Neural Data Science

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Coding Lab 8

```
In [ ]: 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
        %load_ext jupyter_black
        %load_ext watermark
        %watermark --time --date --timezone --updated --python --iversions --wate
       Last updated: 2024-07-02 12:15:58CEST
       Python implementation: CPython
       Python version : 3.12.3
       IPython version : 8.22.2
       sklearn: 1.4.1.post1
       numpy : 1.26.4
       matplotlib: 3.8.3
       seaborn : 0.13.2
```

Task 1: Implement entropy estimators

Grading: 5 pts (basic) + 1 pts (advanced) + 3 pts (bonus)

General framework

Entropy is defined as

Watermark: 2.4.3

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

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: $p(x=X)=\frac{1}{K}$
- ullet "Zipf's law"- distribution: $p(x=X)=rac{1}{Zx}$, 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.

```
In []: 0 * np.log(0)

/var/folders/g_/dvk6nf6n4w71vr5_mf4f1zdm0000gn/T/ipykernel_5272/254522992
2.py:1: RuntimeWarning: divide by zero encountered in log
    0 * np.log(0)
    /var/folders/g_/dvk6nf6n4w71vr5_mf4f1zdm0000gn/T/ipykernel_5272/254522992
2.py:1: RuntimeWarning: invalid value encountered in scalar multiply
    0 * np.log(0)
```

Out[]: nan

Basic

Grading: 5 pts

```
In [ ]:
        def binary_to_integer(binarry_sequence):
            input: binarry_sequence, np.array, shape=(d, )
            output: integer, int
            return sum(2**i * bit for i, bit in enumerate(binarry_sequence[::-1])
        def integer_to_binary(n, d):
            input: n, int
                   d, int (length of the binary sequence)
            output: binary_sequence, np.array, shape=(d, )
            binary_sequence = []
            # Generate the binary representation
            while n > 0:
                binary_sequence.append(n % 2)
                n = n // 2
            # Reverse the sequence to get the correct order
            binary_sequence.reverse()
            # Pad the sequence with leading zeros to ensure length d
            if len(binary_sequence) < d:</pre>
                binary_sequence = [0] * (d - len(binary_sequence)) + binary_seque
            elif len(binary_sequence) > d:
                raise ValueError(f"Integer {n} cannot be represented in {d} bits.
```

```
return np.array(binary_sequence)
def sample_f_uniform_dist(n, d, rng=np.random.default_rng(0)):
    input: n, number of samples
    input: d, number of bits
    input: rng, random number generator
    output: samples, np.array, shape=(n, d)
    # generate n samples of d bits
    return rng.integers(0, 2, (n, d))
# def sample_f_zipf_dist(n, d, alpha=1.1, rng=np.random.default_rng(0)):
#
#
      input: n, number of samples
#
      input: d, number of bits
#
      input: alpha, parameter of Zipf distribution
#
     input: rng, random number generator
#
      output: samples, np.array, shape=(n, d)
#
#
      # generate n samples of d bits
#
      return rng.zipf(a=alpha, size=(n, d)) % 2
def sample_f_zipf_manual_choice(n, num_bits, rng=np.random.default_rng(0)
    .....
    Generates samples from a Zipf distribution with the given alpha param
    and samples either 1 or 0 based on the calculated probabilities.
    Parameters:
    - n: int, number of samples to generate
    - num_bits: int, number of bits in each sample
    - rng: np.random.Generator, random number generator
    Returns:
    - np.array, shape=(n, num_bits), binary samples
    # # Function to calculate the harmonic number H N
    # def harmonic_number(N):
         return np.sum(1.0 / np.arange(1, N + 1))
    # # Number of elements to consider for normalization constant Z
    # N = 1000000 # large number to approximate the infinite sum
    \# Z = harmonic number(N)
    # # Calculate probabilities p(x = k)
    # probabilities = np.zeros(num_bits)
    # for k in range(1, num_bits + 1):
          probabilities[k-1] = 1 / (Z * k)
    N = 2**num bits
```

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

# Generate samples from the Zipf distribution and sample binary value
# samples = np.zeros((n, num_bits), dtype=int)
samples = []
for i in range(n):

# Sample from the Zipf distribution
sample = rng.choice(np.arange(0, N), p=probabilities)
sample = integer_to_binary(sample, num_bits)

# Sample binary value based on the Zipf sample
samples.append(sample)

return np.array(samples)
```

MLE

```
Grading: 1 pts H_{ML} = -\sum_x \hat{p}(x) log(\hat{p}(x))
```

Miller-Maddow corrected

Grading: 1 pts

$$H_{MM}=H_{ML}+rac{d-1}{2n}$$

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

```
In []: 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)

# calculate d hat as the number of phat > 0
dhat = np.sum(phat > 0)

H = entropy_mle(phat) + ((dhat - 1) / (2 * n))

return H
```

Jack-knife corrected

```
Grading: 2 pts \hat{H}_{JK}=N\hat{H}_{ML}-(N-1)\hat{H}_{ML}^{(.)} \hat{H}_{ML}^{(.)}=< H_{ML}^{\lnot i}>
```

