evidence-gamma-normal

April 7, 2022

[1]:
```
import torch
import numpy as np
import matplotlib.pylab as plt

plt.rc('text', usetex=True)
plt.rc('font',**{'family':'sans-serif','serif':['Palatino']})
figSize  = (12, 8)
fontSize = 20
```

1 Notations

Similar to wikipedia.

$$X \sim \Gamma(\alpha, \beta)$$

The probability distribution function is given by

$$f(x; \alpha, \beta) = \frac{x^{\alpha-1} e^{-\beta x} \beta^{\alpha}}{\Gamma(\alpha)}$$

where $\Gamma(\alpha) = (\alpha - 1)!$

α is the shape parameter.

β is the rate parameter (we will fix this parameter to $\beta = 5.0$ throughout this work).

2 PyTorch Notations

Link

`torch.distributions.gamma.Gamma(concentration, rate, validate_args=None)`

Creates a Gamma distribution parameterized by shape concentration and rate.

3 Analysis

3.0.1 Steps

- The data is generated from the Gamma distribution.

- The parameter β is fixed to $\beta = 5.0$.
- Only one parameter, α varied.
- Assume a normal prior on α, that is, $p(\alpha) = \mathcal{N}(\alpha_*, 1)$
- Goal: compute evidence with and without compression.
- Goal: use the score function for compression.
- Goal: compare with the case when a Gaussian likelihood is used.

3.0.2 Bayes' theorem

$$p(\alpha, \beta|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\alpha, \beta)\, p(\alpha, \beta)}{p(\boldsymbol{x})}$$

$p(\beta) = \delta(\beta - 5.0)$. We will ignore β below since it is fixed.

$$p(\alpha|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\alpha)\, p(\alpha)}{p(\boldsymbol{x})}$$

Without Compression

$$p(\boldsymbol{x}) = \int \Gamma(\alpha, \beta = 5.0)\, p(\alpha)\, \mathrm{d}\alpha$$

Assume we have generated N iid samples, $\boldsymbol{x} \in \mathbb{R}^N$:

$$p(\boldsymbol{x}) = \int \prod_{i=1}^{N} f(x_i; \alpha,\, \beta = 5.0)\, p(\alpha)\, \mathrm{d}\alpha$$

We can do this integration numerically (on a grid).

If we assume a Gaussian likelihood,

$$p(\boldsymbol{x}) = \int \prod_{i=1}^{N} f(x_i; \mu,\, \sigma = 1.0)\, p(\mu)\, \mathrm{d}\mu$$

With Compression We will be using the score function, that is,

$$s = \nabla \mathcal{L}$$

where $\mathcal{L}$ is the log-likelihood. We need the derivative of the log-likelihood with respect to α, but evaluated at each sample. The log-likelihood when using the Gamma distribution is:

$$\mathcal{L} = \sum_{i=1}^{N} \log f(x_i; \alpha, \beta = 5.0)$$

and the derivative of the log-likelihood with respect to the parameter, α is:

$$\nabla\mathcal{L} = \nabla \sum_{i=1}^{N} \log f(x_i; \alpha, \beta = 5.0)$$

Therefore, we have compressed N samples (data points) to just 1 number. The likelihood (for the compressed data) is

