

hw3__taylor

April 23, 2021

1 HW3: Hamiltonian Monte Carlo

STATS271/371: Applied Bayesian Statistics

Stanford University. Winter, 2021.

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Due: 11:59pm Friday, April 23, 2021 via GradeScope

In this homework assignment you'll perform MCMC with both Metropolis-Hastings Hamiltonian Monte Carlo. We will investigate the Federalist papers—specifically, modeling the rate at which Hamilton (we're using HMC after all!) uses the word *can* in his papers.

We will fit this model using a negative binomial distribution. That is, for each document n that Hamilton wrote, we have the number of times the word 'can' appears y_n as

$$y_n \sim \text{NB}(\mu_n, r) \quad (1)$$

where

$$\text{NB}(y_n \mid \mu_n, r) = \frac{\Gamma(y_n + r)}{\Gamma(r)\Gamma(y_n + 1)} \left(\frac{r}{\mu_n + r} \right)^r \left(1 - \frac{r}{\mu_n + r} \right)^{y_n} \quad (2)$$

The mean is given by $\mathbb{E}[y_n] = \mu_n$, and r controls the dispersion. Here, we model the mean for document n as

$$\mu_n = \frac{T_n}{1000} \mu \quad (3)$$

where μ is the rate of usage of 'can' per 1000 words and T_n is the number of words in document n (i.e. the document length).

For our model, we will use the following prior for the non-negative parameters,

$$\log \mu \sim \mathcal{N}(0, 9) \quad (4)$$

$$\log r \sim \mathcal{N}(0, 9) \quad (5)$$

In a classic paper, Mosteller and Wallace (JASA, 1963) used likelihood ratios under negative binomial models with different mean rates for Alexander Hamilton and James Madison to infer the

more likely author of disputed Federalist papers. Spoiler alert: while Hamilton wrote the majority of the papers, the 12 disputed papers appear to be Madison's! A key step in their analysis was estimating the NB parameters. While Mosteller and Wallace used a point estimate for each word and author, you'll do full posterior inference, focusing on Hamilton's use of the word *can*.

```
[18]: !wget -nc https://raw.githubusercontent.com/slinderman/stats271sp2021/main/
      ↪ assignments/hw3/federalist_can_hamilton.csv
```

File 'federalist_can_hamilton.csv' already there; not retrieving.

```
[23]: import pandas as pd
import numpy as np
from matplotlib import pyplot as plt

# Load the data
df = pd.read_csv('federalist_can_hamilton.csv')
Ts = np.array(df['Total'])
ys = np.array(df['N'])
# preview data
list(zip(ys, Ts))[:5]
```

```
[23]: [(3, 1622), (5, 2511), (2, 2171), (4, 970), (14, 3095)]
```

1.1 Problem 1 [math]: Show that the negative binomial can be expressed as the marginal distribution of a Poisson with gamma prior

Similar to how the Student's *t* distribution is a marginal of an inverse chi-squared and a Gaussian, show that

$$\text{NB}(y \mid \mu, r) = \int \text{Po}(y \mid \lambda) \text{Ga}(\lambda \mid \alpha, \beta) d\lambda \quad (6)$$

Express the parameters of the negative binomial distribution as a function of the parameters of the gamma distribution. (Assume β is the rate parameter.)

