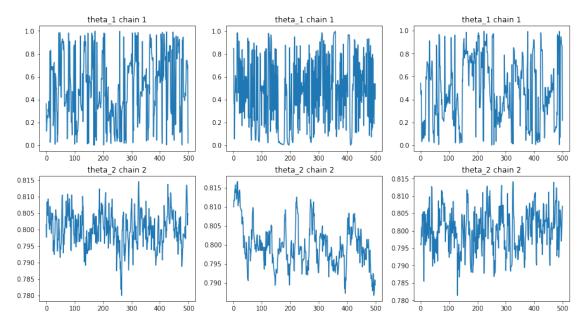
Number of divergences: 0

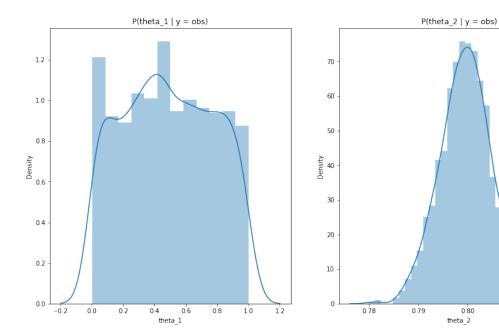
chains = 3 samples = 500

expected theta_1 = 0.4872201681137085 expected theta_2 = 0.8000463843345642 /usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).

warnings.warn(msg, FutureWarning)

/usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).





• NUTS with Uniform priors:

[16]: doing_nuts(model = model, theta1_dist = dist.Uniform(0.,1.), theta2_dist = dist. \neg Uniform(0.,1.), xx = x, yy = y, samples = 500, warmup=1000, chains=3)

0.80

theta 2

0.81

/usr/local/lib/python3.7/dist-packages/pyro/infer/mcmc/api.py:500: UserWarning: num_chains=3 is more than available_cpu=1. Chains will be drawn sequentially. num_chains, available_cpu

Sample [0]: 100%| | 1500/1500 [00:14, 100.50it/s, step size=8.60e-01,

acc. prob=0.903]

Sample [1]: 100%| | 1500/1500 [00:13, 112.41it/s, step size=8.68e-01,

acc. prob=0.875]

| 1500/1500 [00:14, 103.45it/s, step size=8.39e-01, Sample [2]: 100%|

acc. prob=0.914]

	mean	std	median	5.0%	95.0%	n_eff	r_hat
theta_1	0.50	0.29	0.51	0.00	0.89	1296.32	1.00
theta_2	0.80	0.01	0.80	0.79	0.81	1258.25	1.00

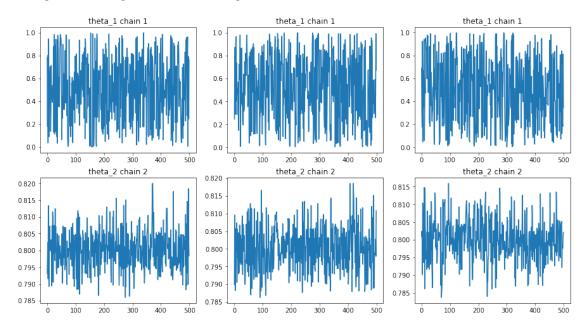
Number of divergences: 0 chains = 3 samples = 500

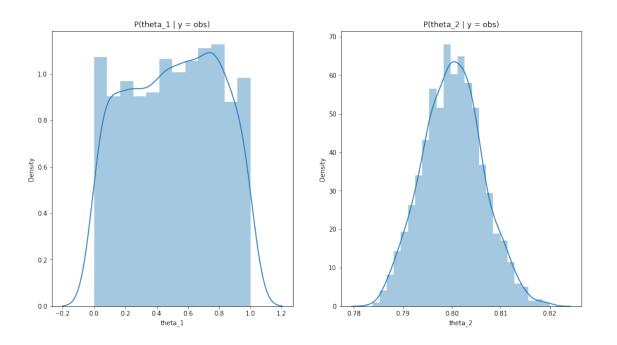
 $expected theta_1 = 0.5046466588973999$ $expected theta_2 = 0.8002350926399231$

/usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).

warnings.warn(msg, FutureWarning)

/usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).