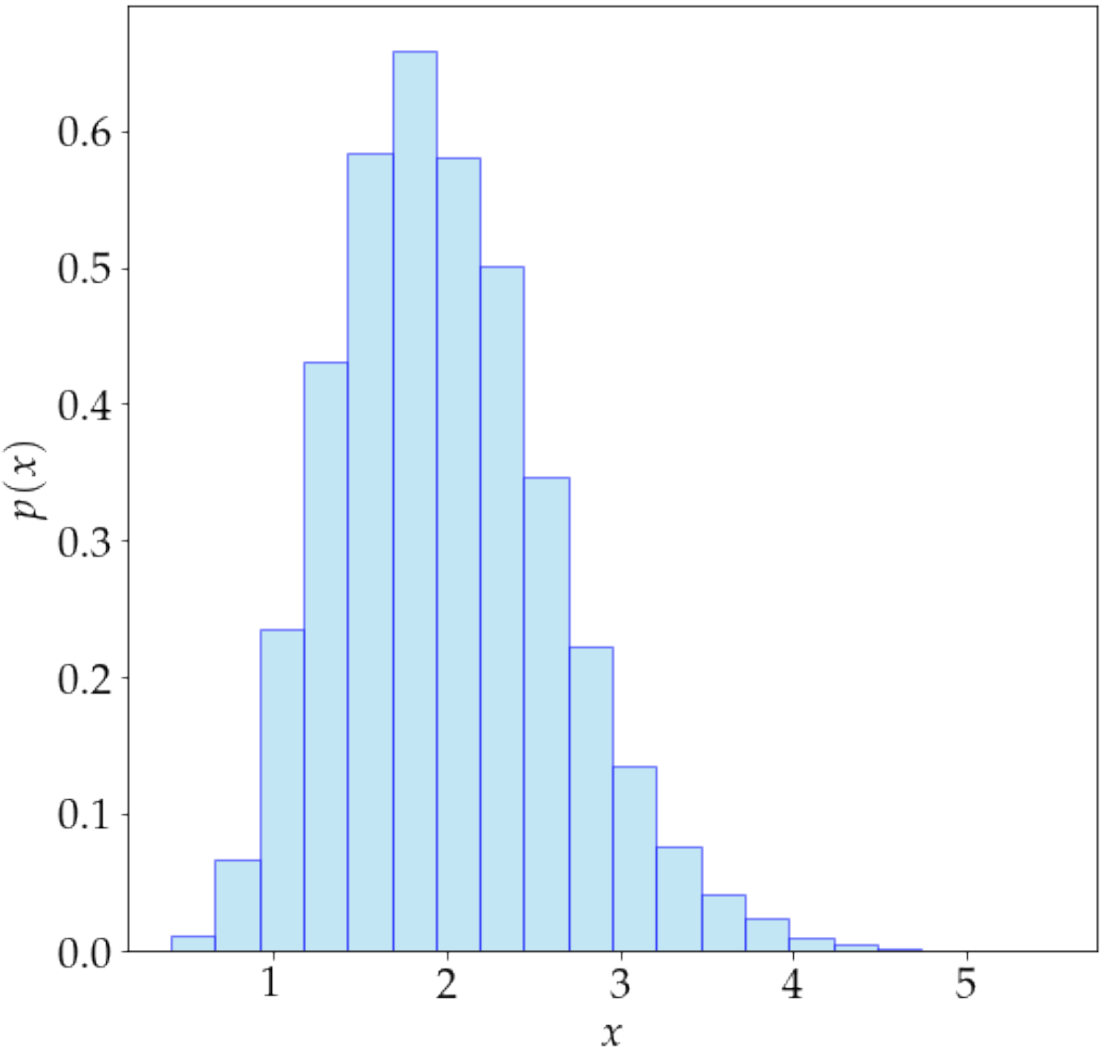
$$p(s|\alpha) = \frac{1}{\sqrt{2\pi\sigma_*^2}} \exp\left[-\frac{1}{2}\frac{(s-s_*)^2}{\sigma_*^2}\right]$$

where $s_* = \nabla\mathcal{L}(\alpha = \alpha_*)$ and $\sigma_*^2 = -\nabla^2\mathcal{L}(\alpha = \alpha_*)$. α_* is a chosen fiducial point.

3.0.3 Explore the Gamma Distribution

[2]:
```
shape = 10.0

# the rate is fixed
rate = 5.0

dist = torch.distributions.gamma.Gamma(shape, rate)

samples = dist.rsample([10000]).view(-1)
```

[3]:
```
plt.figure(figsize=(8,8))
plt.hist(samples, density=True, bins=20, ec='b', alpha=0.5, color='skyblue')
plt.ylabel(r'$p(x)$', fontsize = fontSize)
plt.xlabel(r'$x$', fontsize = fontSize)
plt.tick_params(axis='x', labelsize=fontSize)
plt.tick_params(axis='y', labelsize=fontSize)
plt.show()
```



3.0.4 Data

This is our data vector of size 500 and is fixed throughout the analysis.

[4]:
```
data = dist.rsample([300]).view(-1)
```

4 Gamma Distribution Likelihood

4.0.1 Parameter Estimation Case

We can infer α from the data (sanity check).