$$\begin{aligned}
\int Po(y|\lambda)Ga(\lambda|\alpha, \beta)d\lambda &= \int \frac{\lambda^y e^{-\lambda}}{y!} \frac{\lambda^{\alpha-1} e^{-\beta\lambda}}{\beta^{-\alpha}\Gamma(\alpha)} d\lambda \\
&= \frac{\beta^\alpha}{\Gamma(y+1)\Gamma(\alpha)} \int \lambda^{\alpha+y-1} e^{-\lambda(1+\beta)} d\lambda \\
x = \lambda(1+\beta), \frac{dx}{d\lambda} &= (1+\beta), z = \alpha+y \\
&= \frac{\beta^\alpha}{\Gamma(y+1)\Gamma(\alpha)} \int \left(\frac{x}{1+\beta}\right)^{\alpha+y-1} e^{-x} d\lambda \frac{dx}{d\lambda} (1+\beta)^{-1} \\
&= \frac{\beta^\alpha}{\Gamma(y+1)\Gamma(\alpha)} (1+\beta)^{-z+1} (1+\beta)^{-1} \int x^{z-1} e^{-x} dx \\
&= \frac{\Gamma(\alpha+y)}{\Gamma(y+1)\Gamma(\alpha)} \beta^\alpha (1+\beta)^{-(\alpha+y)} \\
&= \frac{\Gamma(\alpha+y)}{\Gamma(y+1)\Gamma(\alpha)} \beta^\alpha \left(\frac{1}{1+\beta}\right)^\alpha \left(\frac{1}{1+\beta}\right)^y \\
\boxed{\alpha=r}, \frac{1}{1+\beta} &= 1 - \frac{r}{\mu+r} = \frac{\mu}{\mu+r} \implies \boxed{\beta = \frac{r}{\mu}} \\
&= \frac{\Gamma(r+y)}{\Gamma(y+1)\Gamma(r)} \left(\frac{r}{\mu}\right)^r \left(\frac{\mu}{\mu+r}\right)^r \left(1 - \frac{r}{\mu+r}\right)^y \\
&= \frac{\Gamma(r+y)}{\Gamma(y+1)\Gamma(r)} \left(\frac{r}{\mu+r}\right)^r \left(1 - \frac{r}{\mu+r}\right)^y \\
&= NB(y|\mu, r) \\
\implies r = \alpha, \mu &= \frac{\alpha}{\beta}
\end{aligned}$$

1.2 Problem 2: Implement the log joint probability of the model

```
[43]: import autograd.numpy as np

def log_joint(log_mu, log_r, ys=ys, Ts=Ts):
    N = len(ys)
    mu = np.exp(log_mu)
    r = np.exp(log_r)
    mus = (Ts / 1000.0) * mu
    p = r / (mus + r)
    likelihood = (np.sum(np.log(sp.gamma(ys + r)))
                  - np.sum(np.log(sp.gamma(ys + 1)))
                  - N * np.log(sp.gamma(r))
                  + np.sum(ys * np.log(1 - p))
                  + np.sum(r * np.log(p)))
    #likelihood = np.sum(ss.nbinom.logpmf(ys, n=r, p=p))
    r_prior = ss.norm.logpdf(log_r, 0.0, 3.0)
    mu_prior = ss.norm.logpdf(log_mu, 0.0, 3.0)
    return likelihood + r_prior + mu_prior
```

```
[44]: log_joint(ys=ys, Ts=Ts, log_mu=0, log_r=0)
```

[44]: -169.40747146591295

For the following MC implementation problems, sample in $\log(\mu), \log(r)$ space. Initialize with $\log(\mu) = 0, \log(r) = 0$.

1.3 Problem 3: Implement Metropolis-Hastings

Implement and run Metropolis-Hastings with a spherical Gaussian proposal. Try various proposal variances.

```
[39]: def metropolis(log_mu=0,
                    log_r=0,
                    q_sigma = 0.1,
                    iterations=5000,
                    lik=log_joint
                    ):
    """ MCMC approximate inference """
    from scipy.stats import (multivariate_normal,
                             bernoulli)
    from numpy.random import rand
    theta = [log_mu, log_r]
    cache = [theta]
    for i in range(iterations):
        # proposal step
        theta_prime = multivariate_normal.rvs(mean=theta,
                                              cov=np.diag([q_sigma] * 2),
                                              size=1)

        # accept/ reject step
        A = np.exp(lik(theta_prime[0], theta_prime[1])
                  - lik(theta[0], theta[1]))
        a = np.min([1.0, A])
        if bernoulli.rvs(p=a) == 1:
            theta = theta_prime
            cache.append(theta)
    return np.array(cache)
```

```
[40]: mcmc = metropolis()
```