• MCMC with Rescaled Normal priors:

```
doing_mcmc(model = model, theta1_dist = dist.Normal(0.5,0.15), theta2_dist = dist.Normal(0.5,0.15), xx = x, yy = y, samples = 500, warmup=1000, chains=3)
```

/usr/local/lib/python3.7/dist-packages/pyro/infer/mcmc/api.py:500: UserWarning: num_chains=3 is more than available_cpu=1. Chains will be drawn sequentially. num_chains, available_cpu

```
Sample [0]: 100%| | 1500/1500 [00:20, 73.62it/s, step size=8.25e-01, acc. prob=0.974]

Sample [1]: 100%| | 1500/1500 [03:33, 7.03it/s, step size=8.07e-01, acc. prob=0.947]

Sample [2]: 100%| | 1500/1500 [01:14, 20.01it/s, step size=8.82e-01, acc. prob=0.974]
```

	mean	std	median	5.0%	95.0%	n_eff	r_hat
theta_1	0.48	0.17	0.48	0.21	0.77	61.42	1.03
theta 2	-6.98	0.07	-6.96	-7.11	-6.89	2.68	1.64

```
Number of divergences: 0

chains = 3 samples = 500

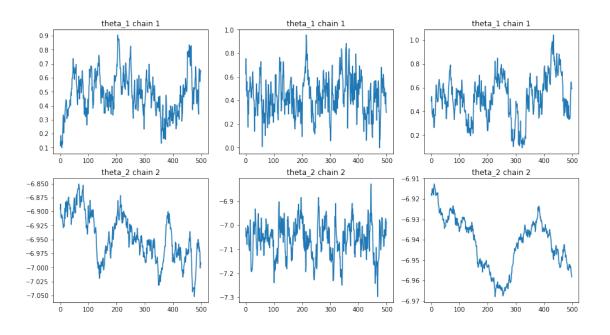
expected theta_1 = 0.47862130403518677

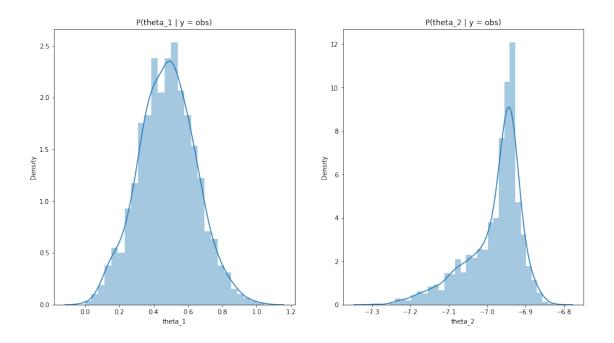
expected theta_2 = -6.981785297393799
```

/usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).

warnings.warn(msg, FutureWarning)

/usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).





• NUTS with Rescaled Normal priors:

```
[19]: doing_nuts(model = model, theta1_dist = dist.Normal(0.5,0.15), theta2_dist = dist.Normal(0.5,0.15), xx = x, yy = y, samples = 500, warmup=1000, chains=3)
```

/usr/local/lib/python3.7/dist-packages/pyro/infer/mcmc/api.py:500: UserWarning: num_chains=3 is more than available_cpu=1. Chains will be drawn sequentially. num_chains, available_cpu

```
Sample [0]: 100%|
                       | 1500/1500 [00:10, 142.40it/s, step size=8.47e-01,
acc. prob=0.909]
                       | 1500/1500 [00:11, 129.17it/s, step size=7.94e-01,
Sample [1]: 100%|
acc. prob=0.931]
                       | 1500/1500 [00:08, 175.07it/s, step size=8.48e-01,
Sample [2]: 100%|
acc. prob=0.915]
                            std
                                   median
                                                5.0%
                                                         95.0%
                                                                    n_{eff}
                                                                              r_hat
                mean
                                                          0.73
                                                                               1.01
   theta 1
                0.49
                           0.14
                                     0.49
                                                0.27
                                                                   848.98
   theta_2
               -1.81
                           3.69
                                     0.80
                                               -7.08
                                                          0.82
                                                                     1.50
                                                                              80.26
```

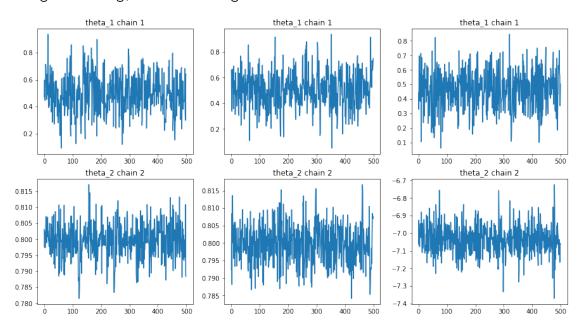
Number of divergences: 0 chains = 3 samples = 500