[5]:
```
def loglike_gamma(data, alpha: float, rate: float = 5.0):
```

```
    alpha = torch.tensor([alpha], dtype = torch.float32)

    rate = torch.tensor([rate], dtype = torch.float32)

    dist = torch.distributions.gamma.Gamma(alpha, rate)

    logp = dist.log_prob(data)

    loglike = torch.sum(logp).item()

    return loglike
```

[6]:
```
def logprior_normal(alpha, mean: float = 10.0, sigma: float = 1.0):

    alpha = torch.tensor([alpha], dtype = torch.float32)

    mean = torch.tensor([mean], dtype = torch.float32)

    sigma = torch.tensor([sigma], dtype = torch.float32)

    dist = torch.distributions.normal.Normal(mean, sigma)

    logprior = dist.log_prob(alpha).item()

    return logprior
```

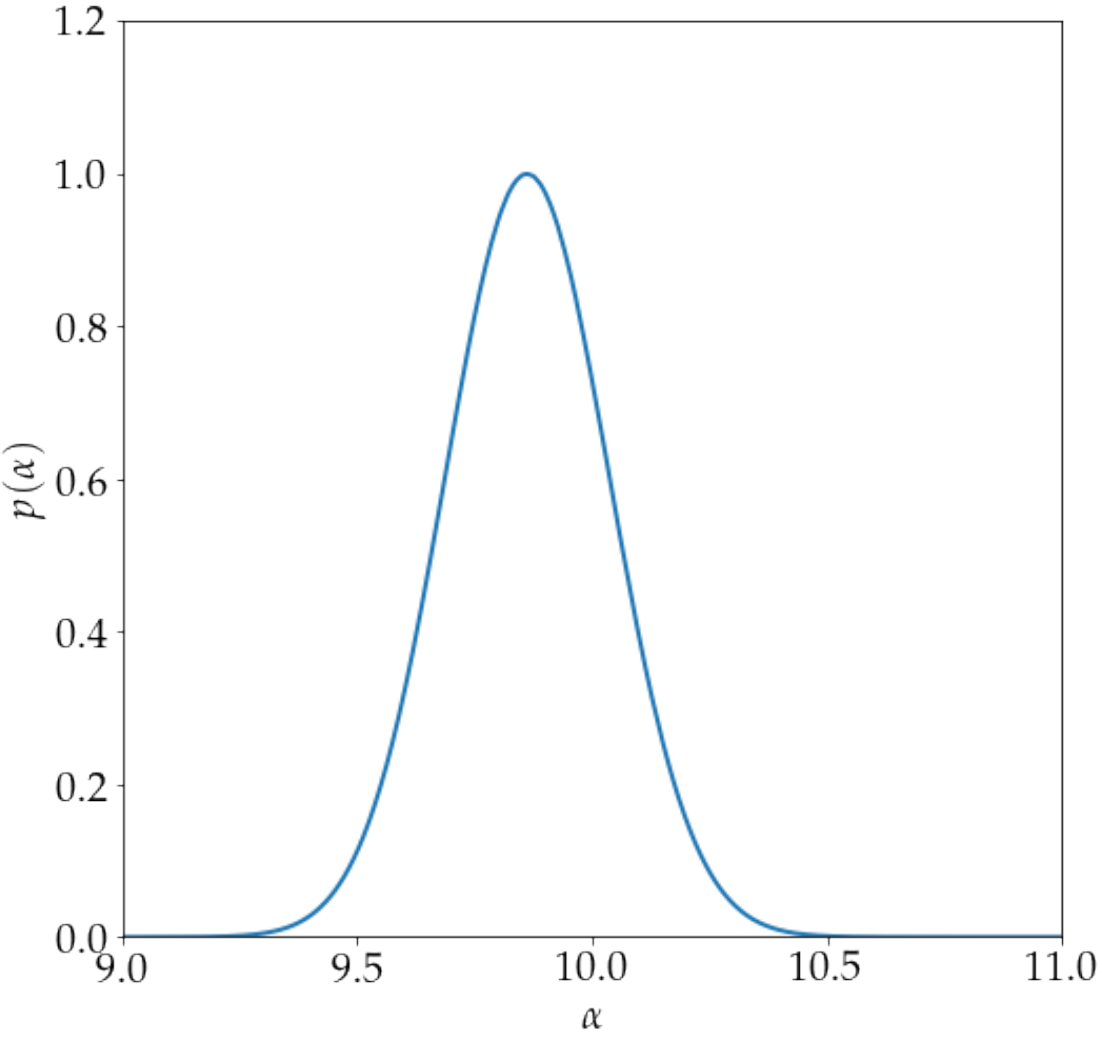
[7]:
```
npoint = 1000
alpha_grid = torch.linspace(9.0, 11.0, npoint)
logpost_gamma = torch.zeros(npoint)
```