1.4 Problem 4: Implement Hamiltonian Monte Carlo

Implement the leapfrog step as a function, and run HMC. Try various step sizes and number of leapfrog steps.

```
[45]: def hamiltonian(log_mu=0.0,
                     log_r=0.0,
                     epsilon = 0.01,
                     iterations=5000,
```

```

        leapfrog_steps=40,
        func=log_joint
    ):
""" HMC approximate inference """
    from scipy.stats import (multivariate_normal,
                             bernoulli)
    from numpy.random import rand
    import autograd.numpy as np
    import autograd.scipy.stats as ss
    import autograd.scipy.special as sp
    from autograd import grad
    from autograd.misc import flatten

    # Setup gradient function
    q, unflatten = flatten([log_mu, log_r])

    def U(params):
        log_mu, log_r = unflatten(params)
        return -log_joint(log_mu, log_r)

    grad_U = grad(U)
    current_q = q
    cache = [q]
    for i in range(iterations):
        # proposal step
        p = multivariate_normal.rvs(mean=[0, 0],
                                     cov=np.diag([1, 1]),
                                     size=1)

        current_p = p

        # First half step
        p = p - epsilon * grad_U(q) / 2

        # Alternate full steps for position and momentum
        for j in range(leapfrog_steps):
            q = q + epsilon * p
            if j != leapfrog_steps-1:
                # Full step when not at end of trajectory
                p = p - epsilon * grad_U(q)

            # half step for momentum at end
            p = p - epsilon * grad_U(q) / 2

            # negate p to make proposal symmetric
            p = -p

        current_U = U(current_q)

```

```

current_K = np.sum(np.power(current_p, 2)) / 2
proposed_U = U(q)
proposed_K = np.sum(np.power(p, 2)) / 2

# accept/ reject step
A = np.exp(current_U - proposed_U + current_K - proposed_K)
a = np.min([1.0, A])
if bernoulli.rvs(p=a) == 1:
    current_q = q
    cache.append(current_q)
return np.array(cache)