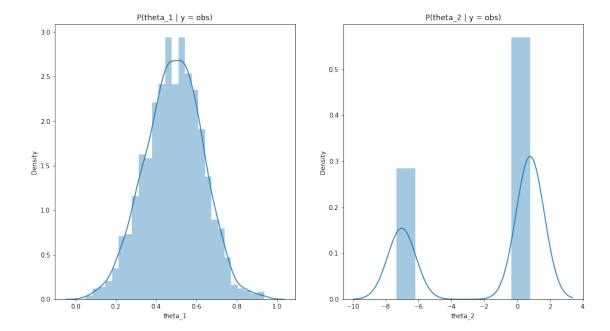
expected theta_1 = 0.4885198175907135expected theta_2 = -1.8113927841186523

/usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).

warnings.warn(msg, FutureWarning)

/usr/local/lib/python3.7/dist-packages/seaborn/distributions.py:2619:
FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).





c. Using either a beta distribution or a uniform distribution as priors for θ_1 and θ_2 lead to similar results. In particular, if we compare the estimates obtained using the HMC algorithm we have that the beta prior gives a better estimate of θ_1 , since the r-value is the same (1.01) and n-eff is higher; however, regarding θ_2 we have that using a uniform distribution gives better results since we have a lower r-value and a higher n-eff, so given this last consideration we can conclude that using a uniform prior gives better results in this case.

If we consider the results obtained using the NUTS algorithm we have that we get the same estimates independently on the prior used, however if we look at the convergence checks we can see that again we get better results for both values by using a uniform prior distribution.

Finally, we can see that using a rescaled normal distribution we get some strange results for the θ_2 parameter: even though we get convergence we can see that the r-values are really far from 1 in both algorithms. θ_1 is estimated just fine, especially by using the NUTS algorithm.

1.1.1 Exercise 2

A bivariate Gibbs sampler for a vector $x=(x_1,x_2)$ draws iteratively from the posterior conditional distributions in the following way: - choose a starting value $p(x_1|x_2^{(0)})$ - for each iteration i: - draw $x_2(i)$ from $p(x_2|x_1^{(i-1)})$ - draw $x_1(i)$ from $p(x_1|x_2^{(i)})$

a. Supposing that samples are drawn from a bivariate normal distribution

$${x_1 \choose x_2} \sim \mathcal{N} \left[{0 \choose 0}, {1 \quad \rho \choose \rho \quad 1} \right],$$

implement a Gibbs sampler function which takes as inputs the parameter rho, the number of iterations iters and the number of warmup draws warmup.

b. Use your implementation of Gibbs sampler to infer the parameters $\theta = (\theta_1, \theta_2)$ from **Exercise** 1.

Solution

a. From the properties of the multivariate normal distribution in the bivariate case we have that in general we can write:

$$\begin{split} x_1 | x_2 &\sim \mathcal{N} \left(\mu_1 + \frac{\rho}{\sigma_2^2} (x_2 - \mu_2), \sigma_1^2 - \frac{\rho^2}{\sigma_2^2} \right) \\ x_2 | x_1 &\sim \mathcal{N} \left(\mu_2 + \frac{\rho}{\sigma_1^2} (x_1 - \mu_1), \sigma_2^2 - \frac{\rho^2}{\sigma_1^2} \right) \end{split}$$

In our case this can be simplified to:

$$x_1 | x_2 \sim \mathcal{N}(\rho x_2, 1 - \rho^2)$$

 $x_2 | x_1 \sim \mathcal{N}(\rho x_1, 1 - \rho^2)$

```
[20]: def gibbs_sampler(rho, warmup, iters):
          x1 = torch.zeros(warmup+iters, 1)
          x2 = torch.zeros(warmup+iters, 1)
          # starting value for x_2
          x2[0] = pyro.sample('x2', dist.Normal(0,1))
          # starting value p(x_1 | x_2^0)
          x1[0] = pyro.sample('x1', dist.Normal(rho*(x2[0].item()), np.
        \rightarrowsqrt(1-rho**2)))
          # iterations
          for i in range(1, warmup+iters):
               # first draw
               x2[i] = pyro.sample('x2', dist.Normal(rho*x1[i-1].item(), np.
        \hookrightarrowsqrt(1-rho**2)))
               #second draw
               x1[i] = pyro.sample('x1', dist.Normal(rho*x2[i].item(), np.
        \rightarrowsqrt(1-rho**2)))
          return x1[warmup:-1], x2[warmup:-1]
```