[8]:
```
for i in range(npoint):

    # the value of alpha
    alpha_value = alpha_grid[i].item()

    # the log-posterior value
    logpost_gamma[i] = loglike_gamma(data, alpha_value)
    logpost_gamma[i] += logprior_normal(alpha_value)
```

[9]:
```
# the pdf normalised by the maximum
pdf_gamma = torch.exp(logpost_gamma - logpost_gamma.max())
```

[10]:
```
plt.figure(figsize = (8,8))
plt.plot(alpha_grid, pdf_gamma, lw = 2.0)
plt.ylabel(r'$p(\alpha)$', fontsize = fontSize)
plt.xlabel(r'$\alpha$', fontsize = fontSize)
```

```
plt.tick_params(axis='x', labelsize=fontSize)
plt.tick_params(axis='y', labelsize=fontSize)
plt.ylim(0.0, 1.2)
plt.xlim(min(alpha_grid), max(alpha_grid))
plt.show()
```



4.0.2 Summary Statistics

[11]:
```
pdf_gamma_norm = pdf_gamma/ torch.trapz(pdf_gamma, alpha_grid)
```

We can calculate the mean and variance as follows:

$$\mathbb{E}[\alpha] = \int \alpha \, p(\alpha|\boldsymbol{x}) \, \mathrm{d}\alpha$$

$$\mathrm{var}[\alpha] = \int \alpha^2 \, p(\alpha|\boldsymbol{x}) \, \mathrm{d}\alpha - \mathbb{E}^2[\alpha]$$

[12]:
```
mean_alpha = torch.trapz(alpha_grid*pdf_gamma_norm, alpha_grid)
```

[13]:
```
var_alpha = torch.trapz(alpha_grid**2 * pdf_gamma_norm, alpha_grid) -␣
↪mean_alpha**2
```

[14]:
```
print(f'The mean is {mean_alpha.item():.4f}')
print(f'The standard deviation is {var_alpha.sqrt().item():.4f}')
```

```
The mean is 9.8626
The standard deviation is 0.1741
```

Good - we expected a value around 10 since the samples (data) were generated from $X \sim \Gamma(10.0, 5.0)$.

4.0.3 Evidence Estimate

We basically need to do a 1D-integration of the posterior (up to a normalisation constant).

[15]:
```
evi_gamma = torch.trapz(pdf_gamma, alpha_grid)
```

[16]:
```
log_evi_gamma = logpost_gamma.max().item() + torch.log(evi_gamma)
```

[17]:
```
log_evi_gamma
```

[17]:
```
tensor(-283.0836)
```

5 Normal Distribution Likelihood

5.0.1 Parameter Estimation Case

[18]:
```
def loglike_normal(data, mean, sigma: float = 1.0):

    mean = torch.tensor([mean], dtype = torch.float32)

    sigma = torch.tensor([sigma], dtype = torch.float32)

    dist = torch.distributions.normal.Normal(mean, sigma)

    logp = dist.log_prob(data)

    loglike = torch.sum(logp).item()

    return loglike
```