```

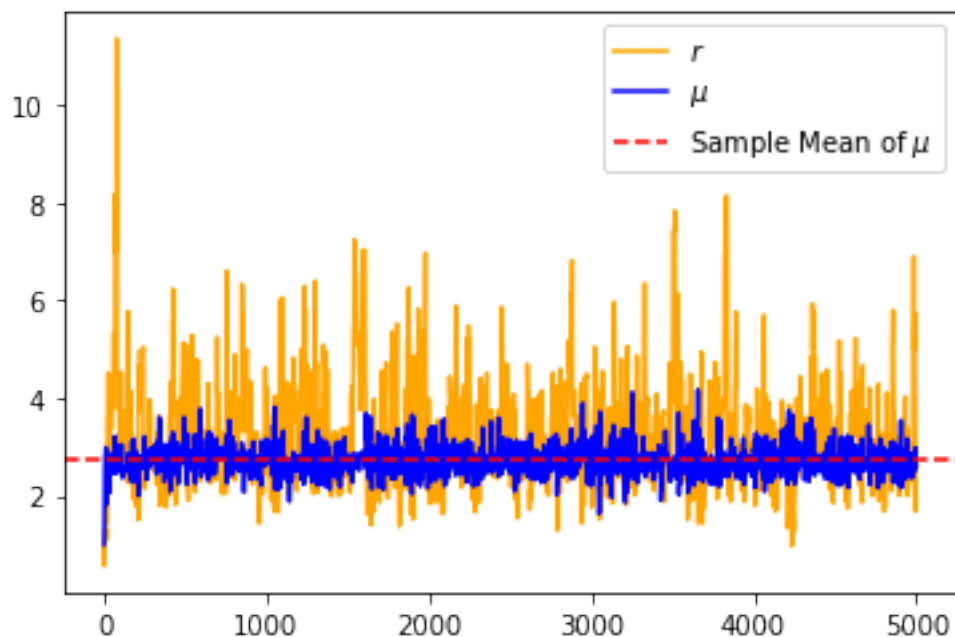
```
[46]: hmc = hamiltonian()
```

1.5 Problem 5: Diagnostics

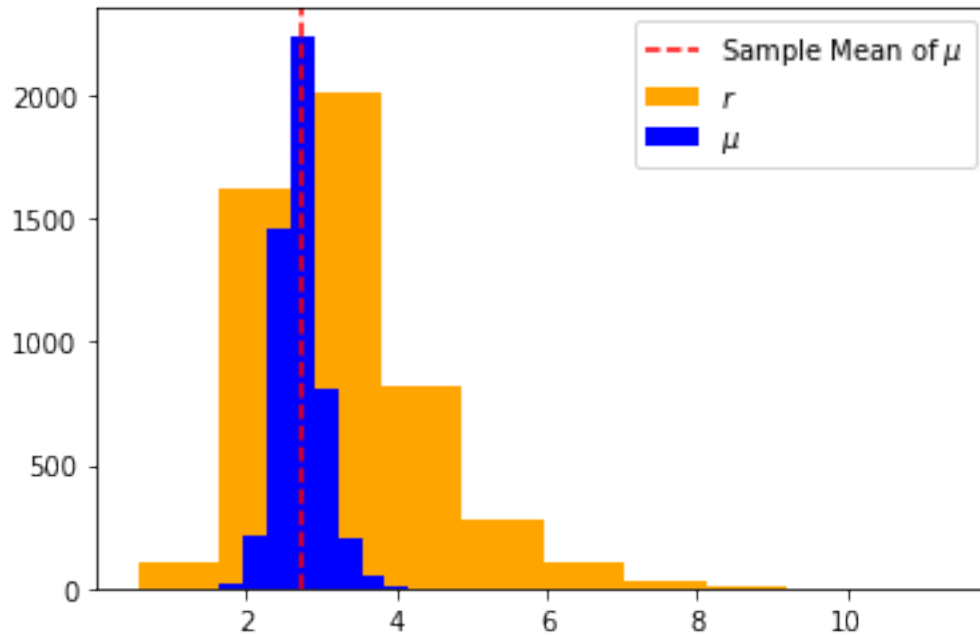
For both algorithms, make trace plots of the parameters and plot histograms of posterior marginals.

```
[47]: plt.plot(np.exp(mcmc[:,1]), color = 'orange', label = r'$r$')
plt.plot(np.exp(mcmc[:,0]), color = 'blue', label = r'$\mu$')
plt.axhline((df.N * 1000 / df.Total).mean(),
            color='red',
            ls='--',
            label=r'Sample Mean of $\mu$')
plt.legend()
plt.show()

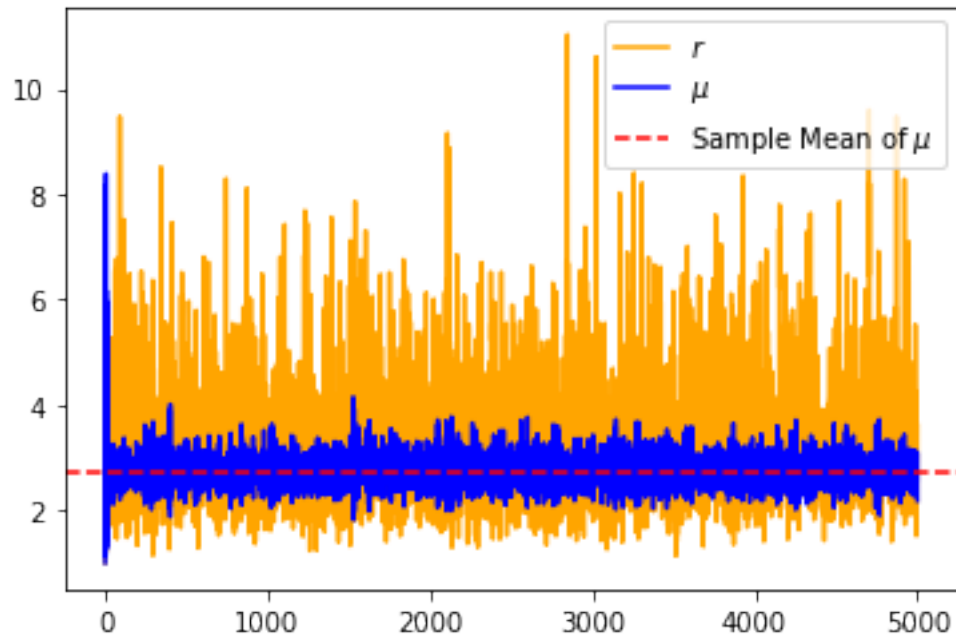
```



```
[48]: plt.hist(np.exp(mcmc[:,1]), color='orange', label = r'$r$')
plt.hist(np.exp(mcmc[:,0]), color='blue', label = r'$\mu$')
plt.axvline((df.N * 1000 / df.Total).mean(), color='red', ls='--',
            label=r'Sample Mean of $\mu$')
plt.legend()
plt.show()
```



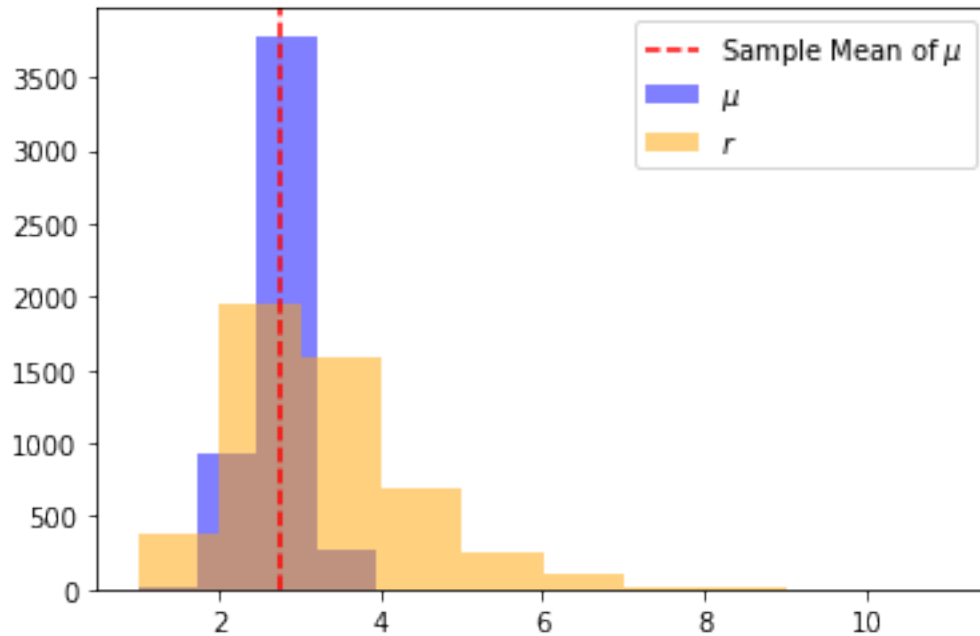
```
[49]: plt.plot(np.exp(hmc[:,1]), color = 'orange', label = r'$r$')
plt.plot(np.exp(hmc[:,0]), color = 'blue', label = r'$\mu$')
plt.axhline((df.N * 1000 / df.Total).mean(),
            color='red',
            ls='--',
            label=r'Sample Mean of $\mu$')
plt.legend()
plt.show()
```



```
[55]: np.std(np.exp(hmc), axis=0)
```

```
[55]: array([0.33120151, 1.12064068])
```

```
[50]: plt.hist(np.exp(hmc[:,0]), color='blue', alpha = 0.5, label = r'$\mu$')
plt.hist(np.exp(hmc[:,1]), color='orange', alpha = 0.5, label = r'$r$')
plt.axvline((df.N * 1000 / df.Total).mean(), color='red', ls='--',
            ↳label=r'Sample Mean of $\mu$')
plt.legend()
plt.show()
```

1.6 Problem 6: Effective Sample Size

Calculate effective sample size for both chains.

```
[2]: import tensorflow_probability as tfp
```

```
[56]: ess = tfp.mcmc.effective_sample_size(mcmc, filter_beyond_positive_pairs=True)
      print(ess.numpy())
```

```
[872.2407521 281.1380704]
```

```
[58]: ess = tfp.mcmc.effective_sample_size(hmc, filter_beyond_positive_pairs=True)
      print(ess.numpy())
```

```
[31502.48369152 2358.65786776]
```

Formatting: check that your code does not exceed 80 characters in line width. If you're working in Colab, you can set *Tools* → *Settings* → *Editor* → *Vertical ruler column* to 80 to see when you've exceeded the limit.

Download your notebook in .ipynb format and use the following commands to convert it to PDF:

```
jupyter nbconvert --to pdf hw3_yourname.ipynb
```

Dependencies:

- nbconvert: If you're using Anaconda for package management,
conda install -c anaconda nbconvert

Upload your .ipynb and .pdf files to Gradescope.