Let's check that this works:

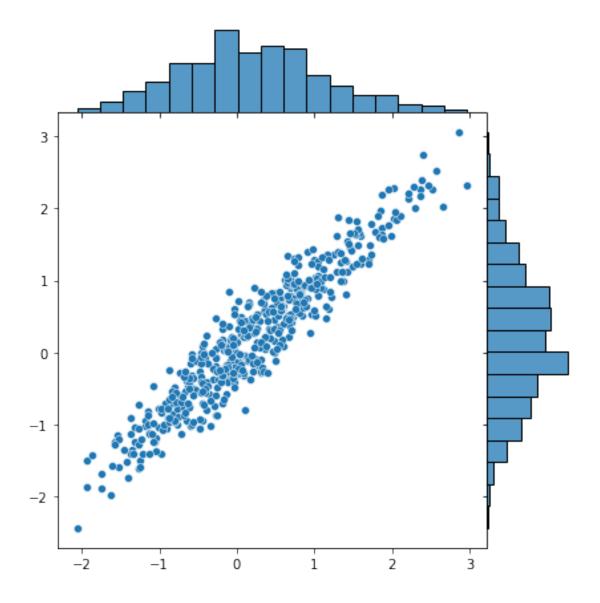
[21]: x1, x2 = gibbs_sampler(0.96, 1000, 500)

[23]: sns.jointplot(np.array(x1[:, 0]), np.array(x2[:, 0]), space = 0)

/usr/local/lib/python3.7/dist-packages/seaborn/_decorators.py:43: FutureWarning: Pass the following variables as keyword args: x, y. From version 0.12, the only valid positional argument will be `data`, and passing other arguments without an explicit keyword will result in an error or misinterpretation.

FutureWarning

[23]: <seaborn.axisgrid.JointGrid at 0x7f090c070c90>



b. Let's define the general case of the previous function:

```
[24]: def gibbs_sampler_general(start, rho, warmup, iters, mu1 = 0, mu2 = 0):
          x1 = torch.zeros(warmup+iters, 1)
          x2 = torch.zeros(warmup+iters, 1)
          x2[0] = start
          # starting value p(x_1 | x_2^0)
          x1[0] = pyro.sample('x1', dist.Normal(mu1 + rho*(x2[0].item()-mu2), np.
        \rightarrowsqrt(1-rho**2)))
          # iterations
          for i in range(1, warmup+iters):
               # first draw
              x2[i] = pyro.sample('x2', dist.Normal(mu2 + rho*(x1[i-1].item()-mu1),_i)
        \rightarrownp.sqrt(1-rho**2)))
               #second draw
              x1[i] = pyro.sample('x1', dist.Normal(mu1 + rho*(x2[i].item()-mu2), np.
        \Rightarrowsqrt(1-rho**2)))
          return x1[warmup:-1], x2[warmup:-1]
```

We need to re-run the NUTS algorithm since we used functions in the previous exercise:

	mean	std	median	5.0%	95.0%	n_eff	${ t r}_{ t hat}$
theta_1	0.50	0.29	0.51	0.03	0.93	7650.97	1.00
${ t theta}_2$	0.80	0.01	0.80	0.79	0.81	7707.00	1.00

Number of divergences: 0

Let's get all the parameters for the distribution of θ_1 and θ_2 :

 $Mu_1 = 0.5024603009223938 Mu_2 = 0.8001969456672668$

Covariance Matrix:

```
[[1. 0.02629717]
[0.02629717 1. ]]
```

Sampling and plotting:

```
[27]: theta1_sample_gibbs, theta2_sample_gibbs = gibbs_sampler_general(0.5, usestimated_rho, 1500, 3000, mu1 = mu1, mu2 = mu2)
```

```
[28]: sns.histplot(theta1_sample_gibbs[:, 0])
  plt.title("histogram for theta1")
  plt.show()
  sns.histplot(theta2_sample_gibbs[:, 0])
  plt.title("histogram for theta2")
  plt.show()
```