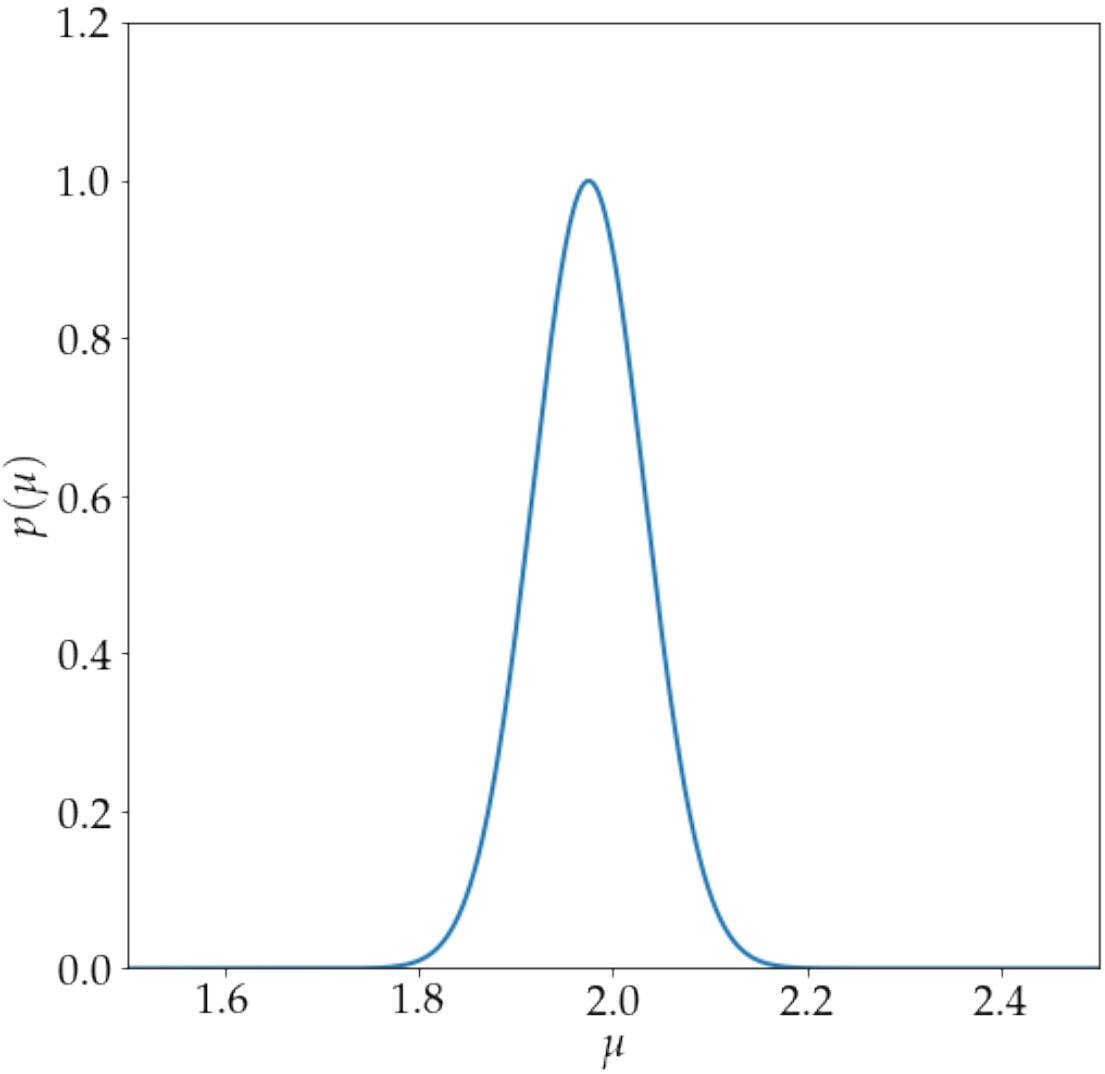
Looking at the Gamma distribution above, the mean is roughly centered on 2.

[19]:
```
npoint = 1000
mu_grid = torch.linspace(1.5, 2.5, npoint)
logpost_normal = torch.zeros(npoint)
```

[20]:
```
for i in range(npoint):

    # the value of alpha
    mu_value = mu_grid[i].item()

    # the log-posterior value
    logpost_normal[i] = loglike_normal(data, mu_value)

    # add the prior contribution with a mean = 2.0 and standard deviation = 1.0
    logpost_normal[i] += logprior_normal(mu_value, 2.0, 1.0)
```

[21]:
```
# the pdf normalised by the maximum
pdf_normal = torch.exp(logpost_normal - logpost_normal.max())
```

[22]:
```
plt.figure(figsize = (8,8))
plt.plot(mu_grid, pdf_normal, lw = 2.0)
plt.ylabel(r'$p(\mu)$', fontsize = fontSize)
plt.xlabel(r'$\mu$', fontsize = fontSize)
plt.tick_params(axis='x', labelsize=fontSize)
plt.tick_params(axis='y', labelsize=fontSize)
plt.ylim(0.0, 1.2)
plt.xlim(min(mu_grid), max(mu_grid))
plt.show()
```



[23]:
```
evi_normal = torch.trapz(pdf_normal, mu_grid)
```

[24]:
```
log_evi_normal = logpost_normal.max().item() + torch.log(evi_normal)
```

[25]:
```
log_evi_normal
```

[25]:
```
tensor(-339.0552)
```

[26]:
```
logBF = log_evi_gamma - log_evi_normal
print(f'The log-Bayes factor between Model 1 (Gamma) and Model 2 (Normal) is␣
 ↪{logBF:.2f}')
```

```
The log-Bayes factor between Model 1 (Gamma) and Model 2 (Normal) is 55.97
```

Good - we expect the Gamma likelihood function to be better compared to a Gaussian likelihood

function.