```
H: float
    Entropy estimate
# insert your code here (2 pt)
# calculate f
x_int = np.apply_along_axis(binary_to_integer, 1, x)
# calculate the histogram
phat = np.histogram(x_int, bins=edges, density=True)[0]
# calculate the number of samples
n = len(x_int)
# sanity check
# print("Sampels: ", n, edges.shape, phat.shape, x_int.shape)
# calculate the estimated entropy Hhat as a mean of each sample entro
Hhat = entropy_mle(phat)
# initialize the sum of the entropy
sum H = 0
# calculate the entropy left out sample
for i in range(n):
    # calculate the phat without the ith sample
    x_int_i = np.delete(x_int, i)
    # calculate the histogram without the ith sample
    phat_i = np.histogram(x_int_i, bins=edges, density=True)[0]
    # calculate the entropy without the ith sample
    H_i = entropy_mle(phat_i)
    # add the entropy to the sum
    sum_H += H_i
# Calculate H_hat_ml_mean
H_hat_ml_mean = sum_H / n
# calculate the jack-knife corrected entropy
H = n * Hhat - (n - 1) * H_hat_ml_mean
return H
```

Coverage-adjusted

Grading: 1 pts

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

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

$$H_{CA} = -\sum_x rac{ ilde{\mathcal{P}_C}(x)log(ilde{\mathcal{P}_C}(x))}{1-(1- ilde{\mathcal{P}_C}(x))^N}$$

```
In [ ]: 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)
\# calculate number fo f_i = 1
f = phat * n
# calculate where f == 1
f_i = np.sum(f == 1)
# calculate C
C = 1 - f_i / n
# calculate P c hat
P_c_hat = phat * C
# calculate the coverage adjusted entropy
\# addjust for P_c_{hat} = 0 to avoid nan
P_c_{hat} = P_c_{hat}[P_c_{hat}] = 0
H = -np.sum((P_c_hat * np.log2(P_c_hat)) / (1 - (1 - P_c_hat) ** n))
return H
```

Advanced

Grading: 1 + 3 pts

JVHW

Grading: 1 pts

```
# datapath = r"C:\Users\Arne.Gittel\Documents\Neuro Master\Neural data sc
# poly entro = None
# def formalize_sample(samp):
#
      samp = np.array(samp)
      if np.any(samp != np.fix(samp)):
#
          raise ValueError("Input sample must only contain integers.")
#
#
      if samp.ndim == 1 or samp.ndim == 2 and samp.shape[0] == 1:
#
          samp = samp.reshape((samp.size, 1))
#
      return samp
# def fingerprint(samp):
#
      """A memory-efficient algorithm for computing fingerprint when wid
#
      large, e.g., wid = 100
#
#
      wid = samp.shape[1]
#
      d = np r_[
#
          np.full((1, wid), True, dtype=bool),
#
          np.diff(np.sort(samp, axis=0), 1, 0) != 0,
#
          np.full((1, wid), True, dtype=bool),
#
      7
#
      f_{col} = []
#
      f_{max} = 0
#
      for k in range(wid):
#
          a = np.diff(np.flatnonzero(d[:, k]))
#
          a max = a max()
          hist, _ = np.histogram(a, bins=a_max, range=(1, a_max + 1))
#
#
          f_col.append(hist)
#
          if a_max > f_max:
#
              f_{max} = a_{max}
      return np.array([np.r_[col, [0] * (f_max - len(col))] for col in f_
# def entro_mat(x, n, g_coeff, c_1):
#
      \# g\_coeff = \{g0, g1, g2, ..., g\_K\}, K: the order of best polynomial
#
      K = len(g\_coeff) - 1
#
      thres = 4 * c 1 * np.log(n) / n
#
      T, X = np.meshgrid(thres, x)
#
      ratio = np.minimum(np.maximum(2 * X / T - 1, 0), 1)
#
      q = np.arange(K).reshape((1, 1, K))
#
      g = g\_coeff.reshape((1, 1, K + 1))
#
      MLE = -X * np.log(X) + 1 / (2 * n)
#
      polyApp = np.sum(
#
          np.concatenate(
#
              (T[..., None], ((n * X)[..., None] - q) / (T[..., None] * (
#
          ).cumprod(axis=2)
#
          * g,
#
          axis=2,
#
      ) - X * np.log(T)
#
      polyfail = np.isnan(polyApp) | np.isinf(polyApp)
#
      polyApp[polyfail] = MLE[polyfail]
```

```
output = ratio * MLE + (1 - ratio) * polyApp
#
      return np.maximum(output, 0)
# def est_entro_JVHW(samp):
#
      """Proposed JVHW estimate of Shannon entropy (in bits) of the input
      This function returns a scalar JVHW estimate of the entropy of samp
#
#
      samp is a vector, or returns a row vector containing the JVHW estim
#
      each column of samp when samp is a matrix.
#
      Input:
#
      ---- samp: a vector or matrix which can only contain integers. The
#
                  data type can be any interger classes such as uint8/int
#
                  uint16/int16/uint32/int32/uint64/int64, or floating-poi
#
                  such as single/double.
#
      Output:
      ---- est: the entropy (in bits) of the input vector or that of eac
#
#
                 of the input matrix. The output data type is double.
#
#
      samp = formalize_sample(samp)
#
      [n, wid] = samp.shape
      n = float(n)
#
      # The order of polynomial is no more than 22 because otherwise floa
#
#
      order = min(4 + int(np.ceil(1.2 * np.log(n))), 22)
#
      global poly_entro
#
      if poly_entro is None:
#
          poly_entro = scipy.io.loadmat(
#
              datapath
#
          ) ["poly entro"]
      coeff = poly_entro[order - 1, 0][0]
#
#
      f = fingerprint(samp)
      prob = np.arange(1, f.shape[0] + 1) / n
#
#
      # Piecewise linear/quadratic fit of c_1
      V1 = np.array([0.3303, 0.4679])
#
      V2 = np.array([-0.530556484842359, 1.09787328176926, 0.184831781602)
#
#
      f1nonzero = f[0] > 0
#
      c_1 = np.zeros(wid)
#
      with np.errstate(divide="ignore", invalid="ignore"):
          if n >= order and f1nonzero.any():
#
              if n < 200:
#
#
                  c_1[f1nonzero] = np.polyval(V1, np.log(n / f[0, f1nonzero]))
#
              else:
#
                  n2f1\_small = f1nonzero \& (np.log(n / f[0]) <= 1.5)
#
                  n2f1\_large = f1nonzero \& (np.log(n / f[0]) > 1.5)
#
                  c_1[n2f1\_small] = np.polyval(V2, np.log(n / f[0, n2f1\_s
#
                  c_1[n2f1_large] = np.polyval(V1, np.log(n / f[0, n2f1_l]))
#
              # make sure nonzero threshold is higher than 1/n
#
              c_1[f1nonzero] = np.maximum(c_1[f1nonzero], 1 / (1.9 * np.l)
#
          prob_mat = entro_mat(prob, n, coeff, c_1)
```

```
return np.sum(f * prob_mat, axis=0) / np.log(2)
In [ ]: ### Necessary functions from https://github.com/EEthinker/JVHW_Entropy_Es
        ### Added comments using ChatGPT fur further understanding
        import scipy.io
        # Path to the polynomial coefficients file (poly_coeff_entro.mat)
        datapath = "../poly_coeff_entro.mat"
        poly_entro = None
        def formalize_sample(samp):
            """Ensure the sample is in the correct format and contains only integ
            This function checks if the input sample contains only integers and r
            it to a column vector if it is a 1D array or a single-row 2D array.
            Input:
            ---- samp: A vector or matrix which should only contain integers. Th
                        data type can be any integer class such as uint8/int8/uin
                        int16/uint32/int32/uint64/int64, or floating-point such a
                        single/double.
            Output:
            ---- samp: A 2D numpy array where each column represents a sequence
                        the input sample. The output ensures that the sample is a
                        column vector if it was a 1D array or a single-row 2D arr
            samp = np.array(samp) # Convert input to a numpy array
            if np.any(samp != np.fix(samp)): # Check if all elements are integer
                raise ValueError("Input sample must only contain integers.")
            if samp.ndim == 1 or (
                samp.ndim == 2 and samp.shape[0] == 1
            ): # If the sample is a 1D array or a single row 2D array
                samp = samp.reshape((samp.size, 1)) # Reshape to a column vector
            return samp
        def fingerprint(samp):
            """Compute the fingerprint of the sample, which is a histogram of fre
            The fingerprint function generates a histogram of frequencies of freq
            for each column in the sample. This is used to represent the sample i
            more compact form which is useful for entropy estimation.
            Input:
            ---- samp: A 2D numpy array where each column represents a sequence.
                        input sample must only contain integers.
            Output:
            ---- f_col: A 2D numpy array where each column represents the finger
                         histogram of the corresponding column in the input sampl
```

wid = samp.shape[1] # Get the number of columns in the sample

1111111

```
# Create a boolean array that marks the changes in sorted sample valu
   d = np.r
       np.full((1, wid), True, dtype=bool), # Add a row of True values
       np.diff(np.sort(samp, axis=0), 1, 0) != 0, # Mark changes in sor
       np.full((1, wid), True, dtype=bool), # Add a row of True values
   1
   f_col = [] # List to store fingerprint histograms for each column
   f_max = 0 # Maximum length of the differences
   for k in range(wid): # Loop over each column
       # Compute the histogram of differences between non-zero entries
       a = np.diff(np.flatnonzero(d[:, k]))
       a_max = a_max()
       hist, _ = np.histogram(a, bins=a_max, range=(1, a_max + 1))
       f_col.append(hist)
       if a_max > f_max: # Update the maximum length of differences
            f_{max} = a_{max}
   # Ensure all histograms have the same length by padding with zeros
    return np.array([np.r_[col, [0] * (f_max - len(col))] for col in f_co
def entro mat(x, n, q coeff, c 1):
   """Calculate the entropy matrix using polynomial approximation.
   This function uses polynomial approximation to estimate the entropy f
   different probabilities based on the input polynomial coefficients an
   a threshold value.
   Input:
   ---- x: A 1D numpy array representing the probabilities of unique co
             in the sample.
          n: The number of observations in the sample.
   g_coeff: A 1D numpy array containing the polynomial coefficients.
     c 1: A 1D numpy array containing the threshold values for each colu
          in the sample.
   Output:
   ---- output: A 2D numpy array representing the entropy matrix for th
                  probabilities. Each column corresponds to a column in t
                  input sample.
    .....
   K = len(g\_coeff) - 1 \# Order of the polynomial
   thres = 4 * c_1 * np.log(n) / n # Calculate the threshold value
   T, X = np.meshgrid(thres, x) # Create a meshgrid for threshold and p
    ratio = np.minimum(
       np.maximum(2 * X / T - 1, 0), 1
    ) # Calculate the ratio for interpolation
   # Prepare for polynomial approximation
   q = np.arange(K).reshape((1, 1, K))
   g = g_coeff.reshape((1, 1, K + 1))
   MLE = -X * np.log(X) + 1 / (2 * n) # Calculate the Maximum Likelihoo
   # Compute polynomial approximation
    polyApp = np.sum(
```

```
np.concatenate(
            (T[..., None], ((n * X)[..., None] - q) / (T[..., None] * (n)
        ).cumprod(
           axis=2
        ) # Cumulative product along the third axis
       * g,
       axis=2,
    -X * np.log(T)
   # Handle cases where polynomial approximation fails (NaN or Inf value
    polyfail = np.isnan(polyApp) | np.isinf(polyApp)
   polyApp[polyfail] = MLE[polyfail]
   # Combine MLE and polynomial approximation using the ratio
   output = ratio * MLE + (1 - ratio) * polyApp
    return np.maximum(output, 0) # Ensure the entropy values are non-neg
def est entro JVHW(samp):
   """Proposed JVHW estimate of Shannon entropy (in bits) of the input s
   This function returns a scalar JVHW estimate of the entropy of samp w
   samp is a vector, or returns a row vector containing the JVHW estimat
   each column of samp when samp is a matrix.
   Input:
   ---- samp: A vector or matrix which can only contain integers. The i
                data type can be any integer class such as uint8/int8/
                uint16/int16/uint32/int32/uint64/int64, or floating-point
                such as single/double.
   Output:
   ---- est: The entropy (in bits) of the input vector or that of each
              of the input matrix. The output data type is double.
   samp = formalize_sample(samp) # Ensure sample format
    [n, wid] = samp.shape # Get the number of rows (n) and columns (wid)
   n = float(n) # Convert the number of rows to a float
   # Determine the order of the polynomial approximation
   order = min(4 + int(np.ceil(1.2 * np.log(n))), 22)
   # Load polynomial coefficients if not already loaded
   global poly entro
   if poly entro is None:
        poly_entro = scipy.io.loadmat(datapath)["poly_entro"]
   coeff = poly_entro[order - 1, 0][0]
   f = fingerprint(samp) # Compute the fingerprint of the sample
   prob = np.arange(1, f.shape[0] + 1) / n # Probability vector for eac
   # Piecewise linear/quadratic fit of c_1
   V1 = np.array([0.3303, 0.4679]) # Coefficients for small values of l
   V2 = np.array(
        [-0.530556484842359, 1.09787328176926, 0.184831781602259]
    ) # Coefficients for large values of log(n/f[0])
```

```
f[0] > 0
            ) # Boolean array indicating non-zero fingerprint values in the firs
            c_1 = np.zeros(wid) # Initialize c_1 with zeros, one for each column
            with np.errstate(
                divide="ignore", invalid="ignore"
            ): # Ignore divide by zero and invalid value warnings
                if n >= order and f1nonzero.any():
                    if n < 200: # Use linear fit for small sample sizes</pre>
                         c_1[f1nonzero] = np.polyval(V1, np.log(n / f[0, f1nonzero
                    else: # Use piecewise quadratic/linear fit for larger sample
                        n2f1\_small = f1nonzero & (np.log(n / f[0]) <= 1.5)
                        n2f1_{large} = f1nonzero & (np.log(n / f[0]) > 1.5)
                         c_1[n2f1_small] = np.polyval(V2, np.log(n / f[0, n2f1_sma
                        c_1[n2f1_large] = np.polyval(V1, np.log(n / f[0, n2f1_lar
                    # Ensure non-zero threshold is higher than 1/n
                    c_1[f1nonzero] = np.maximum(c_1[f1nonzero], 1 / (1.9 * np.log)
                # Compute the entropy matrix for the probabilities
                prob_mat = entro_mat(prob, n, coeff, c_1)
            # Return the estimated entropy in bits
            return np.sum(f * prob_mat, axis=0) / np.log(2)
In [ ]: def entropy_jvhw(x):
            """JVHW estimator of discrete entropy.
            Parameter
            x: np.array, shape=(n_samples, )
                Samples
            Return
            H: float
                Entropy estimate
```

Bonus points: Unseen or Best Upper Bounds estimator

Use the JVHW estimator form https://github.com/EEthinker/JVHW Entro

Grading: 3 bonus pts

return H

insert your code here (1 pt)

 $H = est_entro_JVHW(x)$

f1nonzero = (

```
In []: from scipy.optimize import linprog
from scipy.stats import poisson

# Python implementations of Algorithm 1. of the Matlab code provided for
```

```
def unseen(f):
   Approximates the 'histogram' of a true distribution based on a finger
   Input:
    f -- fingerprint of a sample, where f[i] represents the number of ele
   Output:
   histx -- approximation of the histogram of the true distribution, whe
             that occur with probability x[i]
   x -- probabilities corresponding to histx
   Notes:
   This function approximates the histogram of the true distribution bas
   The sum of probabilities times their respective counts equals 1, ensu
   An estimation of the entropy of the true distribution can be computed
    f = np.array(f).flatten()
    k = np.dot(f, np.arange(1, len(f) + 1))
   # Algorithm parameters
   gridFactor = 1.1
   alpha = 0.5
   xLPmin = 1 / (k * max(10, k))
   maxLPIters = 100000
   # Split the fingerprint
   x = [0]
   histx = [0]
    fLP = np.zeros(len(f))
   for i in range(len(f)):
        if f[i] > 0:
           wind = [
                max(0, i - int(np.ceil(np.sqrt(i)))),
                min(i + int(np.ceil(np.sqrt(i))) + 1, len(f)),
            if sum(f[wind[0] : wind[1]]) < 2 * np.sqrt(i):
                x.append(i / k)
                histx.append(f[i])
                fLP[i] = 0
            else:
                fLP[i] = f[i]
   # If no LP portion, return the empirical histogram
   fmax = np.max(np.where(fLP > 0))
    if fmax == 0:
        return np.array(x[1:]), np.array(histx[1:])
   # Set up the first LP
    LPmass = 1 - np.dot(x, histx)
    fLP = np.append(fLP[:fmax], np.zeros(int(np.ceil(np.sqrt(fmax)))))
    szLPf = len(fLP)
   xLPmax = fmax / k
   xLP = xLPmin * gridFactor ** np.arange(
```

```
int(np.ceil(np.log(xLPmax / xLPmin) / np.log(gridFactor))) + 1
szLPx = len(xLP)
objf = np.zeros(szLPx + 2 * szLPf)
objf[szLPx : szLPx + 2 * szLPf : 2] = 1 / np.sqrt(fLP + 1)
objf[szLPx + 1 : szLPx + 2 * szLPf : 2] = 1 / np.sqrt(fLP + 1)
A = np.zeros((2 * szLPf, szLPx + 2 * szLPf))
b = np.zeros(2 * szLPf)
for i in range(szLPf):
    A[2 * i, :szLPx] = poisson.pmf(i + 1, k * xLP)
    A[2 * i + 1, :szLPx] = -A[2 * i, :szLPx]
    A[2 * i, szLPx + 2 * i] = -1
    A[2 * i + 1, szLPx + 2 * i + 1] = -1
    b[2 * i] = fLP[i]
    b[2 * i + 1] = -fLP[i]
Aeq = np.zeros(szLPx + 2 * szLPf)
Aeq[:szLPx] = xLP
beq = LPmass
options = {"maxiter": maxLPIters, "disp": False}
for i in range(szLPx):
    A[:, i] /= xLP[i]
    Aeq[i] /= xLP[i]
sol = linprog(
    objf,
    A ub=A,
    b_ub=b,
    A_eq=Aeq[np.newaxis, :],
    b_eq=[beq],
    bounds=[(0, None)] * (szLPx + 2 * szLPf),
    options=options,
if sol.status == 0:
    print("Maximum number of iterations reached--try increasing maxLP
if sol.status < 0:</pre>
    print("LP1 solution was not found, still solving LP2 anyway...")
# Solve the 2nd LP
objf2 = np.zeros like(objf)
objf2[:szLPx] = 1
A2 = np.vstack([A, objf])
b2 = np.append(b, sol.fun + alpha)
for i in range(szLPx):
    objf2[i] /= xLP[i]
sol2 = linprog(
    objf2,
    A_ub=A2
    b_ub=b2,
    A_eq=Aeq[np.newaxis, :],
    b_eq=[beq],
    bounds=[(0, None)] * (szLPx + 2 * szLPf),
```

```
if sol2.status != 1:
                print("LP2 solution was not found")
            # Append LP solution to empirical portion of histogram
            sol2.x[:szLPx] /= xLP
            x.extend(xLP)
            histx.extend(sol2.x)
            x, histx = np.array(x), np.array(histx)
             ind = np.argsort(x)
            x = x[ind]
            histx = histx[ind]
            ind = histx > 0
            x = x[ind]
            histx = histx[ind]
            return histx, x
        def makeFinger(v):
            Creates a fingerprint vector from an input vector of integers.
            Input:
            v -- vector of integers
            Output:
            f -- fingerprint vector, where f[i] represents the number of elements
            Notes:
            This function generates a fingerprint vector from the input vector v.
             For each integer i, f[i] counts how many elements in v occur exactly
            h1 = np.histogram(v, bins=np.arange(min(v), max(v) + 2))[0]
             f = np.histogram(h1, bins=np.arange(max(h1) + 2))[0]
            return f[1:]
In [ ]: def estimate_unseen_entropy(samp):
            Estimate the entropy of a sample using the Unseen estimator.
            Parameters
             samp : list of integers
                The sample to estimate the entropy of.
            Returns
            float
                The estimated entropy of the sample.
            111111
            f = makeFinger(samp)
            histx, x = unseen(f)
             return -np.sum(histx * x * np.log2(x))
```

options=options,

```
# Test for unseen estimator
 n = 1024
 k = 10000
 samp = np.random.randint(1, n + 1, k)
 print(samp.shape)
 # Compute corresponding fingerprint
 f = makeFinger(samp)
 # Estimate distribution from which sample was drawn
 h, x = unseen(f)
 # Output entropy of the true distribution Unif[n]
 trueEntropy = np.log2(n)
 print("True entropy:", trueEntropy)
 # Output entropy of the empirical distribution of the sample
 empiricalEntropy = -np.dot(
     f, ((np.arange(1, len(f) + 1) / k) * np.log2(np.arange(1, len(f) + 1))
 print("Empirical entropy:", empiricalEntropy)
 # Output entropy of the recovered histogram [h, x]
 estimatedEntropy = -np.dot(h, x * np.log2(x))
 print("Estimated entropy:", estimatedEntropy)
 entr = estimate_unseen_entropy(samp)
 print("Estimated entropy:", entr)
 p_{test} = 1 / n * np.ones(n) # true distribution
 H_test = -np.sum(p_test * np.log2(p_test)) # true entropy)
 print("True entropy:", H_test)
(10000,)
Maximum number of iterations reached—try increasing maxLPIters
LP2 solution was not found
True entropy: 10.0
Empirical entropy: 9.92683638874989
Estimated entropy: 9.990407741930627
Maximum number of iterations reached—try increasing maxLPIters
LP2 solution was not found
Estimated entropy: 9.990407741930627
True entropy: 10.0
```

Task 2: Distributions

Grading: 4 pts

Uniform distribution

Grading: 2 pts

```
In []: D = 10 # sequence length
N = 2**D # number of possible sequences

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)

```
In [ ]: # insert your code here
        rng = np.random.default_rng(0)
        # Sample from the uniform distribution
        # using sample size of 100 (0.5 pts)
        n1 = 100
        x_100 = sample_f_uniform_dist(n1, D, rng)
        x_100_int = np.apply_along_axis(binary_to_integer, 1, x_100)
        # Sample from the uniform distribution
        # using sample size of 10000 (0.5 pts)
        n2 = 10000
        x_1000 = sample_f_uniform_dist(n2, D, rng)
        x_1000_int = np.apply_along_axis(binary_to_integer, 1, x_1000)
        # Plot the true distribution and
        # the sampled distributions. (0.5 pts)
        print(p.shape, x_100_int.shape, x_100_int[:20], x_1000_int.shape)
        # Plot the true distribution and the sampled distributions
        hist bins = N
        plt.figure(figsize=(20, 10))
        plt.hist(
            x_100_int
            bins=hist_bins,
            density=True,
            alpha=0.5,
            label="Sampled Distribution n=100",
        plt.hist(
            x_1000_{int}
            bins=hist_bins,
            density=True,
            alpha=0.5,
             label="Sampled Distribution n=10000",
```

```
# Plot the true uniform distribution for reference
          plt.plot(p, label="True Distribution", lw=2)
          # plt.hist(p, bins=hist_bins, density=True, alpha=0.5, label="True Distri
          plt.legend()
          plt.xlabel("Integer Value of f_i")
          plt.ylabel("Probability Density")
          plt.title("True Distribution vs Sampled Distributions")
          plt.show()
         (1024,) (100,) [ 897 1023
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                                                                                               306
           686 946
           964 220 788 497 997
                                           821] (10000,)
                                                 True Distribution vs Sampled Distributions
                                                                                            Sampled Distribution n=100
Sampled Distribution n=10000
True Distribution
         0.0200
         0.0175
         0.0125
         0.0100
         0.0075
         0.0050
         0.0025
         0.0000
                                                       Integer Value of f_i
In [ ]: | print(x_100[:10], x_100_int[:10])
         [[1 1 1 0 0 0 0 0 0 0 1]
          [1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1]
          [0\ 1\ 1\ 0\ 0\ 1\ 1\ 0\ 1\ 1]
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          [0 1 0 0 1 1 0 0 0 1]] [ 897 1023 411 592
                                                                     29 631 943
                                                                                         54 826
                                                                                                    30
         5]
```

To do: what I notice

Larger samplesize capture the true underlying distribution better.

When sample size << than possible number of bit combinations (here 1024) some probabilitys are by default to high even when they only occure once while others do not occure at all.

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.

```
In [ ]: sample_sizes = np.round(np.logspace(1, 5, num=10))
        n runs = 30
        rng = np.random.default_rng(1)
        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)
                # sample from the uniform distribution using sample size S and se
                x = sample_f_uniform_dist(int(S), D, rng)
                # convert the binary sequences to integer f
                x_int = np.apply_along_axis(binary_to_integer, 1, x)
                # calculate the histogram
                phat = np.histogram(x_int, bins=edges, density=True)[0]
                # print(np.sum(phat), len(phat), phat * S, np.sum(phat * S))
                # insert your code here
                h_mle[i, j] = entropy_mle(phat)
                h_mm[i, j] = entropy_mm(phat, S)
                h_cae[i, j] = entropy_cae(phat, S)
                # print(x_int.shape, x_int[:10], phat.shape, phat[:10], make_fing
                # h_unseen[i, j] = unseen_estimator(x_int, int(S))
                # print("here", phat * D, np.sum(phat * D))
                h_unseen[i, j] = estimate_unseen_entropy(x_int)
                # cap the number of samples to 1000 for the jack-knife estimator
                if \times int.shape[0] > 1000:
                    x = x[:1000]
                # print(entropy_jk(x, edges))
                h_jk[i, j] = entropy_jk(x, edges)
                # print(entropy_jvhw(x))
                h_jvhw[i, j] = entropy_jvhw(x_int)
```

```
/var/folders/g_/dvk6nf6n4w71vr5_mf4f1zdm0000gn/T/ipykernel_5272/292534620
7.py:46: DeprecationWarning: Conversion of an array with ndim > 0 to a sca
lar is deprecated, and will error in future. Ensure you extract a single e
lement from your array before performing this operation. (Deprecated NumPy
1.25.)
h_jvhw[i, j] = entropy_jvhw(x_int)
```

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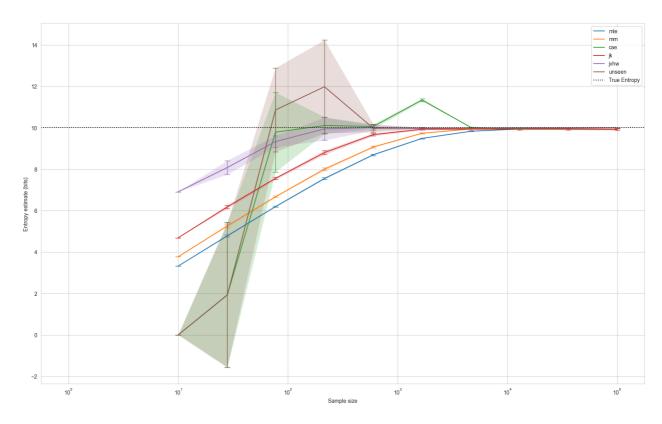
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Plot the resulting average estimate of the entropy for each of the estimators. Which is best? If you implemented everything correctly, this plot should roughly look like in the lecture.

```
plt.fill_between(
    sample_sizes,
    np.mean(h_mm, axis=1) - np.std(h_mm, axis=1),
    np.mean(h_mm, axis=1) + np.std(h_mm, axis=1),
    alpha=0.2,
plt.fill_between(
    sample_sizes,
    np.mean(h_cae, axis=1) - np.std(h_cae, axis=1),
    np.mean(h cae, axis=1) + np.std(h cae, axis=1),
   alpha=0.2,
)
plt.fill_between(
    sample_sizes,
    np.mean(h_jk, axis=1) - np.std(h_jk, axis=1),
    np.mean(h_jk, axis=1) + np.std(h_jk, axis=1),
   alpha=0.2,
plt.fill_between(
    sample_sizes,
    np.mean(h_jvhw, axis=1) - np.std(h_jvhw, axis=1),
    np.mean(h_jvhw, axis=1) + np.std(h_jvhw, axis=1),
   alpha=0.2,
)
plt.fill_between(
    sample_sizes,
    np.mean(h_unseen, axis=1) - np.std(h_unseen, axis=1),
    np.mean(h_unseen, axis=1) + np.std(h_unseen, axis=1),
   alpha=0.2,
)
plt.errorbar(
    sample_sizes,
    np.mean(h_mle, axis=1),
   yerr=np.std(h_mle, axis=1),
    fmt="none", # Do not plot points, only error bars
    capsize=5, # Size of error bar caps
   elinewidth=1, # Thickness of error bar lines
   alpha=0.9, # Transparency
    color="C0", # Match color with 'mle' line
plt.errorbar(
    sample_sizes,
    np.mean(h_mm, axis=1),
   yerr=np.std(h_mm, axis=1),
   fmt="none",
    capsize=5,
   elinewidth=1,
   alpha=0.9,
    color="C1", # Match color with 'mm' line
plt.errorbar(
    sample_sizes,
    np.mean(h_cae, axis=1),
   yerr=np.std(h_cae, axis=1),
```

```
fmt="none",
    capsize=5,
    elinewidth=1,
    alpha=0.9,
    color="C2", # Match color with 'cae' line
plt.errorbar(
    sample_sizes,
    np.mean(h_jk, axis=1),
    yerr=np.std(h_jk, axis=1),
    fmt="none",
    capsize=5,
    elinewidth=1,
    alpha=0.9,
    color="C3", # Match color with 'jk' line
plt.errorbar(
    sample_sizes,
    np.mean(h_jvhw, axis=1),
    yerr=np.std(h_jvhw, axis=1),
    fmt="none",
    capsize=5,
    elinewidth=1,
    alpha=0.9,
    color="C4", # Match color with 'jvhw' line
plt.errorbar(
    sample_sizes,
    np.mean(h_unseen, axis=1),
    yerr=np.std(h_unseen, axis=1),
    fmt="none",
    capsize=5,
    elinewidth=1,
    alpha=0.9,
    color="C5", # Match color with 'unseen' line
)
# plot h_unseen or h_bub here if you implemented them.
plt.axhline(H, color="black", linestyle=":", label="True Entropy")
plt.xlabel("Sample size")
plt.ylabel("Entropy estimate (bits)")
plt.legend()
```

Out[]: <matplotlib.legend.Legend at 0x132f0c170>



JVHW and Jack knive estimators perform best for smaller sample sizes

Zipf distribution

Grading: 2 pts

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)

```
In []: D = 10
N = 2**D

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

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

print(H)
```

7.510649703297878

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

```
In []: # insert your code here
rng = np.random.default_rng(2)
```

```
# Sample from the Zipf distribution
# using sample size of 100 (0.5 pts)
x z 100 = sample f zipf manual choice(n1, D, rng=rng)
x_z_100_int = np.apply_along_axis(binary_to_integer, 1, x_z_100)
# -----
# Sample from the Zipf distribution
# using sample size of 10000 (0.5 pts)
x_z_{10000} = sample_f_zipf_manual_choice(n2, D, rng=rng)
x_z_10000_int = np.apply_along_axis(binary_to_integer, 1, x_z_10000)
print(p.shape, x_z_100.shape, x_z_100[:20], x_z_10000_int.shape)
# Plot the true distribution and the sampled
# distributions. (0.5 pts)
# Plot the true distribution and the sampled distributions
hist bins = N
plt.figure(figsize=(20, 10))
plt.hist(
   x_z_{100_int}
    bins=hist_bins,
   density=True,
   alpha=0.5,
    label="Sampled Distribution n=100",
plt.hist(
   x_z_{10000_int}
    bins=hist_bins,
   density=True,
   alpha=0.5,
    label="Sampled Distribution n=10000",
# Plot the true uniform distribution for reference
plt.plot(p, label="True Distribution", lw=2)
# make y log scale
plt.yscale("log")
plt.legend()
plt.xlabel("Integer Value of f_i")
plt.ylabel("Probability Density")
plt.title("True Distribution vs Sampled Distributions")
plt.show()
```

```
(1024,) (100, 10) [[0 0 0 0 0 0 0 0 1 1]
  [0 0 0 0 0 0 0 1 0 0]
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      0 0 0 0 0 1 1 0 0]
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  [0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1]] (10000,)
                                             True Distribution vs Sampled Distributions
                                                                                             Sampled Distribution n=100
Sampled Distribution n=10000
True Distribution
 10
Probability Density
 10
```

What do we notice:

Same problem regarding sample size we have seen for the uniform distribution, now we see that the probabilitys in the low sample size the sampled values appear ~equally likely (if sampled once) but spread differently over the range of possible integer values (higher values have less amount of sampled values). Even with large sample sizes we see, that for the larger integer values with a very low probability the sampling becomes less accurate.

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.

```
rng = np.random.default_rng(3)
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 Zipf distribution
        # with different sample size (0.5 pts)
        # insert your code here
        # sample from the Zipf distribution using sample size S and seque
        x = sample_f_zipf_manual_choice(int(S), D, rng)
        # convert the binary sequences to integer f
        x_int = np.apply_along_axis(binary_to_integer, 1, x)
        # calculate the histogram
        phat = np.histogram(x_int, bins=edges, density=True)[0]
        # print(np.sum(phat), len(phat))
        # insert your code here
        h_mle[i, j] = entropy_mle(phat)
        h_mm[i, j] = entropy_mm(phat, S)
        h_cae[i, j] = entropy_cae(phat, S)
        h_unseen[i, j] = estimate_unseen_entropy(x_int)
        # cap the number of samples to 1000 for the jack-knife estimator
        if x_int.shape[0] > 1000:
            x = x[:1000]
        h_jk[i, j] = entropy_jk(x, edges)
        h_jvhw[i, j] = entropy_jvhw(x_int)
```

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/var/folders/g_/dvk6nf6n4w71vr5_mf4f1zdm0000gn/T/ipykernel_5272/337808670 9.py:42: DeprecationWarning: Conversion of an array with ndim > 0 to a sca lar is deprecated, and will error in future. Ensure you extract a single e lement from your array before performing this operation. (Deprecated NumPy 1.25.)

h_jvhw[i, j] = entropy_jvhw(x_int)

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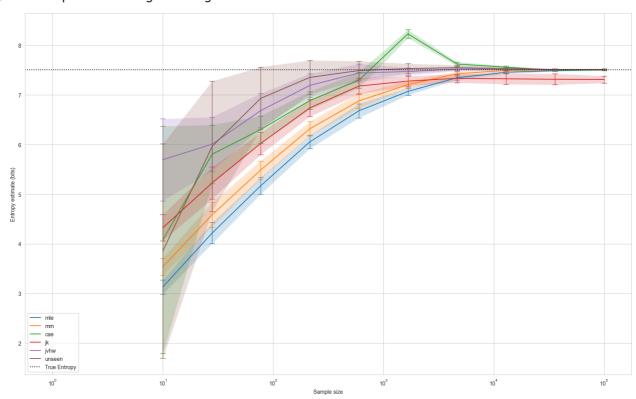
Plot resulting average estimate of the entropy for each of the estimators. Which is best? If you implemented everything correctly, this plot should roughly look like in the lecture.

```
In []: plt.figure(figsize=(20, 12))
        plt.semilogx(sample_sizes, np.mean(h_mle, axis=1), label="mle")
        plt.semilogx(sample_sizes, np.mean(h_mm, axis=1), label="mm")
        plt.semilogx(sample sizes, np.mean(h cae, axis=1), label="cae")
        plt.semilogx(sample_sizes, np.mean(h_jk, axis=1), label="jk")
        plt.semilogx(sample_sizes, np.mean(h_jvhw, axis=1), label="jvhw")
        plt.semilogx(sample_sizes, np.mean(h_unseen, axis=1), label="unseen")
        # plot the standard deviation
        plt.fill between(
            sample_sizes,
            np.mean(h_mle, axis=1) - np.std(h_mle, axis=1),
            np.mean(h_mle, axis=1) + np.std(h_mle, axis=1),
            alpha=0.2,
        plt.fill between(
            sample sizes,
            np.mean(h_mm, axis=1) - np.std(h_mm, axis=1),
            np.mean(h_mm, axis=1) + np.std(h_mm, axis=1),
            alpha=0.2,
        plt.fill_between(
            sample_sizes,
            np.mean(h_cae, axis=1) - np.std(h_cae, axis=1),
            np.mean(h_cae, axis=1) + np.std(h_cae, axis=1),
            alpha=0.2,
        plt.fill between(
            sample_sizes,
```

```
np.mean(h_jk, axis=1) - np.std(h_jk, axis=1),
    np.mean(h_jk, axis=1) + np.std(h_jk, axis=1),
   alpha=0.2,
plt.fill_between(
    sample sizes,
    np.mean(h_jvhw, axis=1) - np.std(h_jvhw, axis=1),
    np.mean(h_jvhw, axis=1) + np.std(h_jvhw, axis=1),
   alpha=0.2,
)
plt.fill_between(
    sample_sizes,
    np.mean(h_unseen, axis=1) - np.std(h_unseen, axis=1),
    np.mean(h_unseen, axis=1) + np.std(h_unseen, axis=1),
   alpha=0.2,
)
plt.errorbar(
    sample_sizes,
    np.mean(h_mle, axis=1),
   yerr=np.std(h_mle, axis=1),
    fmt="none", # Do not plot points, only error bars
    capsize=5, # Size of error bar caps
   elinewidth=1, # Thickness of error bar lines
    alpha=0.9, # Transparency
    color="CO", # Match color with 'mle' line
plt.errorbar(
    sample_sizes,
    np.mean(h mm, axis=1),
   yerr=np.std(h_mm, axis=1),
    fmt="none",
    capsize=5,
   elinewidth=1,
   alpha=0.9,
    color="C1", # Match color with 'mm' line
plt.errorbar(
    sample_sizes,
    np.mean(h_cae, axis=1),
   yerr=np.std(h_cae, axis=1),
   fmt="none",
    capsize=5,
   elinewidth=1,
   alpha=0.9,
    color="C2", # Match color with 'cae' line
plt.errorbar(
    sample_sizes,
    np.mean(h_jk, axis=1),
   yerr=np.std(h_jk, axis=1),
   fmt="none",
    capsize=5,
   elinewidth=1,
   alpha=0.9
    color="C3", # Match color with 'jk' line
```

```
plt.errorbar(
    sample_sizes,
    np.mean(h_jvhw, axis=1),
    yerr=np.std(h_jvhw, axis=1),
    fmt="none",
    capsize=5,
    elinewidth=1,
    alpha=0.9,
    color="C4", # Match color with 'jvhw' line
plt.errorbar(
    sample_sizes,
    np.mean(h_unseen, axis=1),
    yerr=np.std(h_unseen, axis=1),
    fmt="none",
    capsize=5,
    elinewidth=1,
    alpha=0.9,
    color="C5", # Match color with 'unseen' line
# plot h_unseen or h_bub here if you implemented them.
plt.axhline(H, color="black", linestyle=":", label="True Entropy")
plt.xlabel("Sample size")
plt.ylabel("Entropy estimate (bits)")
plt.legend()
```

Out[]: <matplotlib.legend.Legend at 0x14a78b290>



The unseen estimator is not overestimating in this case and performs best on