Coding Lab 8

Neural Data Science

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```
import seaborn as sns
import matplotlib.pyplot as plt
import matplotlib as mpl
import numpy as np

mpl.rc("savefig", dpi=72)
sns.set_style('whitegrid')
%matplotlib inline
```

Task: Implement entropy estimators

General framework

Entropy is defined as

$$H[p] = -\sum_x p_x \log p_x$$

where $p_x = p(x = X)$. Here we assume that X is a discrete random variable and that there are finitely many states K that X can take.

We are interested in the entropy of discrete random variables, because of its relationship with mutual information:

$$I[X|Y] = H[X] - H[X|Y]$$

If we can estimate the entropy well, we can estimate the mutual information well. An application in neuroscience would be estimating the mutual information between a spike train modeled as a sequence of 1 s and 0 s (e.g. $(0, 1, 0, 1, 1)$) and a discrete set of stimuli.

Note that a multivariate binary distribution modeling a spike train can always be mapped to a discrete univariate distribution, $\mathbb{Z}_2 \longrightarrow \mathbb{Z}_+$, by interpreting each binary state $z \in \mathbb{Z}_2$ as its corresponding binary number and computing $f(z) = \sum_i 2^i z_i$.

As discussed in the lecture, the problem is that one always underestimates the true entropy of a distribution from samples. In this exercise you are meant to implement different estimators for discrete entropy and evaluate them on different discrete distributions:

- Uniform distribution:
$$p(x = X) = \frac{1}{K}$$
- "Zipf's law"- distribution:
$$p(x = X) = \frac{1}{Zx}$$
where
$$Z = \sum_k 1/k$$

There is a really good series of blog posts about discrete entropy estimation to be found here, here and here.

Make sure you use binary logarithms throughout.

Implementation of the estimators

Implement the

- maximum likelihood estimator (1 pt)
- miller-maddow corrected estimator (1 pt)
- jack-knife corrected estimator (2 pt)
- coverage adjusted estimator (1 pt).

When implementing the jack-knife estimator, you may want to restrict the amount of resampling for performance reasons e.g. to 1000, even if more samples are available.

By definition, $0 \log 0 = 0$. Adapt the interfaces as needed for your implementation.

In addition, implement or use one of the following more advanced estimators (1+3 pts, extra points if you use your own implementation):

- JVHW estimator with code on github
- Unseen estimator (includes Matlab code in Supplementary)
- Best Upper Bounds estimator (Matlab code available on Ilias)

For this part, you are allowed to use an existing implementation as well.

MLE

$$H_{ML} = -\sum_x \hat{p}(x) log(\hat{p}(x))$$

```
def entropy_mle(phat):
    '''Maximum likelihood or plug-in estimator of discrete entropy

    Parameter
    ---------

    phat: np.array, shape=(n_bins, )
        Estimate of the distribution / histogram

    Return
    ------
    H: float
        Entropy estimate
    '''
    # insert your code here (1 pt)
    # where is phat zero, calulate with 0log0 = 0
    H = -np.sum([p * np.log2(p) if p != 0 else 0 for p in phat])
    return H
```

Miller-Maddow corrected

$$H_{MM} = H_{ML} + \frac{\hat{d} - 1}{2n}$$

$$\hat{d} = \#[\hat{p}(x) > 0]$$

```
def entropy_mm(phat, n):
    '''Miller-Maddow corrected estimator of discrete entropy
    Parameters
    ----------

    phat: np.array, shape=(n_bins, )
        Estimate of the distribution / histogram

    n:  int
        Number of samples


    Return
    ------

    H: float
        Entropy estimate
    '''

    # insert your code here (1 pt)
    dhat = np.sum(phat > 0)
    H = entropy_mle(phat) + (dhat - 1) / (2 * n)

    return H
```

Jack-knife corrected

$$\hat{H}_{JK} = N\hat{H}_{ML} - (N-1)\hat{H}_{ML}^{(.)}$$

$$\hat{H}_{ML}^{(.)} =< H_{ML}^{\neg i} >$$

```
def entropy_jk(x, edges, max_resamples=1000):
    '''Jack-knife corrected estimator of discrete entropy