6 Compression - Score Function

[27]:
```
def score_compression_gamma(data, alpha: float, rate: float = 5.0):

    alpha = torch.tensor([alpha], dtype = torch.float32)

    # we need the derivatives with respect to the shape parameter
    alpha.requires_grad = True

    rate = torch.tensor([rate], dtype = torch.float32)

    dist = torch.distributions.gamma.Gamma(alpha, rate)

    # the log-likelihood
    log_like = dist.log_prob(data).sum()

    # gradient of log-likelihood with respect to shape (alpha)
    grad_log_like = torch.autograd.grad(log_like, alpha, create_graph=True)[0]

    # the second derivative with respect to shape (alpha)
    hessian = torch.autograd.grad(grad_log_like, alpha)[0]

    return grad_log_like.item(), hessian.item()
```

We will choose $\alpha = 10.0$ as the expansion (fiducial) point. We can also quickly compute the Maximum Likelihood Estimator (MLE), that is, find α_{MLE} for which $\nabla\mathcal{L} = 0$ and this happens at:

$$\alpha_{\text{MLE}} = \frac{\beta}{N}\sum_{i=1}^{N} x_i$$

In our work, $\beta = 5.0$. So we want just compute α_{MLE}.

[28]:
```
# Maximum likelihood estimate
torch.mean(data).item() * 5.0
```

[28]:
```
9.87557053565979
```

[29]:
```
# compress the data at the shape parameter = 10.0

s_data, h_data = score_compression_gamma(data, 10.0)
```

[30]:
```
print(f'Error estimate of the score: {np.sqrt(-1.0 / h_data):.4f}')
```

```
Error estimate of the score: 0.1780
```

[31]:
```
print(f'Previously, we estimated the standard deviation of the shape parameter␣
↪using the posterior as: {var_alpha.sqrt().item():.4f}')
```

```
Previously, we estimated the standard deviation of the shape parameter using the
posterior as: 0.1741
```

7 ISSUE below

The pdf is *always* centred on the expansion point? and the error estimate on α does not look good!

[32]:
```
def loglike_gamma_score(alpha, data, score, hessian, rate: float = 5.0):

    grad, _ = score_compression_gamma(data, alpha, rate)

    # print(grad)

    # calculate the variance (inverse of hessian)
    var = torch.tensor([-1. / hessian])

    std = torch.sqrt(var)

    gaussian = torch.distributions.normal.Normal(score, std)

    loglike = gaussian.log_prob(torch.tensor([grad]))

    return loglike
```

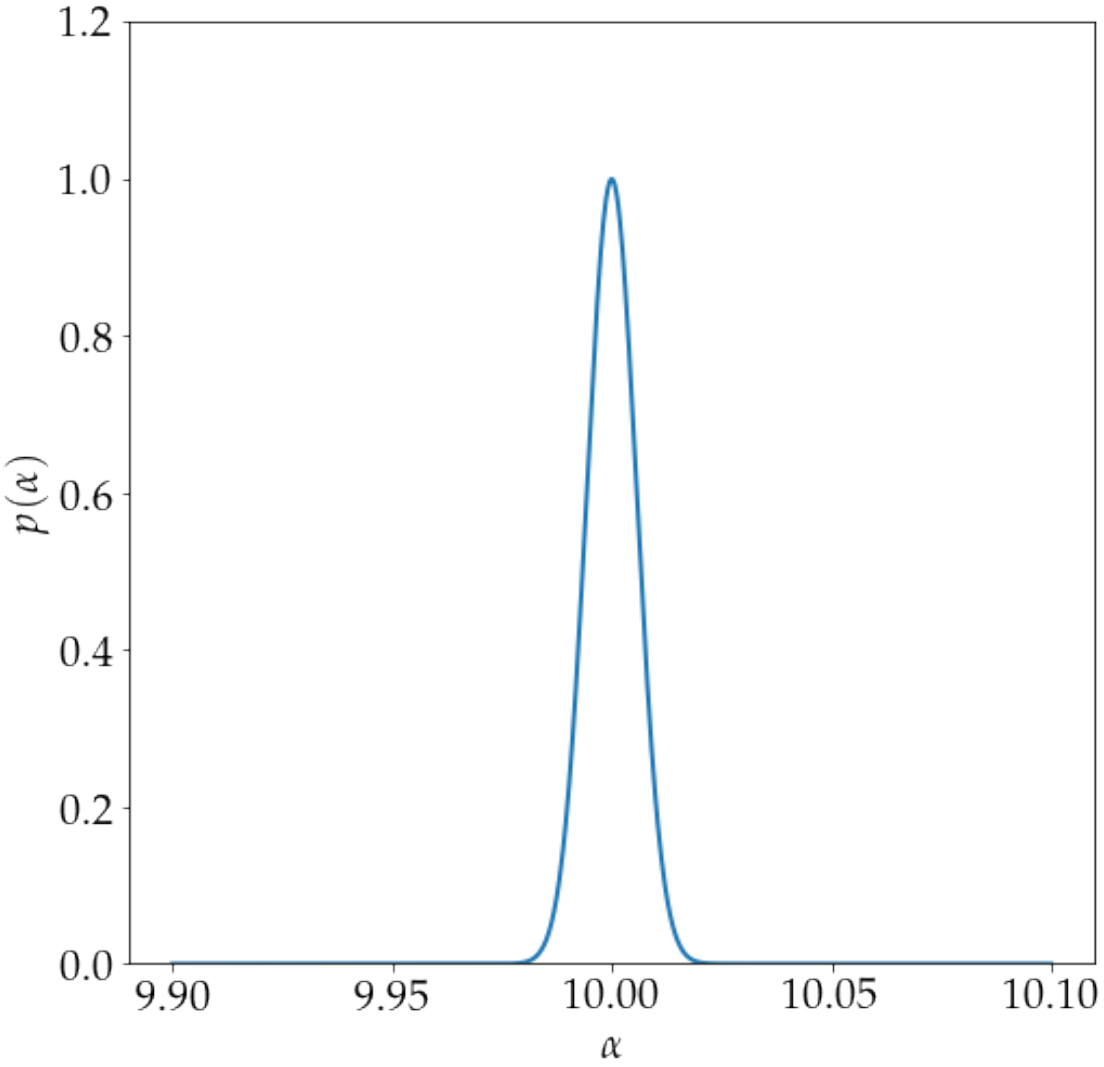
[33]:
```
logpost_gamma_score = torch.zeros(npoint)
```

[34]:
```
alpha_test = torch.linspace(9.90, 10.10, 1000)
for i in range(npoint):

    # the value of alpha
    alpha_value = alpha_test[i].item()

    # the log-posterior value
    logpost_gamma_score[i] = loglike_gamma_score(alpha_value, data, s_data,␣
↪h_data, rate = 5.0)
    logpost_gamma_score[i] += logprior_normal(alpha_value, 10.0, 1.0)
```

[35]:
```
# the pdf normalised by the maximum
pdf_gamma_score = torch.exp(logpost_gamma_score - logpost_gamma_score.max())
```

[36]:
```
plt.figure(figsize = (8,8))
plt.plot(alpha_test, pdf_gamma_score, lw = 2.0)
plt.ylabel(r'$p(\alpha)$', fontsize = fontSize)
plt.xlabel(r'$\alpha$', fontsize = fontSize)
```

```
plt.tick_params(axis='x', labelsize=fontSize)
plt.tick_params(axis='y', labelsize=fontSize)
plt.ylim(0.0, 1.2)
# plt.xlim(min(alpha_grid), max(alpha_grid))
plt.show()
```