    Parameters
    ----------
    x: np.array, shape=(n_samples, )
        Samples

    edges: np.array, shape=(n_bins, )
        Histogram bin edges
    max_resamples: int, optional (default=1000)
        Maximum number of resamples to use for the jack-knife estimator


    Return
    ------

    H: float
        Entropy estimate
    '''
    if len(x) > 1000:
        max_resamples = 1000
    else:
        max_resamples = len(x)
    phat = np.histogram(x, bins=edges)[0] / len(x)
    n = len(x)
    H_forloop = np.zeros(max_resamples)
    for i in range(max_resamples):
        x_i = np.delete(x, i)
        phat_i = np.histogram(x_i, bins=edges)[0] / (n - 1)
        H_i = entropy_mle(phat_i)
        H_forloop[i]= H_i
    H_dot = np.mean(H_forloop)

    H = n * entropy_mle(phat) - (n - 1) * H_dot
    return H
```

Coverage-adjusted

$$C = 1 - \frac{\# f_i = 1}{N}$$

$$\hat{P}_C = \hat{P} \cdot C$$

$$H_{CA} = -\sum_x \frac{\hat{P}_C(x) log(\hat{P}_C(x))}{1 - (1 - \hat{P}_C(x))^N}$$

```
def entropy_cae(phat, n):
    '''coverage-adjusted estimator of discrete entropy

    Parameters
    ----------

    phat: np.array, shape=(n_bins, )
        Estimate of the distribution / histogram

    n: int
        Number of samples.


    Return
    ------

    H: float
        Entropy estimate
    '''

    # insert your code here (1 pt)
    # calulate singletons in phat
    unique, counts = np.unique(phat, return_counts=True)
    singletons = unique[counts == 1]

    if singletons.size == 0:
        singletons = 1
    else:
        singletons = np.sum(counts==1)

    C = 1 - (singletons)/n
    PC = phat * C
    PCs = [p * np.log2(p) if p != 0 else 0 for p in PC]
    H = -np.nansum(PCs / (1 - ((1 - PC) ** n)))
    return H
```

JVHW

```
import est_entro as ee

def entropy_jvhw(x):
    '''JVHW estimator of discrete entropy.

    Parameter
    ---------
    x: np.array, shape=(n_samples, )
        Samples

    Return
    ------
    H: float
        Entropy estimate
    '''

    # insert your code here (1 pt)
    H = ee.est_entro_JVHW(x)

    return H
```

Optional: Unseen or Best Upper Bounds estimator

```
# insert your code here

# ------------------------------------------
# Port Unseen or Best Upper Bounds estimator
# from MatLab to Python. (3 bonus pts)
# ------------------------------------------

import numpy as np
from scipy.stats import poisson
from scipy.optimize import linprog

def unseen(f):
    """
    Input: fingerprint f, where f[i] represents number of elements that
    appear i times in a sample. Thus sum(i*f[i]) = sample size.
    Output: approximation of 'histogram' of true distribution. Specifically,
    histx[i] represents the number of domain elements that occur with
    probability x[i]. Thus sum(x[i]*histx[i]) = 1, as distributions have
    total probability mass 1.
    An approximation of the entropy of the true distribution can be computed
    as: Entropy = (-1)*sum(histx.*x.*log(x))
    """
    f = np.array(f)
    k = np.sum(np.arange(len(f)) * f)  # total sample size

    # algorithm parameters
    grid_factor = 1.1  # the grid of probabilities will be geometric, with this ratio.
    alpha = 0.5  # the allowable discrepancy between the returned solution and the "best"
    x_lp_min = 1 / (k * max(10, k))  # minimum allowable probability.
    max_lp_iters = 1000  # the 'MaxIter' parameter for scipy's linprog LP solver.

    # Split the fingerprint into the 'dense' portion for which we solve an LP to yield the
    # and 'sparse' portion for which we simply use the empirical histogram
    x = np.array([0])
    histx = np.array([0])
    f_lp = np.zeros(len(f))
    for i in range(len(f)):
        if f[i] > 0:
            wind = [max(1, i - int(np.ceil(np.sqrt(i)))), min(i + int(np.ceil(np.sqrt(i)))
            if np.sum(f[wind[0]:wind[1]]) < 2 * np.sqrt(i):
                x = np.append(x, i / k)
                histx = np.append(histx, f[i])
                f_lp[i] = 0
            else:
                f_lp[i] = f[i]

    # If no LP portion, return the empirical histogram
    f_max = np.max(np.where(f_lp > 0))
    if len(f_max) == 0:
        x = x[1:]
        histx = histx[1:]
    if np.min(np.shape(f_max)) == 0:
        x = x[1:]
        histx = histx[1:]
        return histx, x
```

```
# Set up the first LP
lp_mass = 1 - np.dot(x, histx)  # amount of probability mass in the LP region
f_lp = np.append(f_lp[:f_max], np.zeros(int(np.ceil(np.sqrt(f_max)))))
sz_lp_f = len(f_lp)
x_lp_max = f_max / k
x_lp = x_lp_min * np.power(grid_factor, np.arange(int(np.ceil(np.log(x_lp_max / x_lp_m
sz_lp_x = len(x_lp)
objf = np.zeros(sz_lp_x + 2 * sz_lp_f)
objf[sz_lp_x::2] = 1 / np.sqrt(f_lp + 1)  # discrepancy in ith fingerprint expectation
objf[(sz_lp_x+1)::2] = 1 / np.sqrt(f_lp + 1)  # weighted by 1/sqrt(f(i) + 1)
A = np.zeros((2 * sz_lp_f, sz_lp_x + 2 * sz_lp_f))
b = np.zeros(2 * sz_lp_f)
for i in range(sz_lp_f):
    A[2*i-1, :sz_lp_x] = poisson.pmf(i+1, k * x_lp)
    A[2*i, :sz_lp_x] = -A[2*i-1, :sz_lp_x]
    A[2*i-1, sz_lp_x+2*i-1] = -1
    A[2*i, sz_lp_x+2*i] = -1
    b[2*i-1] = f_lp[i]
    b[2*i] = -f_lp[i]
Aeq = np.zeros(sz_lp_x + 2 * sz_lp_f)
Aeq[:sz_lp_x] = x_lp
beq = lp_mass

# Solve the 1st LP
res_lp1 = linprog(objf, A_ub=A, b_ub=b, A_eq=Aeq, b_eq=beq, bounds=(0, None), method='
                  options={'maxiter': max_lp_iters})
if res_lp1.status == 0:
    print('maximum number of iterations reached--try increasing max_lp_iters')
if res_lp1.status < 0:
    print('LP1 solution was not found, still solving LP2 anyway...')

# Solve the 2nd LP, which minimizes support size subject to incurring at most alpha wo
# (of the objective function in the previous LP).
objf2 = np.zeros(sz_lp_x + 2 * sz_lp_f)
objf2[:sz_lp_x] = 1
A2 = np.vstack((A, objf1))
b2 = np.append(b, res_lp1.fun + alpha)
for i in range(sz_lp_x):
    objf2[i] = objf2[i] / x_lp[i]  # rescaling for better conditioning
res_lp2 = linprog(objf2, A_ub=A2, b_ub=b2, A_eq=Aeq, b_eq=beq, bounds=(0, None), metho
                  options={'maxiter': max_lp_iters})
# append LP solution to empirical portion of histogram
sol2 = res_lp2.x[:sz_lp_x] / x_lp
x = np.append(x, x_lp)
histx = np.append(histx, sol2)
ind = np.argsort(x)
x = x[ind]
histx = histx[ind]
ind = np.where(histx > 0)
x = x[ind]
histx = histx[ind]

return x
```

Uniform distribution

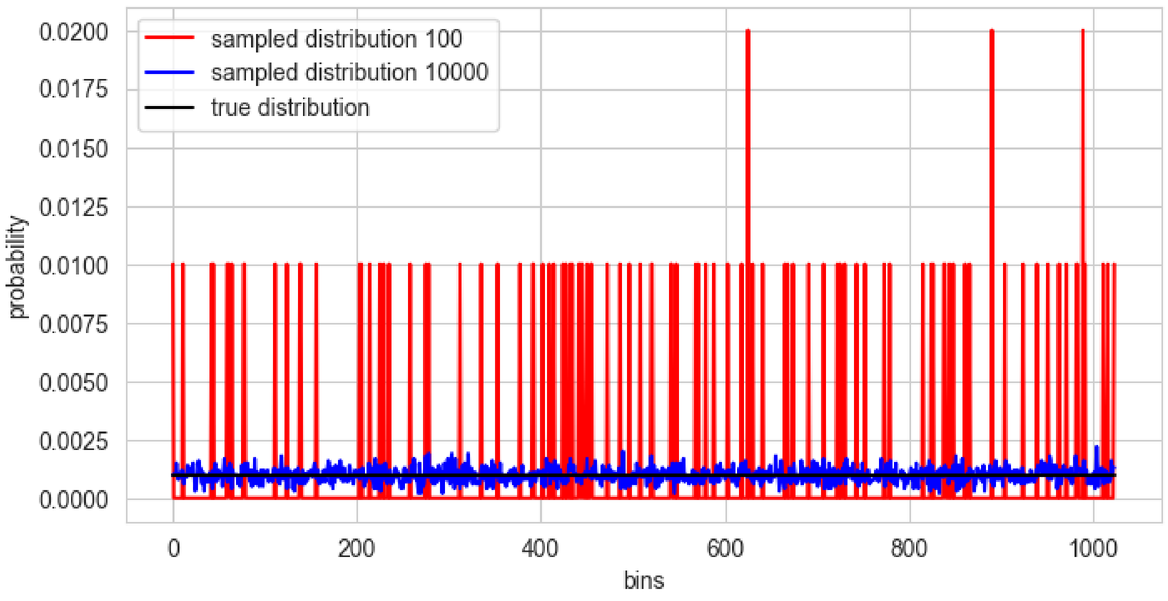
```
D = 10
N = 2**D

p = 1/N * np.ones(N)   # true distribution

H = - np.sum(p * np.log2(p))  # true entropy

print(H)
```

```
10.0
```

Sample from the uniform distribution using sample sizes of 100 and 10000. Plot the true distribution and the sampled distributions. What do you notice? (2 pt)

```
# insert your code here

# ------------------------------------
# Sample from the uniform distribution
# using sample size of 100 (0.5 pts)
# ------------------------------------
uniform_samples = np.random.choice(N, size=100, p=p)
#uniform_samples = np.random.randint(low=0, high=D ,size=100)

# ------------------------------------
# Sample from the uniform distribution
# using sample size of 10000 (0.5 pts)
# -----------------------------------
uniform_samples_2 = np.random.choice(N, size=10000, p=p)

#uniform_samples_2 = np.random.randint(low=0, high=D ,size=10000)

# -----------------------------------
# Plot the true distribution and
# the sampled distributions. (0.5 pts)
# -----------------------------------

fig, ax = plt.subplots(1, 1, figsize=(8, 4))
# plot the true distribution

# plot the sampled distribution
ax.plot(np.histogram(uniform_samples, bins=N)[0] / 100, 'r', label='sampled distribution 1
ax.plot(np.histogram(uniform_samples_2, bins=N)[0] / 10000, 'b', label='sampled distributi
ax.plot(p, 'k', label='true distribution')

ax.set_xlabel('bins')
ax.set_ylabel('probability')
ax.legend(loc='best')

# we noticed that the sampled distribution is not as smooth as the true distribution becau
# but if you would to enlarge the sample size, the sampled distribution will be more smoot
```

```
<matplotlib.legend.Legend at 0x154049010>
```



Use the framework below to generate samples of different size (logarithmically spaced between 10 and 100000) and evaluate the different entropy estimators for multiple runs.

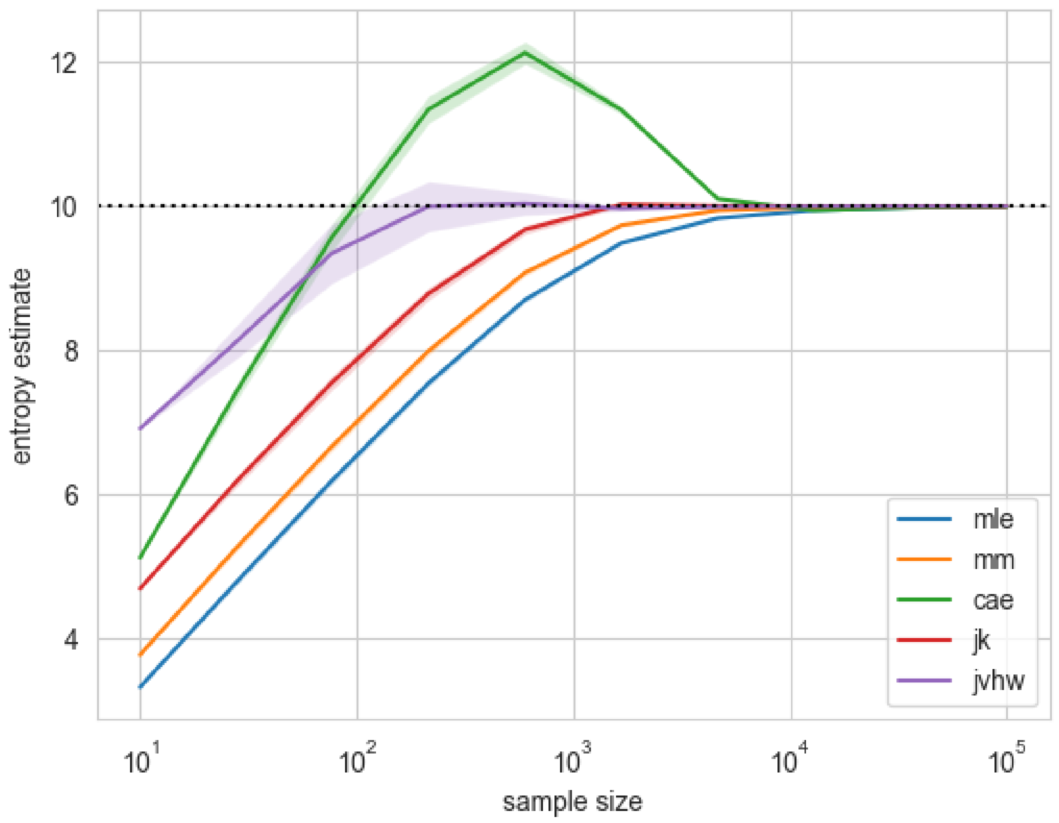
```
sample_sizes = np.round(np.logspace(1,5,num=10))
n_runs = 30

edges = np.arange(-0.5, N, 1)

h_mle  = np.zeros((len(sample_sizes), n_runs))
h_mm   = np.zeros((len(sample_sizes), n_runs))
h_jk   = np.zeros((len(sample_sizes), n_runs))
h_cae  = np.zeros((len(sample_sizes), n_runs))
h_jvhw = np.zeros((len(sample_sizes), n_runs))
h_unseen = np.zeros((len(sample_sizes), n_runs))

# add h_unseen or h_bub here if you implemented them.

for i, S in enumerate(sample_sizes):
    for j in np.arange(n_runs):

        # -----------------------------------
        # Sample from the uniform distribution
        # with different sample size (0.5 pts)
        # -------------------------------------
        x = np.random.choice(N, size=int(S), p=p)
        phat = np.histogram(x, bins=edges)[0] / S
        # insert your code here
        zip_h_mle[i,j]  = entropy_mle(phat)
        h_mm[i,j]   = entropy_mm(phat, S)
        h_cae[i,j]  = entropy_cae(phat, S)
        h_jk[i,j]   = entropy_jk(x, edges)
        h_jvhw[i,j] = entropy_jvhw(x)
        # add h_unseen or h_bub here if you implemented them.
        #h_unseen[i,j] = unseen(x)
```

```
/var/folders/6f/4s63gb612m185fbsprljhfmh0000gn/T/ipykernel_9254/1409420637.py:34: RuntimeWar
  H = -np.nansum(PCs / (1 - ((1 - PC) ** n)))
/var/folders/6f/4s63gb612m185fbsprljhfmh0000gn/T/ipykernel_9254/641789983.py:29: Deprecation
  h_jvhw[i,j] = entropy_jvhw(x)
```

Plot the resulting average estimate of the entropy for each of the estimators. Which is best? If you implemented everything correctly, this plot should roughly look like in the lecture.

```
plt.figure()
plt.semilogx(sample_sizes, np.mean(h_mle,  axis=1), label='mle')
plt.fill_between(sample_sizes, np.mean(h_mle, axis=1) - np.std(h_mle, axis=1), np.mean(h_m
plt.semilogx(sample_sizes, np.mean(h_mm,   axis=1), label='mm')
plt.fill_between(sample_sizes, np.mean(h_mm, axis=1) - np.std(h_mm, axis=1), np.mean(h_mm,
plt.semilogx(sample_sizes, np.mean(h_cae,  axis=1), label='cae')
plt.fill_between(sample_sizes, np.mean(h_cae, axis=1) - np.std(h_cae, axis=1), np.mean(h_c
plt.semilogx(sample_sizes, np.mean(h_jk,   axis=1), label='jk')
plt.fill_between(sample_sizes, np.mean(h_jk, axis=1) - np.std(h_jk, axis=1), np.mean(h_jk,
plt.semilogx(sample_sizes, np.mean(h_jvhw, axis=1), label='jvhw')
plt.fill_between(sample_sizes, np.mean(h_jvhw, axis=1) - np.std(h_jvhw, axis=1), np.mean(h

# plot h_unseen or h_bub here if you implemented them.

plt.axhline(H, color='black', linestyle=':')
plt.xlabel('sample size')
plt.ylabel('entropy estimate')
plt.legend()
```

```
<matplotlib.legend.Legend at 0x1555ee710>
```



Zipf distribution

Zipf's law refers to a family of power law like distributions for which $p_k \sim 1/k^d$. We will simply use $d = 1$ here.

Adapt the framework above to sample from a Zipf distribution and evaluate the estimators for this case. Are there differences to the uniform case? (2 pts)

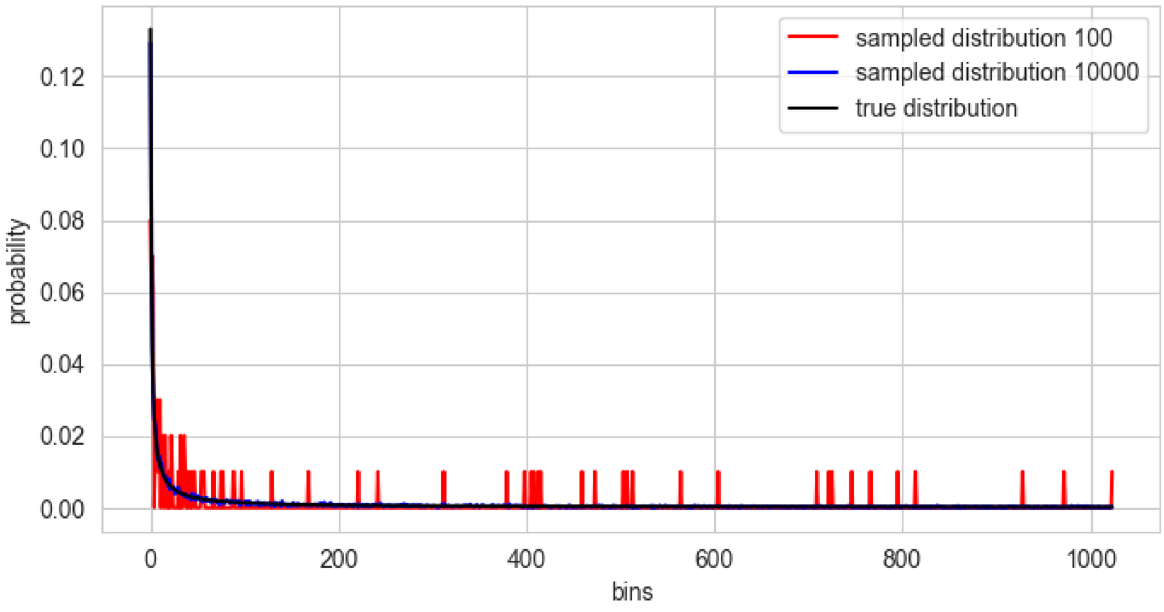
```
D = 10
N = 2**D

p = 1/(np.arange(0,N)+1)     # true distribution
p = p/np.sum(p)

H_zipf = - np.sum(p * np.log2(p))  # true entropy

print(H_zipf)
```

```
7.510649703297878
```

Sample from the Zipf distribution using sample sizes of 100 and 10000. In this case, the function `random.choice` is very helpful for sampling. Plot the true distribution and the sampled distributions. What do you notice?

```
# insert your code here

# ---------------------------------------
# Sample from the Zipf distribution
# using sample size of 100 (0.5 pts)
# ---------------------------------------
zipf_samples = np.random.choice(N, size=100, p=p)

# ---------------------------------------
# Sample from the Zipf distribution
# using sample size of 10000 (0.5 pts)
# ---------------------------------------
zipf_samples_2 = np.random.choice(N, size=10000, p=p)

# ---------------------------------------
# Plot the true distribution and the sampled
# distributions. (0.5 pts)
# ---------------------------------------
fig, ax = plt.subplots(1, 1, figsize=(8, 4))
# plot the true distribution

ax.plot(np.histogram(zipf_samples, bins=N)[0] / 100, 'r', label='sampled distribution 100'
ax.plot(np.histogram(zipf_samples_2, bins=N)[0] / 10000, 'b', label='sampled distribution
ax.plot(p, 'k', label='true distribution')
ax.set_xlabel('bins')
ax.set_ylabel('probability')
ax.legend(loc='best')


# we noticed that the sampled distribution is not as smooth as the true distribution becau
```

```
<matplotlib.legend.Legend at 0x1546d2810>
```



Use the framework below to generate samples of different size (logarithmically spaced between 10 and 100000) and evaluate the different entropy estimators for multiple runs.

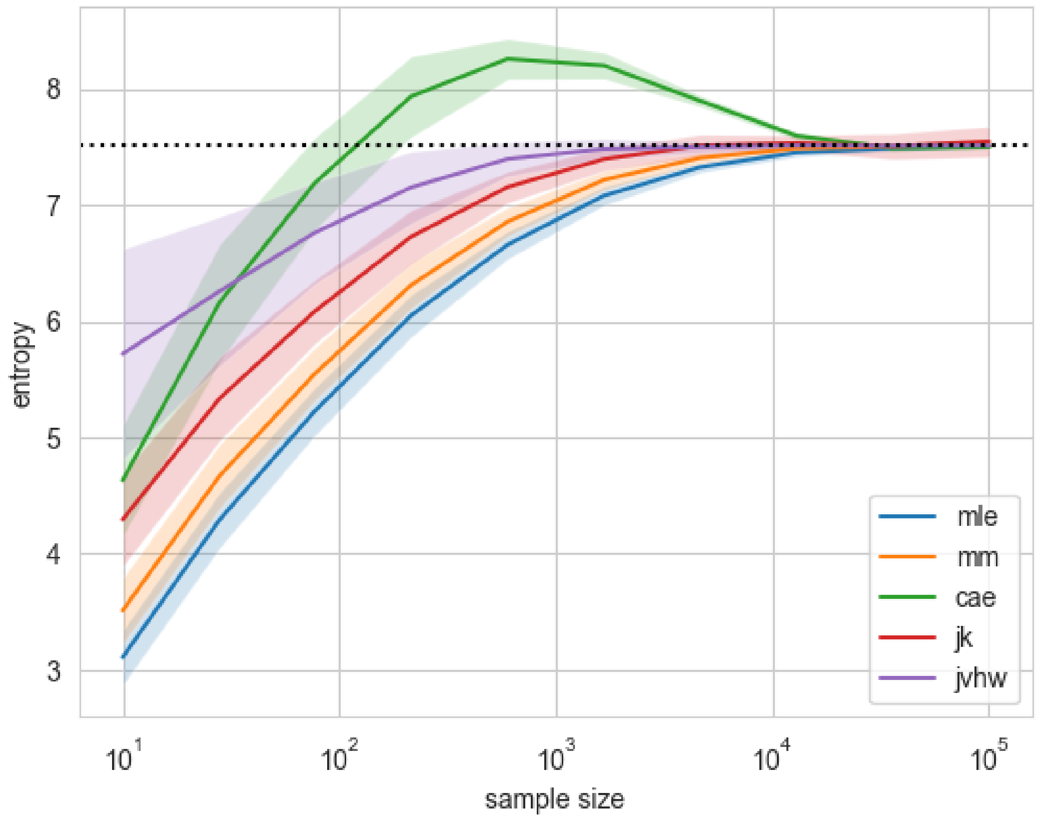
```
sample_sizes = np.round(np.logspace(1,5,num=10))
n_runs = 30

edges = np.arange(-0.5, N, 1)

zip_h_mle  = np.zeros((len(sample_sizes), n_runs))
zip_h_mm   = np.zeros((len(sample_sizes), n_runs))
zip_h_jk   = np.zeros((len(sample_sizes), n_runs))
zip_h_cae  = np.zeros((len(sample_sizes), n_runs))
zip_h_jvhw = np.zeros((len(sample_sizes), n_runs))

# add h_unseen or h_bub here if you implemented them.

for i, S in enumerate(sample_sizes):
    for j in np.arange(n_runs):

        # ---------------------------------------
        # Sample from the Zipf distribution
        # with different sample size (0.5 pts)
        # ---------------------------------------
        x = np.random.choice(N, size=int(S), p=p)
        phat = np.histogram(x, bins=edges)[0] / S

        # insert your code here

        zip_h_mle[i,j]  = entropy_mle(phat)
        zip_h_mm[i,j]   = entropy_mm(phat, S)
        zip_h_cae[i,j]  = entropy_cae(phat, S)
        zip_h_jk[i,j]   = entropy_jk(x, edges)
        zip_h_jvhw[i,j] = entropy_jvhw(x)
```

```
/var/folders/6f/4s63gb612m185fbsprljhfmh0000gn/T/ipykernel_9254/1409420637.py:34: RuntimeWarn
  H = -np.nansum(PCs / (1 - ((1 - PC) ** n)))
/var/folders/6f/4s63gb612m185fbsprljhfmh0000gn/T/ipykernel_9254/47445998.py:30: DeprecationWa
  zip_h_jvhw[i,j] = entropy_jvhw(x)
```

Plot resulting average estimate of the entropy for each of the estimators. Which is best? If you implemented everything correctly, this plot should roughly look like in the lecture.

```
plt.figure()

plt.semilogx(sample_sizes, np.mean(zip_h_mle,  axis=1), label='mle')
# plot std error
plt.fill_between(sample_sizes, np.mean(zip_h_mle,  axis=1) - np.std(zip_h_mle,  axis=1), n

plt.semilogx(sample_sizes, np.mean(zip_h_mm,   axis=1), label='mm')
plt.fill_between(sample_sizes, np.mean(zip_h_mm,  axis=1) - np.std(zip_h_mm,  axis=1), np.

plt.semilogx(sample_sizes, np.mean(zip_h_cae,  axis=1), label='cae')
plt.fill_between(sample_sizes, np.mean(zip_h_cae,  axis=1) - np.std(zip_h_cae,  axis=1), n

plt.semilogx(sample_sizes, np.mean(zip_h_jk,   axis=1), label='jk')
plt.fill_between(sample_sizes, np.mean(zip_h_jk,  axis=1) - np.std(zip_h_jk,  axis=1), np.

plt.semilogx(sample_sizes, np.mean(zip_h_jvhw, axis=1), label='jvhw')
plt.fill_between(sample_sizes, np.mean(zip_h_jvhw,  axis=1) - np.std(zip_h_jvhw,  axis=1),

# plot h_unseen or h_bub here if you implemented them.
plt.ylabel('entropy')
plt.xlabel('sample size')
plt.axhline(H_zipf, color='black', linestyle=':')
plt.legend()
```

```
<matplotlib.legend.Legend at 0x1558bf250>
```



Key differences between the two distributions:

- Zipfs law is a power law distribution, while the uniform distribution is a constant distribution, which means that the probability of each event is the same.
- The standard deviation in the plots are higher in the Zipf distribution than in the uniform distribution.
- The Zipf distribution has a lower entropy than the uniform distribution.
- The esitmation starts at a lower entropy in the Zipf distribution than in the uniform distribution.