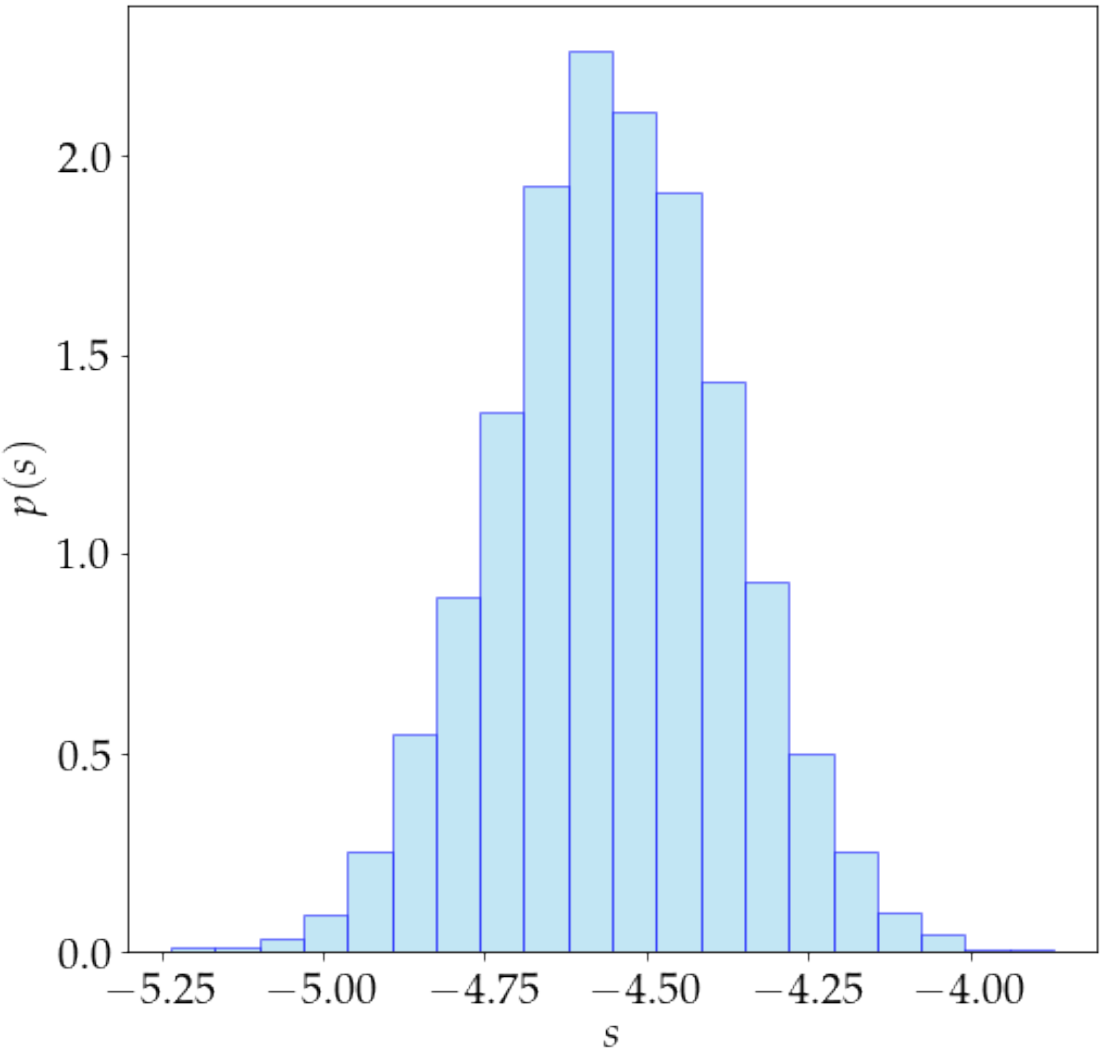


7.0.1 Test

We can just sample the score, given the score function calculated at $\alpha = 10.0$ and the error estimate. This looks good but we would expect the error estimate on α to be of the same width (since the Hessian is just the second derivative of the log-likelihoood with respect to the parameter α). Maybe not - maybe we need a lot of data for the likelihood to peak. Maybe the likelihood surface is too broad.

[37]:
```
gaussian_test = torch.distributions.normal.Normal(s_data, np.sqrt(-1.0 /␣
↪h_data))
```

[38]:
```
plt.figure(figsize=(8,8))
plt.hist(gaussian_test.rsample([10000]), density=True, bins=20, ec='b', alpha=0.
↪5, color='skyblue')
plt.ylabel(r'$p(s)$', fontsize = fontSize)
plt.xlabel(r'$s$', fontsize = fontSize)
plt.tick_params(axis='x', labelsize=fontSize)
plt.tick_params(axis='y', labelsize=fontSize)
plt.show()
```



[ ]: