Ali Al Kadhim and Harrison B. Prosper Department of Physics, Florida State University

```
import numpy as np; import pandas as pd
import scipy as sp; import scipy.stats as st
import torch; import torch.nn as nn
from numba import njit
from sklearn.preprocessing import StandardScaler; from
sklearn.model_selection import train_test_split
import matplotlib as mp; import matplotlib.pyplot as plt;
#reset matplotlib stle/parameters
import matplotlib as mpl
mpl.rcParams.update(mpl.rcParamsDefault)
plt.style.use('seaborn-deep')
mp.rcParams['agg.path.chunksize'] = 10000
font_legend = 15; font_axes=15
# %matplotlib inline
import copy; import sys; import os
from IPython.display import Image, display
import optuna
#sometimes jupyter doesnt initialize MathJax automatically for latex,
so do this
import ipywidgets as wid; wid.HTMLMath('$\LaTeX$')
```

{"version_major":2,"version_minor":0,"model_id":"3029f2222dd247b582617
2e9f69ad1be"}

Table of Contents

Background and Problem Statement

In particle physics, the most important experiment is a counting experiment, represented by a Poisson probability model.Suppose we have a count experiment, we we observe in each bin (or channel) k a count n_k. Given N total channels, the probability of obtaining the observed result is given by the Poisson

$$\prod_{k=1}^{N} \frac{e^{-\left(\epsilon_k \sigma + b_k\right)} \left(\epsilon_k \sigma + b_k\right)^{n_k}}{n_k!}$$

Where σ, the cross section (the parameter of interest), b_k is expected background for the k th channel (the nuissance parameter). ϵ_k is the "acceptance parameter", for the kth channel, which is typically a product of the detector efficiency, branching fraction, and luminosity.

This is the prototype of many statistical models in astronomy and particle physics in which data are binned and the count in each bin consist a priori of the sum of counts from signal and background. Written in terms of the simplified 2-parameter model, the expected count in each bin k takes the form

\begin{equation} n_{exp}=\theta+\nu \end{equation}

Where n_{exp} is the expected signal count, θ is the unknown mean count, which is the parameter of interest (the cross section), and ν is the background unknown mean count, which is the nuissance parameter.

The two-parameter problem

the conditional probability of observing n signal counts and m background counts in a single channel is given by

$$P(n,m \mid \theta,\nu)=L(\theta,\nu)=\frac{e^{-(\theta+\nu)}(\theta+\nu)^{n}}{n!}\frac{e^{-\nu}\nu^{m}}{m!}$$

Where, once the counts n and m have been observed becomes the likelihood $L(\theta,\nu)$. The objective now is to derive confidence intervals or limits for the parameter of interest θ. What makes this challenging is the presence of nuissance parameter ν. In the Bayesian approach, nuissance parameters are assigned priors $\pi(\nu)d\nu$ and are integrated out in order to arrive at the posterior for θ in a process called marginalization. Frequentist methods deal with nuissance parameters by profiling them the likelihood in order to arrive at their MLEs.

The typical way to arrive at confidence intervals that guarantee coverage is the Neyman-Pearson construction. However, it does not deal with the existence of nuissance parameters....

the Poisson mean¿$\theta+\nu$, and the probability model is given by

$$p(N,M\vee\theta,\nu)=\text{Poiss}(N;\theta+\nu)\,\text{Poiss}(M;\nu)=L(\theta,\nu)=\frac{e^{-(\theta+\nu)}(\theta+\nu)^{N}}{N!}\frac{e^{-\nu}\nu^{M}}{M!}$$

Where ν is the nuissance parameter, θ is the paramter of interest, for which we want to estimate confidence intervals or (upper) limits.

Observed Data:

- N (observed counts for signal)
- M (observed counts for background)

Parameters:

- θ: parameter of interest, proportional σ in HEP (unknown signal mean)

- ν: nuissance parameter (unknown background mean)

Auxiliary (simulated) Data (simulated on-the-fly for each observation)

- n: expected signal count

- m: expected backround count

The standard procedure for removal of nuissance parameters is Bayesian marginalization, but in this study we adopt LFI with frequentest methods.

In this notebook we generate data comprising the quadruplets $(Z_i, \theta_i, \nu_i, N_i, M_i)$ where

$ \begin{align} \theta & \sim \textrm{uniform}(0, 20), \ \nu & \sim \textrm{uniform}(0, 20), \ n & \sim \textrm{poisson}(\theta + \nu),\ m & \sim \textrm{poisson}(\nu),\ N & \sim \textrm{uniform}(0,10),\ M & \sim \textrm{uniform}(0, 10), \textrm{ and } \ Z & = I[\lambda_{\textrm{gen}} \leq \lambda_D (D, \theta)], \end{align} $

where the size of each of these samples is B', I is the indicator function, and $\lambda_D(D, \theta) = \lambda(N, M, \theta)$ is our chosen test statistic

$$\lambda = -2 \log \frac{p(n, m \vee \theta, \hat{\nu}(\theta))}{p(n, m \vee \hat{\theta}, \hat{\nu}(\theta))} = -2 \log \frac{L_{\text{prof}}(n, m, \theta, \hat{\nu}(\theta))}{L_{\text{prof}}(n, m, \hat{\theta}_{\text{MLE}}, \hat{\nu}(\theta))},$$

where $L_{\text{prof}}(n, m, \theta, \hat{\nu}(\theta))$ is the profiled likelihood. The maximum likelihood estimate of $\hat{\theta}$ is given by

$$\hat{\theta}_{\text{MLE}} = n - m$$

.

Low-count data can sometimes yield spurious results, where the MLE of a parameter of interest θ, could yield a negative result. In the case that θ is the cross section, yielding a negative result is non-physical, which leads to the ad-hoc fix: taking ignoring the MLE solution and taking $\hat{\theta} = 0$ when $n < m$,

$$\hat{\theta}_{\text{non-MLE}} = \begin{cases} n - m & n > m \\ 0 & n \leq m \end{cases}$$

$$\log p(n, m \vee \theta, \nu) = -(\theta + \nu) + n \log(\theta + \nu) \vee - \nu + m \log \nu + \text{constants}$$

The MLE $\hat{\nu}(\theta)$ is attained by solving $\frac{\partial \log p(n, m \vee \theta, \nu)}{\partial \nu} = 0$ leading to

$$\hat{\nu}(\theta) = \left(g + \sqrt{g^2 + 8 m \theta}\right) / 4$$

where $g \equiv n + m - 2\theta$.

Where $L_{\text{prof}}(n, m, \theta, \hat{\nu}(\theta))$ is the profiled likelihood - that is - the likelihood function when the nuissance parameters are replaced by their maximum likelihood estimates (MLE) for a given value of the parameter of interest. The test statistic in Eq. (1) is used due to its well-known behavior of it converging to ti a χ^2_k variate with k degrees of freedom, according to Wilk's Theorem, where k is the number of free parameters (parameters of interest after the nuissance parameters have been replaecd by their MLEs).

Clearly, our choice of using the test statistic above is motivated by the Neyman-Pearson Lemma Instead of using different statistics for LFI as in the Ann Lee paper, we use this one since in Ann lee's paper, for example the ACORE statistic

$$\Lambda\left(D;\Theta_0\right) := \log \frac{\sup_{\theta_0 \in \Theta_0} \prod_{i=1}^{n} O\left(X_i^{\text{obs}};\theta_0\right)}{\sup_{\theta \in \Theta} \prod_{i=1}^{n} O\left(X_i^{\text{obs}};\theta\right)}$$

, since the odds $\mathbb{O}\left(\mathbf{X}_{i}^{\
text {obs }}\right) $, are merely estimates of the likelihood, and not the likelihood itselt, therefore Wilk's theorem is not guaranteed to work, even if we have a large sample size.

```
def mkdir(dir_):
    """make a directory without overwriting what's in it if it
exists"""
    # assert isinstance(dir_, str)
    try:
        os.system('mkdir -p %s' % str(dir_) )
    except Exception:
        pass

mkdir('utils')

# %writefile 'src/utils.py'

def import_base_stack():
    import numpy as np; import pandas as pd
    import scipy as sp; from numba import njit

@njit
def DR(s, theta):
    return sp.special.gammainc(s, theta)

@njit
def DL(s, theta):
    return 1 - sp.special.gammainc(s+1, theta)


def L_prof(n,m,theta):
    k=1
    k1 = k+1
    k2 = 0.5/k1
    g = n+m - k1*theta
    nu_hat = k2* (g+ np.sqrt(g*g +4*k1*m*theta))
    p1 = st.poisson.pmf(n, mu = theta + nu_hat)
    p2 = st.poisson.pmf(m, mu = k * nu_hat)

    return p1*p2



def theta_hat(n,m, MLE=True):
    theta_hat = n-m
    if not MLE:
        theta_hat = theta_hat * (theta_hat > 0)
    return theta_hat

# @njit
def lambda_test(theta, n, m, MLE=True):
    Ln = L_prof(n,m,theta)
    Ld = L_prof(n,m, theta_hat(n,m, MLE))
    lambda_  = -2*np.log(Ln/Ld)
    return np.array(lambda_)
```

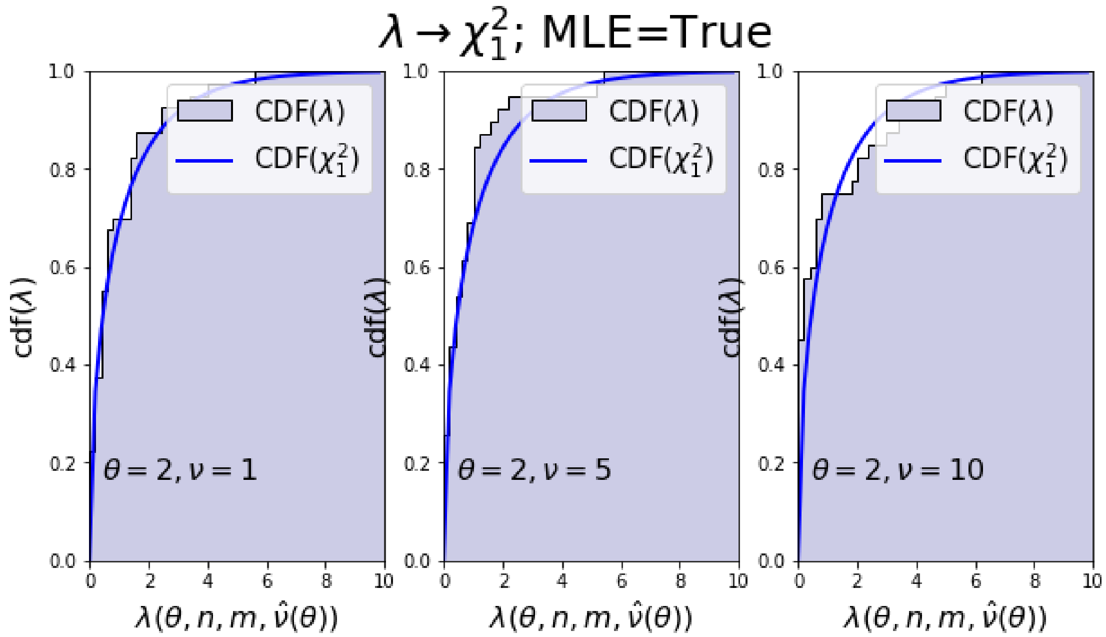
Prior to reporting the results of our method, we validate that our method by comparing it to the well-known results of Wilk's Theorem. That is, the test statistic $\lambda(\theta, n, m, \nu(\theta))$ should be distributed as a χ_1^2 (a χ^2 distribution with a number of degrees of freedom equal to the number of free parameters left in our problem).

We test this theorem with our algorithm, but stopping at step 9. We then histogram the comulative distribution function (CDF) of $\lambda(\theta)$ for a given (fixed) θ and ν, and compare it to the analystical CDF of a χ_1^2 distribtion. The figure (below) shows that the results of our test statistic does indeed agree with what we expect from Wilk's Theorem.

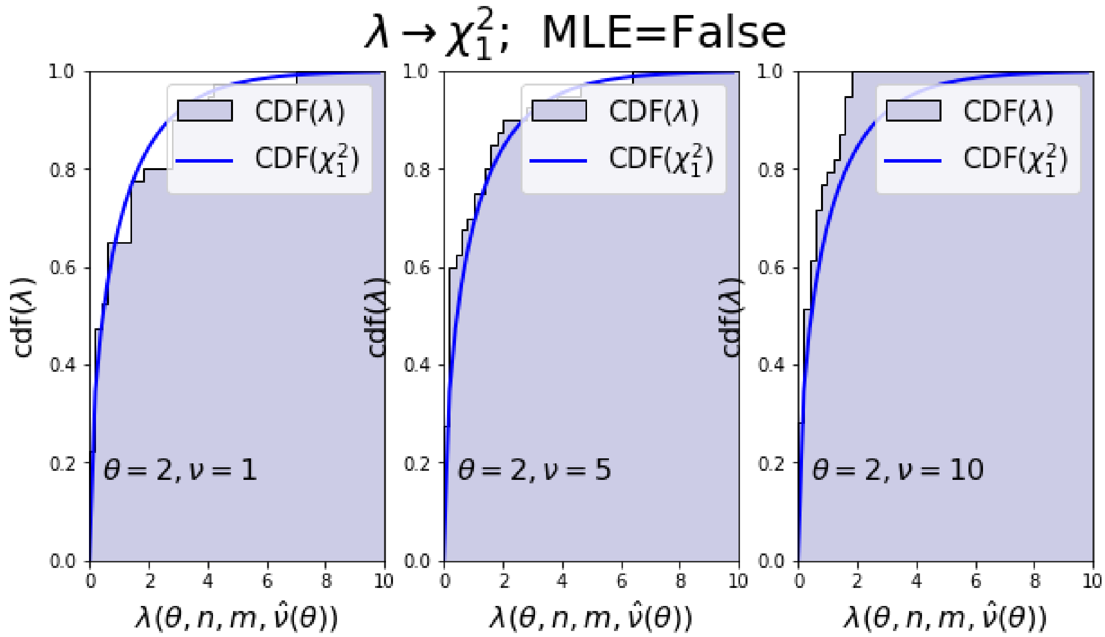
```
chi2_exp_size=40

def run_sim(theta, nu, MLE, lambda_size):
    """Sample n ~ Pois(theta+nu),
              m ~ Pois(nu),
    and compute
              lambda(theta, n, m)

    return: (n, m, lambda_), where each are np arrays of length
lambda_size
    """
    n = st.poisson.rvs(theta+nu, size=lambda_size)
    m = st.poisson.rvs(nu, size=lambda_size)
    lambda_ = lambda_test(theta, n, m, MLE=MLE)
    return (n, m, lambda_)

def run_sims(points, MLE):
    """
    Run an entire simulation, that is, generate n and m from
    run_sim above, and calculate lambda, for

    input: a tuple of (theta, nu) scalars

    Reurns:df, lambda_results

    where lambda_results is a list of tuples
        (n, m, lambda_, theta, nu)
    and df is just a dataframe of [n,m,lambda,theta,nu]
    """
    lambda_results=[]
    df=pd.DataFrame()
    for p in points:
        theta, nu = p
        df['theta']=theta
        df['nu']=nu
        n, m, lambda_ = run_sim(theta, nu, MLE, lambda_size
=chi2_exp_size)
        df['n'] = n
        df['m'] = m
        df['lambda']=lambda_
        lambda_results.append((n, m, lambda_, theta, nu))

        print( '\n \n (theta, nu) =  (%.f, %.f) \n ' % (theta, nu) )
        print(f'\t \t with associated n =  {n}, \n \n \t \t m = {m}, \
n \n \t \t lambda = {lambda_}'  )
    return df, lambda_results

def plot_one(lambda_, theta, nu, ax):
    """Histogram the CDF of  lambda_t =
-2log(Lp(theta)/Lp(theta_hat)),
    for a given (fixed) theta and nu.
    Also, plot the actual CDF of a chi^2 distribution with 1 free
parameter
    (since only theta is left after we profile nu) """
    ftsize = 16; xmin= 0; xmax= 10
    ymin= 0; ymax= 1
    x_range = (xmin, xmax)
    y_range = (ymin, ymax)
    ax.set_xlim(x_range); ax.set_ylim(y_range)
    ax.set_xlabel(r'$\lambda (\theta, n, m, \hat{\nu}(\theta))
$',fontsize=ftsize)
    ax.set_ylabel(r'cdf$(\lambda)$', fontsize=ftsize)
    ##########HISTOGRAM CDF OF LAMBDA####################
    ax.hist(lambda_, bins=5*xmax, range=x_range,
    color=(0.8,0.8,0.9),
    density=True, cumulative=True,
    histtype='stepfilled', edgecolor='black', label=r'CDF$(\lambda)$')
    ############################################################
    ########### HISTOGRAM CDF OF THE CHI2 OF OF X WITH 1 DOF
    #x is not theta, that's the whole point of Wilks thm, x is an
arbitrary RV
    x = np.arange(0, xmax, 0.2)
    y = st.chi2.cdf(x, 1)
    ax.plot(x, y, color='blue',
    linewidth=2, label=r'CDF$(\chi^2_1)$')
    # annotate
    xwid = (xmax-xmin)/12
    ywid = (ymax-ymin)/12
    xpos = xmin + xwid/2
    ypos = ymin + ywid*2
    ax.text(xpos, ypos,
    r'$ \theta = %d, \nu = %d$' % (theta, nu),
    fontsize=ftsize)
    ax.legend(loc='upper right',fontsize=15)
```

1. Generate one scalar θ and one scalar ν
2. Generate $\lambda(\theta,\nu)$ of size N. Observe that the distribution of this λ will approach the CDF of a $\chi^2_{dof}(x)$ of an RV of one dof (since θ is the only free parameter left), confirming Wilk's theorem
3. Observe that this test statistc will be dependent on the value of ν in the non-MLE case, which is not desirable since we want to be insensetive to nuissance parameters for maximal statistal power

```
#points=(theta,nu)
points_1 = (2, 1)
points_2 = (2, 5)
points_3 = (2, 10)
MLE=True
_, _ , lambda_1 = run_sim(theta=points_1[0], nu=points_1[1], MLE=MLE,
lambda_size=chi2_exp_size)
_, _ , lambda_2 = run_sim(theta=points_2[0], nu=points_2[1], MLE=MLE,
lambda_size=chi2_exp_size)
_, _ , lambda_3 = run_sim(theta=points_3[0], nu=points_3[1], MLE=MLE,
lambda_size=chi2_exp_size)

fig, ax = plt.subplots(1,3, figsize=(10,5))
plot_one(lambda_1, points_1[0], points_1[1], ax[0])
plot_one(lambda_2, points_2[0], points_2[1], ax[1])
plot_one(lambda_3, points_3[0], points_3[1], ax[2])
fig.suptitle(r'$\lambda \rightarrow \chi^2_1$; MLE=%s' % str(MLE),
fontsize=25); plt.show()
```



```
#points=(theta,nu)
points_1 = (2, 1)
points_2 = (2, 5)
points_3 = (2, 10)
MLE=False
_, _ , lambda_1 = run_sim(theta=points_1[0], nu=points_1[1], MLE=MLE,
lambda_size=chi2_exp_size)
_, _ , lambda_2 = run_sim(theta=points_2[0], nu=points_2[1], MLE=MLE,
lambda_size=chi2_exp_size)
_, _ , lambda_3 = run_sim(theta=points_3[0], nu=points_3[1], MLE=MLE,
lambda_size=chi2_exp_size)

fig, ax = plt.subplots(1,3, figsize=(10,5))
plot_one(lambda_1, points_1[0], points_1[1], ax[0])
plot_one(lambda_2, points_2[0], points_2[1], ax[1])
plot_one(lambda_3, points_3[0], points_3[1], ax[2])
fig.suptitle(r'$\lambda \rightarrow \chi^2_1$;  MLE=False',
fontsize=25); plt.show()
```



As shall be discussed later in this notebook, one way of calculating p-value for θ corresponding to an observed $\{N,M\}$ pair (which will still be dependent on ν) is by calculating the test statistic at the $\{N,M\}$ pair and calculating

$$p_\theta(\nu)=\text{Prob}(\lambda_{gen}(n,m;\theta,\nu)\le\lambda_D(N,M;\theta,\nu))=\int_{\lambda_D}^{\infty} f(\lambda_{gen}(n,m \mid \theta,\nu) \mid H_{null})\,d\lambda_{gen},$$

where f is the PDF of λ. We see from above that the statistic λ is an approximate sampling distribution of the χ^2 PDF, proving Wilk's theorem, and hence the p-value could also be caluclated by

$$p_\theta(\nu)=\int_{\chi^2}^{\infty} f(z;k)\,dz$$

where k is the number of degrees of freedom (free parameters) which is 1 in the 2-parameter problem , and $f(z;k)$ is the χ^2 PDF. This p-value can then easily be computed (e.g. yielding $p-1-\alpha(1-F_{\chi^2}[\theta,\nu])$, where $ F_{\chi^2}$ is the comulative χ^2 distribution function (as a function of θ and ν).

Generate 6 pairs (tuples) of (θ,ν) values

```
points = [(theta, nu) for theta, nu in
           zip(np.random.randint(low=1,high=4,size=3),
               np.random.randint(low=0,high=4,size=3))]
```

```
df, results = run_sims(points, MLE=True)
```

```
 (theta, nu) =  (2, 0)

            with associated n =  [2 5 4 3 1 3 2 0 1 1 1 2 1 1 2 4 1 1
2 3 1 1 3 3 1 4 3 2 1 3 4 2 2 3 0 3 2
 0 3 2],

            m = [0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0
 0 0 0],

            lambda = [-0.          2.93147181  1.54517744  0.43279065
0.61370564  0.43279065
 -0.          4.          0.61370564  0.61370564  0.61370564 -0.
  0.61370564  0.61370564 -0.          1.54517744  0.61370564
0.61370564
 -0.          0.43279065  0.61370564  0.61370564  0.43279065
0.43279065
  0.61370564  1.54517744  0.43279065 -0.          0.61370564
0.43279065
  1.54517744 -0.         -0.          0.43279065  4.
0.43279065
 -0.          4.          0.43279065 -0.        ]


 (theta, nu) =  (2, 3)

            with associated n =  [5 9 5 9 3 6 4 4 6 2 8 4 4 5 2 7 5 3
5 4 6 5 5 8 7 4 6 2 5 2 4 7 4 5 7 4 4
 3 9 8],

            m = [3 4 6 5 4 1 5 3 5 4 6 8 5 5 3 2 4 5 3 5 5 3 3 0 4 9 2
4 4 3 5 2 0 1 4 2 3
 3 2 2],

            lambda = [-0.          0.7165121   0.80229178  0.29075642
1.2288131   1.47928694
  0.97179616  0.1396362   0.09005222  2.51359335 -0.
2.96578989
  0.97179616  0.39239727  1.66020193  1.07969347  0.10956358
1.92861676
 -0.          0.97179616  0.09005222 -0.         -0.
7.09035489
  0.09206738  3.7531945   0.52939123  2.51359335  0.10956358
1.66020193
  0.97179616  1.07969347  1.54517744  0.74478362  0.09206738 -0.
  0.1396362   0.63419698  2.52578322  1.75504047]


 (theta, nu) =  (1, 0)
```

```
            with associated n =  [2 0 0 1 1 1 1 2 0 2 2 0 0 3 2 3 1 3
1 3 0 1 1 3 0 1 1 4 1 0 0 2 3 2 1 0 2
 1 0 0],

            m = [0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0
 0 0 0],

            lambda = [ 0.77258872  2.          2.         -0.
-0.         -0.
 -0.          0.77258872  2.          0.77258872  0.77258872  2.
  2.          2.15888308  0.77258872  2.15888308 -0.
2.15888308
 -0.          2.15888308  2.         -0.         -0.
2.15888308
  2.         -0.         -0.          3.54517744 -0.          2.
  2.          0.77258872  2.15888308  0.77258872 -0.          2.
  0.77258872 -0.          2.          2.        ]
```

```
df.head()
```

```
   theta  nu  n  m    lambda
0      1   0  2  0  0.772589
1      1   0  0  0  2.000000
2      1   0  0  0  2.000000
3      1   0  1  0 -0.000000
4      1   0  1  0 -0.000000
```

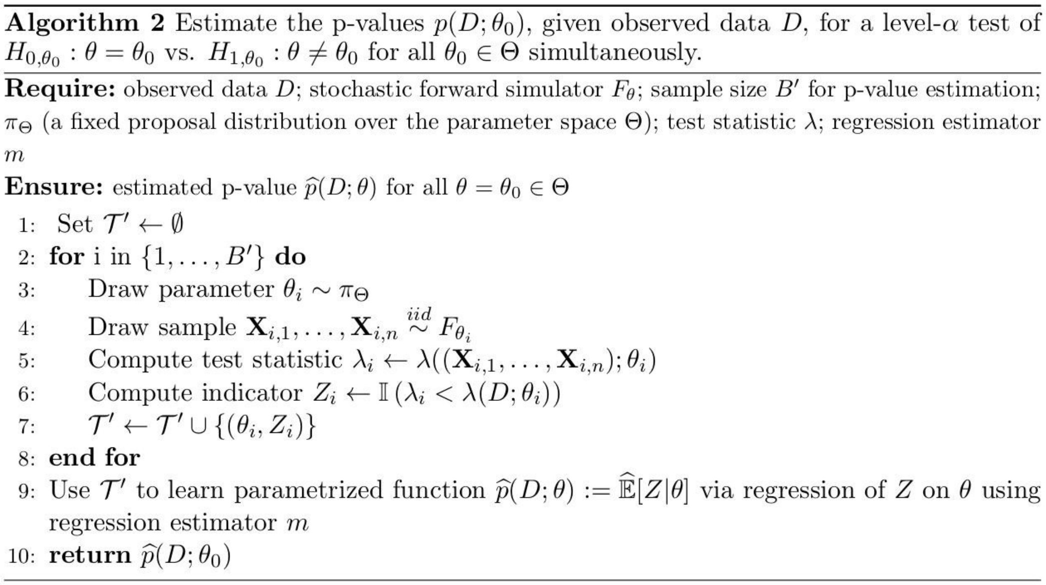
```
n, m, lambda_, theta, nu =results[1]
print(f'results[1] =  (n1, m1, lambda1, theta1, nu1) =  (  \n {n}, \n
{m}, \n {lambda_}, \n {theta}, \n {nu})' )
print(f'''\n (n.shape, m.shape, lambda_.shape, theta.size, nu.size) =
      ({n.shape}, \t {m.shape}, \t {lambda_.shape}, \t {theta.size}, \
t {nu.size})''')
```

```
results[1] =  (n1, m1, lambda1, theta1, nu1) =  (
 [5 9 5 9 3 6 4 4 6 2 8 4 4 5 2 7 5 3 5 4 6 5 5 8 7 4 6 2 5 2 4 7 4 5
7 4 4
 3 9 8],
 [3 4 6 5 4 1 5 3 5 4 6 8 5 5 3 2 4 5 3 5 5 3 3 0 4 9 2 4 4 3 5 2 0 1
4 2 3
 3 2 2],
 [-0.          0.7165121   0.80229178  0.29075642  1.2288131
1.47928694
  0.97179616  0.1396362   0.09005222  2.51359335 -0.
2.96578989
  0.97179616  0.39239727  1.66020193  1.07969347  0.10956358
1.92861676
 -0.          0.97179616  0.09005222 -0.         -0.
7.09035489
  0.09206738  3.7531945   0.52939123  2.51359335  0.10956358
1.66020193
  0.97179616  1.07969347  1.54517744  0.74478362  0.09206738 -0.
  0.1396362   0.63419698  2.52578322  1.75504047],
 2,
 3)

 (n.shape, m.shape, lambda_.shape, theta.size, nu.size) =
      ((40,),    (40,),     (40,),     1,    1)
```

Generate Training data (or take a look at the saved training data)

We then generate training data where the number of training examples is B' according to Alg. 2 of Anne Lee et al. (shown below). The training data now has ${\theta, \nu, N, M } $ as training features and Z as the target. We then use Pytorch to build MLP regression model with average quadratic loss to estimate the distribution of Z, $E[Z \vee \theta, v]$, which according to Alg. 2 is the p-value.

```
algorithm2 = Image('images/Algorithm2.jpg'); display(algorithm2)
```



```
Algorithm 2 Estimate the p-values $p(D;\theta_0)$, given observed data $D$, for a level-$\alpha$ test of
$H_{0,\theta_0}: \theta = \theta_0$ vs. $H_{1,\theta_0}: \theta \neq \theta_0$ for all $\theta_0 \in \Theta$ simultaneously.
Require: observed data $D$; stochastic forward simulator $F_\theta$; sample size $B'$ for p-value estimation;
$\pi_\Theta$ (a fixed proposal distribution over the parameter space $\Theta$); test statistic $\lambda$; regression estimator $m$
Ensure: estimated p-value $\widehat{p}(D;\theta)$ for all $\theta = \theta_0 \in \Theta$
Set $\mathcal{T}' \leftarrow \emptyset$
for i in $\{1, \ldots, B'\}$ do
    Draw parameter $\theta_i \sim \pi_\Theta$
    Draw sample $\mathbf{X}_{i,1}, \ldots, \mathbf{X}_{i,n} \overset{iid}{\sim} F_{\theta_i}$
    Compute test statistic $\lambda_i \leftarrow \lambda((\mathbf{X}_{i,1}, \ldots, \mathbf{X}_{i,n}); \theta_i)$
    Compute indicator $Z_i \leftarrow \mathbb{I}(\lambda_i < \lambda(D;\theta_i))$
    $\mathcal{T}' \leftarrow \mathcal{T}' \cup \{(\theta_i, Z_i)\}$
end for
Use $\mathcal{T}'$ to learn parametrized function $\widehat{p}(D;\theta) := \widehat{\mathbb{E}}[Z|\theta]$ via regression of $Z$ on $\theta$ using
regression estimator $m$
return $\widehat{p}(D;\theta_0)$
```

As we know, the p-value is the probability under the null hypothesis H_{null} (which is in this case parameterized by θ) of finding data of equal or greater *incompatibility* with the predictions of H_{null}. Therefore, in our case, the p-value under the null hypothesis (defined by θ) is given by

$$p_\theta(v) = \text{Prob}(\lambda_{gen}(n,m;\theta,v) \le \lambda_D(N,M;\theta,v)) = \int_{\lambda_D}^{\infty} f(\lambda_{gen}(n,m \mid \theta,v) \mid H_{null}) \, d\lambda_{gen},$$

where f is the PDF of λ. In the strict frequentist approach, θ is rejected only if the p-value is less than the significance level of a hypothesis test α (i.e. accepeted if $p_\theta(v) \le \alpha$)

After calculating the p-value, one can then

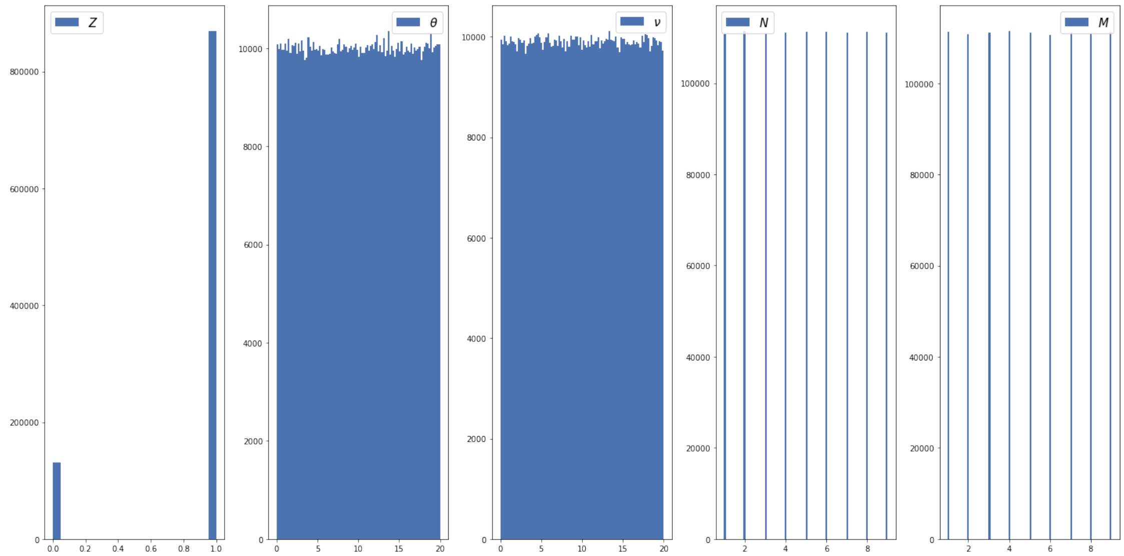
In our study we approximate this integral as the histogram of θ weighted by Z divided by the histogram of θ, and denote this histogram as h. We compare this exact p-value with the outcome of our MLP, $\hat{p}(\theta, v, N, M)$ for the case where $\hat{\theta}$ is taken as the MLE in Fig. below we see almost perfect match.

```
train_df = 
pd.read_csv('data/two_parameters_theta_0_20_1000k_Examples_MLE_True.cs
v')
train_df.describe()
```

```
           Unnamed: 0                Z            theta               nu 
\
count  1000000.000000  1000000.000000  1000000.000000  1000000.000000   

mean    499999.500000        0.869337       10.002658        9.999062   

std     288675.278933        0.337032        5.777129        5.772508   

min          0.000000        0.000000        0.000013        0.000034   

25%     249999.750000        1.000000        4.994221        4.996941   

50%     499999.500000        1.000000       10.005912        9.997695   

75%     749999.250000        1.000000       15.001766       14.996255   

max     999999.000000        1.000000       19.999969       19.999976   


                    N               M  
count  1000000.000000  1000000.000000  
mean         5.001477        4.999767  
std          2.581041        2.582273  
min          1.000000        1.000000  
25%          3.000000        3.000000  
50%          5.000000        5.000000  
75%          7.000000        7.000000  
max          9.000000        9.000000  
```

```
bins_ = 'auto'
fig, ax = plt.subplots(nrows=1, ncols=5, figsize=(20,10))
ax[0].hist(train_df['Z'], bins=bins_, label=r'$Z$')
ax[1].hist(train_df['theta'], bins=bins_, label=r'$\theta$')
ax[2].hist(train_df['nu'], bins=bins_, label=r'$\nu$')
ax[3].hist(train_df['N'], bins=bins_, label=r'$N$')
ax[4].hist(train_df['M'], bins=bins_, label=r'$M$')
```

```
[ax[i].legend(fontsize=font_legend) for i in range(5)]
plt.tight_layout(); plt.show()
```



Generate data according to:

$ \begin{align} \theta & \sim \textrm{uniform}(0, 20), \ \nu & \sim \textrm{uniform}(0, 20), \ n & \sim \textrm{poisson}(\theta + \nu),\ m & \sim \textrm{poisson}(\nu),\ N & \sim \textrm{uniform}(0,10),\ M & \sim \textrm{uniform}(0, 10), \textrm{ and } \ Z & = I[\lambda_{\textrm{gen}} \leq \lambda_D (D, \theta)], \end{align} $

```
thetaMin, thetaMax =  0, 20
numin, numax = 0, 20
Nmin, Nmax =  1,10
Mmin, Mmax =  1 , 10

def generate_training_data(Bprime, MLE, save_data=False):
    """Generate the training data, that is, features=[theta, nu, N,
M], targets=Z"""
    #sample theta and nu from uniform(0,20)
    theta = st.uniform.rvs(thetaMin, thetaMax, size=Bprime)
    # nu = st.uniform.rvs(nuMin, nuMax, size=Bprime)
    nu= st.uniform.rvs(numin, numax, size=Bprime)
    #n,m ~ F_{\theta,\nu}, ie our simulator. sample n from a Poisson
with mean theta+nu
    n = st.poisson.rvs(theta+ nu, size=Bprime)
    #sample m from a poisson with mean nu
    m = st.poisson.rvs(nu, size=Bprime)
    #sample our observed counts (N,M), which take the place of D
    N = np.random.randint(Nmin, Nmax, size=Bprime)
    M = np.random.randint(Mmin, Mmax, size=Bprime)
    SUBSAMPLE=10
    print('n=', n[:SUBSAMPLE])
    print('m=', m[:SUBSAMPLE])
    print('N=', N[:SUBSAMPLE])
    print('M=', M[:SUBSAMPLE])
    lambda_gen = lambda_test(theta, n, m, MLE)
    print('lambda_gen= ', lambda_gen[:SUBSAMPLE])
    lambda_D = lambda_test(theta, N, M, MLE)
    print('lambda_D= ', lambda_D[:SUBSAMPLE])
    #if lambda_gen <= lambda_D: Z=1, else Z=0
    Z = (lambda_gen <= lambda_D).astype(np.int32)

    data_2_param = {'Z' : Z, 'theta' : theta, 'nu': nu, 'N':N, 'M':M}

    data_2_param = pd.DataFrame.from_dict(data_2_param)
    if save_data:
        data_2_param.to_csv('data/two_parameters_theta_%s_%s_
%sk_Examples_MLE_%s.csv' %\
                            (str(thetaMin), str(thetaMax),
str(int(Bprime/1000)), str(MLE)) )

    print('\n')
    print(data_2_param.describe())
    return data_2_param

Train_data_MLE_True = generate_training_data(Bprime=1000000, MLE=True,
save_data=True)
```

```
n= [15 17  4 20  9 31 12 18 26 12]
m= [ 9  9  1  0  0  5  4  8 14  7]
N= [8 6 3 2 5 9 6 8 1 9]
M= [7 6 6 9 8 5 8 1 6 6]
lambda_gen=  [0.22041922 0.59769146 0.70458812 0.15167097 1.59159138
3.72210763
 1.44015718 0.21793792 0.27341912 2.61956417]
lambda_D=  [ 3.19597616  1.32802053  1.95898303 35.34006927
5.32754169  6.69370749
 12.47100404  0.04426842 18.81476063  4.93279847]


                    Z           theta              nu               N
\
count  1000000.000000  1000000.000000  1000000.000000  1000000.000000

mean         0.870055       10.001843       10.000098        4.999642

std          0.336243        5.774806        5.771397        2.581812

min          0.000000        0.000008        0.000020        1.000000

25%          1.000000        4.999020        4.999096        3.000000

50%          1.000000        9.997342       10.002818        5.000000
```

```
75%          1.000000       15.006256       14.988187        7.000000

max          1.000000       19.999982       19.999990        9.000000


                    M
count  1000000.000000
mean         4.994021
std          2.581949
min          1.000000
25%          3.000000
50%          5.000000
75%          7.000000
max          9.000000
```

Write Custom Data Loader

```
# %writefile data/dataloader.py

def split_t_x(df, target, source):
    # change from pandas dataframe format to a numpy
    # array of the specified types
    t = np.array(df[target])
    x = np.array(df[source])
    return t, x

def get_batch(x, batch_size):
    # the numpy function choice(length, number)
    # selects at random "batch_size" integers from
    # the range [0, length-1] corresponding to the
    # row indices.
    rows    = np.random.choice(len(x), batch_size)
    batch_x = x[rows]
    # batch_x.T[-1] = np.random.uniform(0, 1, batch_size)
    return batch_x


def get_data_sets(simulate_data, batchsize):
    """write custom data generator because who wants to read pytorch's
DataLoader source code
    (and its sometimes slow for some reason)"""
    # if simulate_data:
    #     Train_data_MLE_True = generate_training_data(Bprime=100000,
MLE=True, save_data=False)

    # if SUBSAMPLE:
```

```
    #     data=load_df('data/TWO_PARAMETERS_TRAINING_DATA_1M.csv',
SUBSAMPLE=10000)#This is MLE DATA!
    # else:
    #     data=load_df('data/TWO_PARAMETERS_TRAINING_DATA_1M.csv')
    # data=load_df('data/TWO_PARAMETERS_TRAINING_DATA_1M.csv')
    data =
pd.read_csv('data/two_parameters_theta_0_20_1000k_Examples_MLE_True.cs
v',
                 # nrows=SUBSAMPLE,
                 usecols=['Z','theta','nu', 'N', 'M']
                )
    train_data, test_data = train_test_split(data,
                                         test_size=0.02)
    #split the train data (0.8 of whole set) again into 0.8*0.8=0.64
of whole set
    # train_data, valid_data = train_test_split(train_data,
test_size=0.2)
    train_data = train_data.reset_index(drop=True)
    # valid_data = valid_data.reset_index(drop=True)
    test_data  = test_data.reset_index(drop=True)

    target='Z'
    source = ['theta','nu','N','M']
    train_t, train_x = split_t_x(train_data, target=target,
source=source)
    # valid_t, valid_x = split_t_x(valid_data, target=target,
source=source)
    test_t,  test_x  = split_t_x(test_data,  target=target,
source=source)

    def training_set_features():
            #start with an infinite loop, so that you can keep calling
next (i.e. set = train_set(); set.next() ) until you run out of
training examples
        while True:
            #get a random batch of the defined size
            batch_x = get_batch(train_x, batchsize)
            #print('batch_x', batch_x)
            #index of one of the items in our examples
            yield batch_x

    def evaluation_set_features():
        #start with an infinite loop, so that you can keep calling
next (i.e. set = train_set(); set.next() ) until you run out of
training examples
        while True:
            batch_x = get_batch(test_x,batchsize)
            #index of one of the items in our examples
            yield batch_x
    def training_set_targets():
            #start with an infinite loop, so that you can keep calling
next (i.e. set = train_set(); set.next() ) until you run out of
training examples
        while True:
            #get a random batch of the defined size
            batch_x = get_batch(train_t, batchsize)
            #print('batch_x', batch_x)
            #index of one of the items in our examples
            yield batch_x

    def evaluation_set_targets():
            #start with an infinite loop, so that you can keep calling
next (i.e. set = train_set(); set.next() ) until you run out of
training examples
        while True:
            #get a random batch of the defined size
            batch_x = get_batch(test_t, batchsize)
            #print('batch_x', batch_x)
            #index of one of the items in our examples
            yield batch_x

    return training_set_features, training_set_targets,
evaluation_set_features, evaluation_set_targets

training_set_features, training_set_targets, evaluation_set_features,
evaluation_set_targets = get_data_sets(simulate_data=True,
batchsize=300)

first_features_batch = next(training_set_features())
print('first features batch \n', first_features_batch[:5])
print('\nfirst features batch shape \n', first_features_batch.shape)

first features batch
 [[19.52477661  6.51129404  2.          4.        ]
 [ 9.35131833 12.84672943  1.          6.        ]
 [ 0.61313754 13.7363275   7.          9.        ]
 [ 7.02718582 17.24384141  4.          7.        ]
 [14.6905525  16.97985822  5.          4.        ]]

first features batch shape
 (300, 4)

def binsize(data_df_or_Bprime):
    """ decide on the number of bins in a histogram according to
Struge's rule"""
    if isinstance(data_df_or_Bprime,pd.core.frame.DataFrame):
        bin_count = int(np.ceil(np.log2(data_df_or_Bprime.shape[0])) +
1)
```

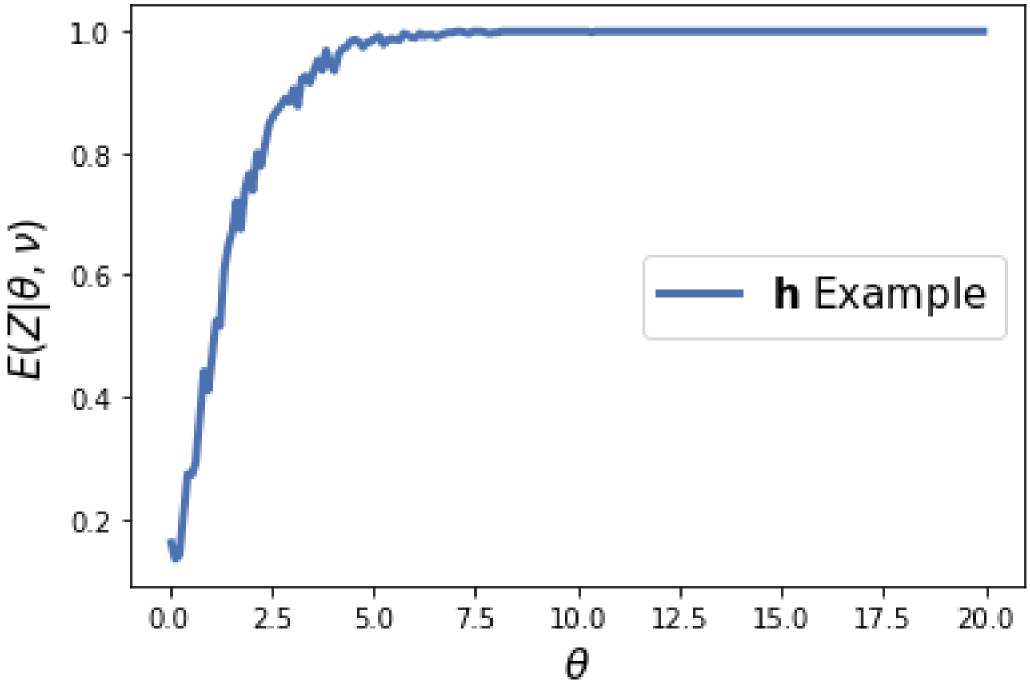
```
    elif isinstance(data_df_or_Bprime, int):
        bin_count = int(np.ceil(np.log2(data_df_or_Bprime)) + 1)
    return bin_count
```

Plot the histogrammed function the histogrammed function $h(\tilde{\theta}, \nu, N, M) = h(\theta_{min}, \theta_{max}, \nu, N, M)$ where $\tilde{\theta}$ means that it is simulated (inside the function).

```
def make_hist_data(Bprime,
              thetamin, thetamax,
              nu, N, M,
                nbins,
             MLE=True):

    theta = st.uniform.rvs(thetamin, thetamax, size=Bprime)
    n = st.poisson.rvs(theta + nu, size=Bprime)
    m = st.poisson.rvs(nu, size=Bprime)

    Z = (lambda_test(theta, n, m, MLE=MLE) <
         lambda_test(theta, N, M, MLE=MLE)).astype(np.int32)

    thetarange = (thetamin, thetamax)
    # bins = binsize(Bprime)

    # weighted histogram   (count the number of ones per bin)
    y1, bb = np.histogram(theta,
                          bins=nbins,
                          range=thetarange,
                          weights=Z)

    # unweighted histogram (count number of ones and zeros per bin)
    yt, _ = np.histogram(theta,
                         bins=nbins,
                         range=thetarange)

    y =  y1 / yt

    return y, bb

h, h_bins = make_hist_data(Bprime=1000,
                           thetamin=0,thetamax=20,
                           nu=3,N=1,M=1,
                           nbins=200, MLE=True)
h
```

```
array([0.25      , 0.28571429, 0.        , 0.33333333, 0.42857143,
       0.        , 0.33333333, 0.16666667, 0.16666667, 0.28571429,
       0.33333333, 0.25      , 0.71428571, 1.        , 0.66666667,
       0.75      , 0.71428571, 0.625     , 0.75      , 0.66666667,
       1.        , 0.875     , 0.8       , 1.        , 0.625     ,
       0.5       , 1.        , 0.81818182, 1.        , 0.8       ,
       1.        , 1.        , 1.        , 1.        , 0.66666667,
       1.        , 1.        , 1.        , 0.85714286, 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       0.5       , 0.85714286, 1.        , 1.        , 0.9       ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 0.66666667, 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ,
       1.        , 1.        , 1.        , 1.        , 1.        ])

def plot_one_hist(Bprime, thetamin, thetamax, nu, N, M, MLE, nbins,
ax):
    counts, bins= make_hist_data(Bprime,
              thetamin, thetamax,
              nu, N, M,
            nbins,
             MLE)
    bin_centers = (bins[1:]+bins[:-1])/2
    ax.plot(bin_centers, counts, label= r'$\mathbf{h}$ Example', lw=3)
    ax.set_xlabel(r'$\theta$',fontsize=font_axes)
    ax.set_ylabel(r'$E(Z|\theta,\nu)$',fontsize=font_axes)
    ax.legend(loc='center right',fontsize=font_legend)

fig= plt.figure();ax=fig.add_subplot()
```

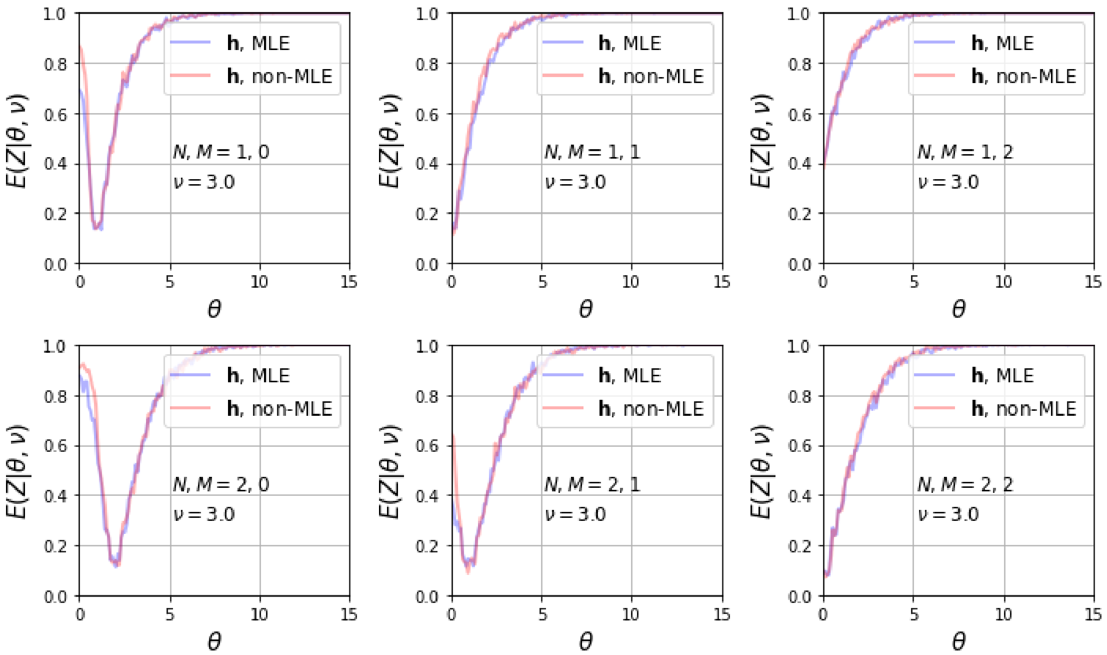
```
#Example:
plot_one_hist(Bprime=100000, thetamin=0,thetamax=20,
nu=3,N=1,M=1,MLE=True, nbins=200, ax=ax)
```



Plot the histogrammed approximations for the MLE vs non-MLE cases for a single value of ν

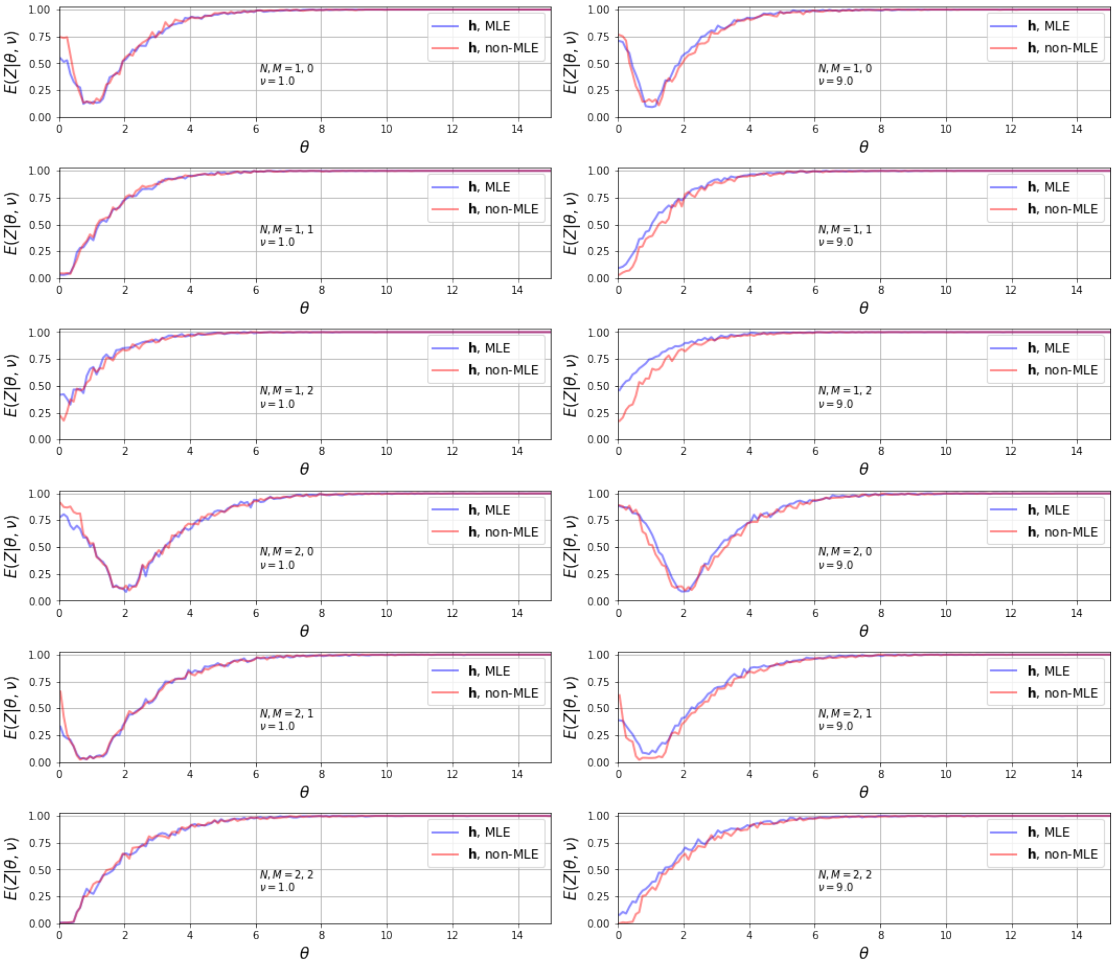
```
def plot_data_one_nu(Bprime, thetamin, thetamax, nu, D, MLE,
              FONTSIZE=15,
              func=None,
              fgsize=(10, 6)):

    # make room for 6 sub-plots
    fig, ax = plt.subplots(nrows=2,
                           ncols=3,
                           figsize=fgsize)

    # padding
    plt.subplots_adjust(hspace=0.01)
    plt.subplots_adjust(wspace=0.20)

    # use flatten() to convert a numpy array of
    # shape (nrows, ncols) to a 1-d array.
    ax = ax.flatten()

    for j, (N, M) in enumerate(D):

        y, bb = make_hist_data(Bprime,
                              thetamin, thetamax,
                              nu, N, M,
                              nbins=200,
                              MLE=True)

        ax[j].set_xlim(thetamin, thetamax-5)
        ax[j].set_ylim(0, 1)
        ax[j].set_xlabel(r'$\theta$', fontsize=FONTSIZE)
        ax[j].set_ylabel(r'$E(Z|\theta, \nu)$', fontsize=FONTSIZE)

        x = (bb[1:]+bb[:-1])/2
        ax[j].plot(x, y, 'b', lw=2, label='$\mathbf{h}$, MLE',
alpha=0.3)
        #h is histogram approximation

        y_nonMLE, bb_nonMLE = make_hist_data(Bprime,
                              thetamin, thetamax,
                              nu, N, M,
                              nbins=200,
                              MLE=False)


        x_nonMLE = (bb_nonMLE[1:]+bb_nonMLE[:-1])/2
        ax[j].plot(x_nonMLE, y_nonMLE, 'r', lw=2, label='$\mathbf{h}$,
non-MLE',alpha=0.3)


        if func:
            p, _ = func(nu, N, M)
            ax[j].plot(x, p, 'r', lw=2, label='f')
            #f is model approximation

        ax[j].grid(True, which="both", linestyle='-')
        ax[j].text(5.1, 0.42, r'$N, M = %d, %d$' % (N, M),
fontsize=font_legend-3
                   # fontsize=FONTSIZE
                  )

        ax[j].text(5.1, 0.30, r'$\nu = %5.1f$' % nu,
fontsize=font_legend-3
                   # fontsize=FONTSIZE
                  )

        ax[j].legend(loc='upper right',fontsize=font_legend-3)

    # hide unused sub-plots
    for k in range(j+1, len(ax)):
        ax[k].set_visible(False)

    plt.tight_layout()
    plt.show()
```

```
D = [ (N, M) for N in range(1,3) for M in range(3)]
plot_data_one_nu(Bprime=100000, thetamin=0, thetamax=20, nu=3, D=D,
MLE=True)
```



Plot the histogrammed approximations for the MLE vs non-MLE cases for multiple values of ν, indicating the dependence on the nuissance parameter

```
def plot_data(Bprime, thetamin, thetamax, D, MLE,
              FONTSIZE=15,
              func=None,
              fgsize=(15, 13)):

    # make room for 6 sub-plots
    fig, ax = plt.subplots(nrows=6,
                           ncols=2,
                           figsize=fgsize)

    # padding
    plt.subplots_adjust(hspace=0.01)
    plt.subplots_adjust(wspace=0.20)

    # use flatten() to convert a numpy array of
    # shape (nrows, ncols) to a 1-d array.
    # ax = ax.flatten()

    for j, (N, M) in enumerate(D):
        NU1=1
        y, bb = make_hist_data(Bprime,
                              thetamin, thetamax,
                               NU1, N, M,
                              nbins=200,
                              MLE=True)

        ax[j, 0].set_xlim(thetamin, thetamax-5)
        ax[j, 0].set_ylim(0, 1.03)
        ax[j, 0].set_xlabel(r'$\theta$', fontsize=FONTSIZE)
        ax[j, 0].set_ylabel(r'$E(Z|\theta, \nu)$', fontsize=FONTSIZE)

        x = (bb[1:]+bb[:-1])/2
        ax[j, 0].plot(x, y, 'b', lw=2, label='$\mathbf{h}$, MLE',
alpha=0.45)
        #h is histogram approximation

        y_nonMLE, bb_nonMLE = make_hist_data(Bprime,
                              thetamin, thetamax,
                              NU1, N, M,
                              nbins=200,
                              MLE=False)


        x_nonMLE = (bb_nonMLE[1:]+bb_nonMLE[:-1])/2
        ax[j, 0].plot(x_nonMLE, y_nonMLE, 'r', lw=2, label='$\
mathbf{h}$, non-MLE',alpha=0.45)

        ax[j, 0].grid(True, which="both", linestyle='-')
        ax[j, 0].text(6.1, 0.42, r'$N, M = %d, %d$' % (N, M),
                   # fontsize=FONTSIZE
                  )

        ax[j, 0].text(6.1, 0.30, r'$\nu = %5.1f$' % NU1,
                   # fontsize=FONTSIZE
                  )

        ax[j, 0].legend(loc='upper right', fontsize=font_legend-3)
        ############define second nu value to see difference
        NU2=9
        y, bb = make_hist_data(Bprime,
                              thetamin, thetamax,
                               NU2, N, M,
                              nbins=200,
                              MLE=True)

        ax[j, 1].set_xlim(thetamin, thetamax-5)
        ax[j, 1].set_ylim(0, 1.03)
        ax[j, 1].set_xlabel(r'$\theta$', fontsize=FONTSIZE)
        ax[j, 1].set_ylabel(r'$E(Z|\theta, \nu)$', fontsize=FONTSIZE)

        x = (bb[1:]+bb[:-1])/2
        ax[j, 1].plot(x, y, 'b', lw=2, label='$\mathbf{h}$, MLE',
alpha=0.45)
        #h is histogram approximation
        y_nonMLE, bb_nonMLE = make_hist_data(Bprime,
                              thetamin, thetamax,
                              NU1, N, M,
                              nbins=200,
                              MLE=False)


        x_nonMLE = (bb_nonMLE[1:]+bb_nonMLE[:-1])/2
        ax[j, 1].plot(x_nonMLE, y_nonMLE, 'r', lw=2, label='$\
mathbf{h}$, non-MLE',alpha=0.45)


        ax[j, 1].grid(True, which="both", linestyle='-')
        ax[j, 1].text(6.1, 0.42, r'$N, M = %d, %d$' % (N, M),
                   # fontsize=FONTSIZE
                  )

        ax[j, 1].text(6.1, 0.30, r'$\nu = %5.1f$' % NU2,
                   # fontsize=FONTSIZE
                  )

        ax[j, 1].legend(loc='upper right', fontsize=font_legend-3)

        if func:
            p, _ = func(nu, N, M)
            ax[j, 0].plot(x, p, 'r', lw=2, label='f')
            #f is model approximation



    # hide unused sub-plots
    for k in range(j+1, len(ax)):
        ax[k].set_visible(False)

    plt.tight_layout()
    plt.show()

D = [ (N, M) for N in range(1,3) for M in range(3)]
plot_data(Bprime=100000, thetamin=0, thetamax=20, D=D, MLE=True)
```



ML

```
def getwholedata(MLE_or_nonMLE, valid=False):
    if MLE:
        data = 
pd.read_csv('data/two_parameters_theta_0_20_1000k_Examples_MLE_True.csv',
                     # nrows=SUBSAMPLE,
                     usecols=['Z','theta','nu', 'N', 'M']
                    )

    else:
        data = 
pd.read_csv('data/two_parameters_theta_0_20_1000k_Examples_MLE_False.csv',
             # nrows=SUBSAMPLE,
             usecols=['Z','theta','nu', 'N', 'M']
            )
    train_data, test_data = train_test_split(data, test_size=0.2)
    #split the train data (0.8 of whole set) again into 0.8*0.8=0.64
of whole set


    train_data = train_data.reset_index(drop=True)
    test_data  = test_data.reset_index(drop=True)

    target='Z'
    source = ['theta','nu','N','M']

    train_t, train_x = split_t_x(train_data, target=target,
source=source)
    test_t,  test_x  = split_t_x(test_data,  target=target,
source=source)
    print('train_t shape = ', train_t.shape, '\n')
    print('train_x shape = ', train_x.shape, '\n')

    if valid:
        #if you want to also make a validation data set
        train_data, valid_data = train_test_split(train_data,
test_size=0.2)
        valid_data = valid_data.reset_index(drop=True)
        valid_t, valid_x = split_t_x(valid_data, target=target,
source=source)


    return train_t, train_x, test_t,  test_x


# n_iterations=50
```

Define Model, which will approximate the expectation value above

```
class Model(nn.Module):

    def __init__(self, n_inputs=4, n_nodes=20, n_layers=5):

        # call constructor of base (or super, or parent) class
        super(Model, self).__init__()

        self.layers = []

        # create input layer
        self.layer0 = nn.Linear(n_inputs, n_nodes)
        self.layers.append(self.layer0)

        # create "hidden" layers
        for l in range(1, n_layers):
            cmd = 'self.layer%d = nn.Linear(%d, %d)' % \
            (l, n_nodes, n_nodes)
            exec(cmd)
            cmd = 'self.layers.append(self.layer%d)' % l
            exec(cmd)

        # create output layer
        cmd = 'self.layer%d = nn.Linear(%d, 1)' % (n_layers, n_nodes)
        exec(cmd)
        cmd = 'self.layers.append(self.layer%d)' % n_layers
        exec(cmd)

    # define (required) method to compute output of network
    def forward(self, x):
        y = x
        for layer in self.layers[:-1]:
            y = layer(y)
            y = torch.relu(y)
        y = self.layers[-1](y)
        y = torch.sigmoid(y)
        return y

model = Model()
print(model)
```

```
Model(
  (layer0): Linear(in_features=4, out_features=20, bias=True)
  (layer1): Linear(in_features=20, out_features=20, bias=True)
  (layer2): Linear(in_features=20, out_features=20, bias=True)
  (layer3): Linear(in_features=20, out_features=20, bias=True)
  (layer4): Linear(in_features=20, out_features=20, bias=True)
  (layer5): Linear(in_features=20, out_features=1, bias=True)
)
```

```
def average_quadratic_loss(f, t, x):
    # f and t must be of the same shape
    return  torch.mean((f - t)**2)
def average_loss(f, t):
    # f and t must be of the same shape
    return  torch.mean((f - t)**2)

def validate(model, avloss, inputs, targets):
    # make sure we set evaluation mode so that any training specific
    # operations are disabled.
    model.eval() # evaluation mode

    with torch.no_grad(): # no need to compute gradients wrt. x and t
        x = torch.from_numpy(inputs).float()
        t = torch.from_numpy(targets).float()
        # remember to reshape!
        o = model(x).reshape(t.shape)
    return avloss(o, t, x)


def get_features_training_batch(x, t, batch_size):
    # the numpy function choice(length, number)
    # selects at random "batch_size" integers from
    # the range [0, length-1] corresponding to the
    # row indices.
    rows    = np.random.choice(len(x), batch_size)
    batch_x = x[rows]
    batch_t = t[rows]
    # batch_x.T[-1] = np.random.uniform(0, 1, batch_size)
    return (batch_x, batch_t)


def train(model, optimizer, avloss,
          batch_size,
          n_iterations, traces,
          step, window, MLE):

    # to keep track of average losses
    xx, yy_t, yy_v, yy_v_avg = traces

    n = len(valid_x)

    if MLE:
        train_t, train_x, test_t,  test_x =
getwholedata(MLE_or_nonMLE=True, valid=False)
    else:
        train_t, train_x, test_t,  test_x =
getwholedata(MLE_or_nonMLE=False, valid=False)

    print('Iteration vs average loss')
    print("%10s\t%10s\t%10s" % \
          ('iteration', 'train-set', 'valid-set'))

    # training_set_features, training_set_targets,
evaluation_set_features, evaluation_set_targets =
get_data_sets(simulate_data=False, batchsize=batch_size)

    for ii in range(n_iterations):

        # set mode to training so that training specific
        # operations such as dropout are enabled.


        model.train()

        # get a random sample (a batch) of data (as numpy arrays)
        #Harrison-like Loader
        batch_x, batch_t = get_features_training_batch(train_x,
train_t, batch_size)

        #Or Ali's Loader
        # batch_x, batch_t = next(training_set_features()),
next(training_set_targets())
        # batch_x_eval, batch_t_eval =
next(evaluation_set_features()), next(evaluation_set_targets())

        with torch.no_grad(): # no need to compute gradients
            # wrt. x and t
            x = torch.from_numpy(batch_x).float()
            t = torch.from_numpy(batch_t).float()


        outputs = model(x).reshape(t.shape)

        # compute a noisy approximation to the average loss
        empirical_risk = avloss(outputs, t, x)

        # use automatic differentiation to compute a
        # noisy approximation of the local gradient
        optimizer.zero_grad()       # clear previous gradients
        empirical_risk.backward()   # compute gradients

        # finally, advance one step in the direction of steepest
        # descent, using the noisy local gradient.
        optimizer.step()            # move one step

        if ii % step == 0:


            #using Harrison-like loader
            acc_t = validate(model, avloss, train_x[:n], train_t[:n])
            acc_v = validate(model, avloss, test_x[:n], test_t[:n])

            #using Ali's loader
            # acc_t = validate(model, avloss, batch_x, batch_t)
            # acc_v = validate(model, avloss, batch_x_eval,
batch_t_eval)


            yy_t.append(acc_t)
            yy_v.append(acc_v)

            # compute running average for validation data
            len_yy_v = len(yy_v)
            if   len_yy_v < window:
                yy_v_avg.append( yy_v[-1] )
            elif len_yy_v == window:
                yy_v_avg.append( sum(yy_v) / window )
            else:
                acc_v_avg  = yy_v_avg[-1] * window
                acc_v_avg += yy_v[-1] - yy_v[-window-1]
                yy_v_avg.append(acc_v_avg / window)

            if len(xx) < 1:
                xx.append(0)
                print("%10d\t%10.6f\t%10.6f" % \
                      (xx[-1], yy_t[-1], yy_v[-1]))
            else:
                xx.append(xx[-1] + step)

                print("\r%10d\t%10.6f\t%10.6f\t%10.6f" % \
                          (xx[-1], yy_t[-1], yy_v[-1], yy_v_avg[-1]),
                      end='')

    print()
    return (xx, yy_t, yy_v, yy_v_avg)

def plot_average_loss(traces, ftsize=18,save_loss_plots=False):

    xx, yy_t, yy_v, yy_v_avg = traces

    # create an empty figure
    fig = plt.figure(figsize=(6, 4.5))
    fig.tight_layout()

    # add a subplot to it
    nrows, ncols, index = 1,1,1
    ax  = fig.add_subplot(nrows,ncols,index)

    ax.set_title("Average loss")

    ax.plot(xx, yy_t, 'b', lw=2, label='Training')
    ax.plot(xx, yy_v, 'r', lw=2, label='Validation')
    #ax.plot(xx, yy_v_avg, 'g', lw=2, label='Running average')

    ax.set_xlabel('Iterations', fontsize=ftsize)
    ax.set_ylabel('average loss', fontsize=ftsize)
    ax.set_xscale('log')
    ax.set_yscale('log')
    ax.grid(True, which="both", linestyle='-')
    ax.legend(loc='upper right')
    if save_loss_plots:

plt.savefig('images/loss_curves/IQN_'+N+T+'_Consecutive_2.png')
        print('\nloss curve saved in
images/loss_curves/IQN_'+N+target+'_Consecutive.png')
```

```
    # if show_loss_plots:
    plt.show()
```

Define my regularized regression model. Since the values are on the same scales, it is not necessary to include batchnormalization or to normalize the data

```
class RegularizedRegressionModel(nn.Module):
    #inherit from the super class
    def __init__(self, nfeatures, ntargets, nlayers, hidden_size, 
dropout):
        super().__init__()
        layers = []
        for _ in range(nlayers):
            if len(layers) ==0:
                #inital layer has to have size of input features as 
its input layer
                #its output layer can have any size but it must match 
the size of the input layer of the next linear layer
                #here we choose its output layer as the hidden size 
(fully connected)
                layers.append(nn.Linear(nfeatures, hidden_size))
                #batch normalization
                # layers.append(nn.BatchNorm1d(hidden_size))
                #Dropout seems to worsen model performance
                layers.append(nn.Dropout(dropout))
                #ReLU activation 
                layers.append(nn.ReLU())
            else:
                #if this is not the first layer (we dont have layers)
                layers.append(nn.Linear(hidden_size, hidden_size))
                # layers.append(nn.BatchNorm1d(hidden_size))
                #Dropout seems to worsen model performance
                layers.append(nn.Dropout(dropout))
                layers.append(nn.ReLU())
                #output layer:
        layers.append(nn.Linear(hidden_size, ntargets)) 

        # ONLY IF ITS A CLASSIFICATION, ADD SIGMOID
        layers.append(nn.Sigmoid())
            #we have defined sequential model using the layers in 
oulist 
        self.model = nn.Sequential(*layers)


    def forward(self, x):
        return self.model(x)
```

Make a hyperparameter Tuning Workflow

Use Optuna (axriv:1907.10902) for hyperparameter tuning. The search space for the hyperparameters that I'm tuning is defined in the params dictionary:

```
    params = {
      "nlayers": trial.suggest_int("nlayers",1,13),
      "hidden_size": trial.suggest_int("hidden_size", 2, 130),
      "dropout": trial.suggest_float("dropout", 0.1,0.5),
      "optimizer_name" : trial.suggest_categorical("optimizer_name",
["Adam", "RMSprop"]),
      "learning_rate": trial.suggest_float("learning_rate", 1e-5, 1e-
2),
      "batch_size": trial.suggest_int("batch_size", 1000, 10000)

    }

class Engine:
    """loss, training and evaluation"""
    def __init__(self, model, optimizer, batch_size):
                 #, device):
        self.model = model
        #self.device= device
        self.optimizer = optimizer
        self.batch_size=batch_size

    #the loss function returns the loss function. It is a static
method so it doesn't need self
    # @staticmethod
    # def loss_fun(targets, outputs):
    #   tau = torch.rand(outputs.shape)
    #   return torch.mean(torch.where(targets >= outputs,
    #                                   tau * (targets - outputs),
    #                                   (1 - tau)*(outputs -
targets)))

#     This loss combines a Sigmoid layer and the BCELoss in one single
class. This version is more numerically stable than using a plain
Sigmoid followed by a BCELoss as,
#     by combining the operations into one layer

    def train(self, x, t):
        """the training function: takes the training dataloader"""
        self.model.train()
        final_loss = 0
        for iteration in range(n_iterations):
            self.optimizer.zero_grad()
            batch_x, batch_t = get_features_training_batch(x, t,
self.batch_size)#x and t are train_x and train_t
```

```
            # with torch.no_grad():
            inputs=torch.from_numpy(batch_x).float()
            targets=torch.from_numpy(batch_t).float()
            outputs = self.model(inputs)
            loss = average_quadratic_loss(outputs, targets, inputs)
            loss.backward()
            self.optimizer.step()
            final_loss += loss.item()

        return final_loss / self.batch_size

    def evaluate(self, x, t):
        """the training function: takes the training dataloader"""
        self.model.eval()
        final_loss = 0
        for iteration in range(n_iterations):
            batch_x, batch_t = get_features_training_batch(x, t,
self.batch_size)#x and t are train_x and train_t

            # with torch.no_grad():
            inputs=torch.from_numpy(batch_x).float()
            targets=torch.from_numpy(batch_t).float()
            outputs = self.model(inputs)
            loss =average_quadratic_loss(outputs, targets, inputs)
            final_loss += loss.item()
        return final_loss / self.batch_size



EPOCHS=1
def run_train(params, save_model=False):
    """For tuning the parameters"""

    model =  RegularizedRegressionModel(
              nfeatures=train_x.shape[1],
                ntargets=1,
                nlayers=params["nlayers"],
                hidden_size=params["hidden_size"],
                dropout=params["dropout"]
                )
    # print(model)


    learning_rate= params["learning_rate"]
    optimizer_name = params["optimizer_name"]

    # optimizer = torch.optim.Adam(model.parameters(),
lr=params["learning_rate"])
```

```
    optimizer = getattr(torch.optim, optimizer_name)
(model.parameters(), lr=learning_rate)

    eng=Engine(model, optimizer, batch_size=params["batch_size"])
    best_loss = np.inf
    early_stopping_iter=10
    early_stopping_coutner=0

    for epoch in range(EPOCHS):
        train_loss = eng.train(train_x, train_t)
        valid_loss=eng.evaluate(test_x, test_t)

        print(f"{epoch} \t {train_loss} \t {valid_loss}")
        if valid_loss<best_loss:
            best_loss=valid_loss
            if save_model:
                model.save(model.state_dict(), "model_m.bin")
        else:
            early_stopping_coutner+=1
        if early_stopping_coutner > early_stopping_iter:
            break
    return best_loss

# run_train()

def objective(trial):
    params = {
      "nlayers": trial.suggest_int("nlayers",1,13),
      "hidden_size": trial.suggest_int("hidden_size", 2, 130),
      "dropout": trial.suggest_float("dropout", 0.1,0.5),
      "optimizer_name" : trial.suggest_categorical("optimizer_name",
["Adam", "RMSprop"]),
      "learning_rate": trial.suggest_float("learning_rate", 1e-5, 1e-
2),
      "batch_size": trial.suggest_int("batch_size", 1000, 10000)

    }
    # all_losses=[]

    temp_loss = run_train(params,save_model=False)
    # all_losses.append(temp_loss)
    return temp_loss

def tune_hyperparameters():
    print('Getting best hyperparameters')
    study=optuna.create_study(direction="minimize")
    study.optimize(objective, n_trials=10)
    best_trial = study.best_trial
    print('best model parameters', best_trial.params)
    best_params=best_trial.params#this is a dictionary
    filename='best_params/best_params_Test_Trials.csv'
    param_df=pd.DataFrame({
                            'n_layers':best_params["nlayers"],
                            'hidden_size':best_params["hidden_size"],
                            'dropout':best_params["dropout"],

'optimizer_name':best_params["optimizer_name"],
                            'learning_rate':
best_params["learning_rate"],
                            'batch_size':best_params["batch_size"] },
                                    index=[0]
    )

    param_df.to_csv(filename)
```

Don't run the one cell below, unless you want to tune!

```
tune_hyperparameters()
```

Load the dictionary of the best hyperparameters that was saved from our hyperparameter tuning workflow, and retrieve the values

```
BEST_PARAMS = pd.read_csv('best_params/best_params_Test_Trials.csv')
print(BEST_PARAMS)

n_layers = int(BEST_PARAMS["n_layers"])
hidden_size = int(BEST_PARAMS["hidden_size"])
dropout = float(BEST_PARAMS["dropout"])
optimizer_name = BEST_PARAMS["optimizer_name"].to_string().split()[1]
learning_rate =  float(BEST_PARAMS["learning_rate"])
batch_size = int(BEST_PARAMS["batch_size"])
```

```
   Unnamed: 0  n_layers  hidden_size  dropout optimizer_name 
learning_rate  \
0           0         4           11  0.13208        RMSprop 
0.006398   

   batch_size  
0        1000  
```

Define network node shapes, parameters, and training data

```
BATCHSIZE=batch_size
training_set_features, training_set_targets, evaluation_set_features, 
evaluation_set_targets = \
get_data_sets(simulate_data=False, batchsize=BATCHSIZE)

sample_x=next(training_set_features())#this is just to get the 
dimenstions of one batch
sample_y=next(training_set_targets())
#(batchsize,5) for mass
```

```
print('sample x shape', sample_x.shape)
print('sample t shape', sample_y.shape)

n_features = sample_x.shape[1]
print('\n')



model =  RegularizedRegressionModel(
    nfeatures=sample_x.shape[1],
    ntargets=1,
    nlayers=n_layers,
    hidden_size=hidden_size,
    dropout=dropout
    )

print(model)
```

```
sample x shape (1000, 4)
sample t shape (1000,)


RegularizedRegressionModel(
  (model): Sequential(
    (0): Linear(in_features=4, out_features=11, bias=True)
    (1): Dropout(p=0.1320798105984151, inplace=False)
    (2): ReLU()
    (3): Linear(in_features=11, out_features=11, bias=True)
    (4): Dropout(p=0.1320798105984151, inplace=False)
    (5): ReLU()
    (6): Linear(in_features=11, out_features=11, bias=True)
    (7): Dropout(p=0.1320798105984151, inplace=False)
    (8): ReLU()
    (9): Linear(in_features=11, out_features=11, bias=True)
    (10): Dropout(p=0.1320798105984151, inplace=False)
    (11): ReLU()
    (12): Linear(in_features=11, out_features=1, bias=True)
    (13): Sigmoid()
  )
)
```

Chose whose model (Ali or Harrison) and paramers and train

```
def initiate_whose_model(Ali_or_Harrison, MLE):
    whose_model='Ali'

    if whose_model=='Harrison':
        n_layers=5
        hidden_size=5
        dropout=0
        learning_rate=int(1e-3)
        batch_size=64
        optimizer     = torch.optim.Adam(model.parameters(),
lr=int(1e-3))
        model=Model()
    elif whose_model=='Ali':
        n_layers = int(BEST_PARAMS["n_layers"])
        hidden_size = int(BEST_PARAMS["hidden_size"])
        dropout = float(BEST_PARAMS["dropout"])
        optimizer_name =
BEST_PARAMS["optimizer_name"].to_string().split()[1]
        learning_rate =  float(BEST_PARAMS["learning_rate"])
        batch_size = int(BEST_PARAMS["batch_size"])
        model =  RegularizedRegressionModel(
            nfeatures=sample_x.shape[1],
            ntargets=1,
            nlayers=n_layers,
            hidden_size=hidden_size,
            dropout=dropout
            )
        optimizer = getattr(torch.optim, str(optimizer_name) )
(model.parameters(), lr=learning_rate)

    return n_layers, hidden_size, dropout, optimizer_name,
learning_rate, batch_size, model, optimizer

n_layers, hidden_size, dropout, optimizer_name, learning_rate,
batch_size, model_MLE, optimizer_MLE = initiate_whose_model('Ali',
MLE=True)
print(optimizer_MLE)
print('\n\n')
print(model_MLE)

#also initiate non-MLE model
n_layers, hidden_size, dropout, optimizer_name, learning_rate,
batch_size, model_nonMLE, optimizer_nonMLE =
initiate_whose_model('Ali', MLE=False)
```

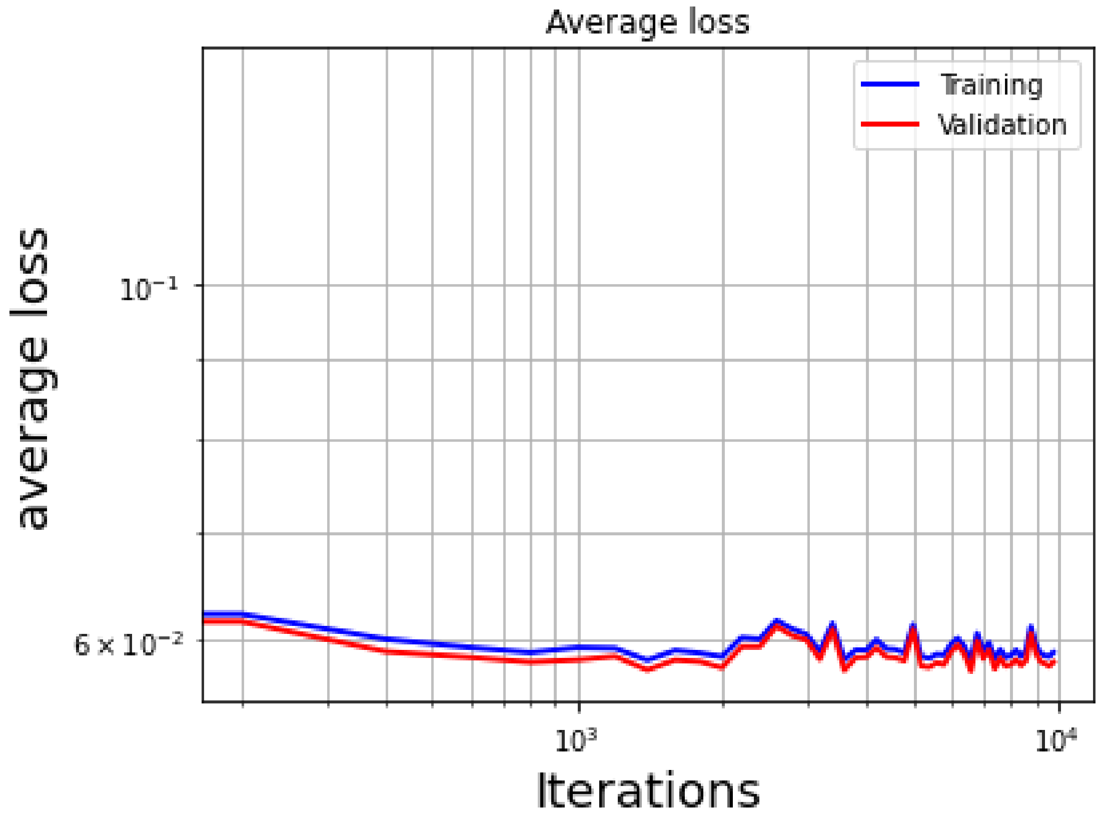
```
RMSprop (
Parameter Group 0
    alpha: 0.99
    centered: False
    eps: 1e-08
    lr: 0.0063975512794992
    momentum: 0
    weight_decay: 0
)



RegularizedRegressionModel(
  (model): Sequential(
    (0): Linear(in_features=4, out_features=11, bias=True)
    (1): Dropout(p=0.1320798105984151, inplace=False)
    (2): ReLU()
    (3): Linear(in_features=11, out_features=11, bias=True)
    (4): Dropout(p=0.1320798105984151, inplace=False)
    (5): ReLU()
    (6): Linear(in_features=11, out_features=11, bias=True)
    (7): Dropout(p=0.1320798105984151, inplace=False)
    (8): ReLU()
    (9): Linear(in_features=11, out_features=11, bias=True)
    (10): Dropout(p=0.1320798105984151, inplace=False)
    (11): ReLU()
    (12): Linear(in_features=11, out_features=1, bias=True)
    (13): Sigmoid()
  )
)
```

Train MLE model

```
BATCHSIZE=batch_size
traces_MLE = ([], [], [], [])
traces_step = 200


n_iterations=10000
traces_MLE= train(model=model_MLE,
              optimizer=optimizer_MLE,
              avloss=average_quadratic_loss,
              batch_size=BATCHSIZE,
              n_iterations=n_iterations,
              traces=traces_MLE,
              step=traces_step,
              window=200,
                MLE=True)
```

```
train_t shape =  (800000,)

train_x shape =  (800000, 4)

Iteration vs average loss
 iteration  train-set  valid-set
         0   0.134987   0.134437
      9800   0.058935   0.058109   0.058109
```

```
# n_iterations=10000
# BATCHSIZE=500
# traces= train(model=model, optimizer=optimizer,
avloss=average_quadratic_loss,
#           batch_size=BATCHSIZE,
#           n_iterations=n_iterations, traces=traces,
#           step=traces_step, window=100)

plot_average_loss(traces_MLE)
```

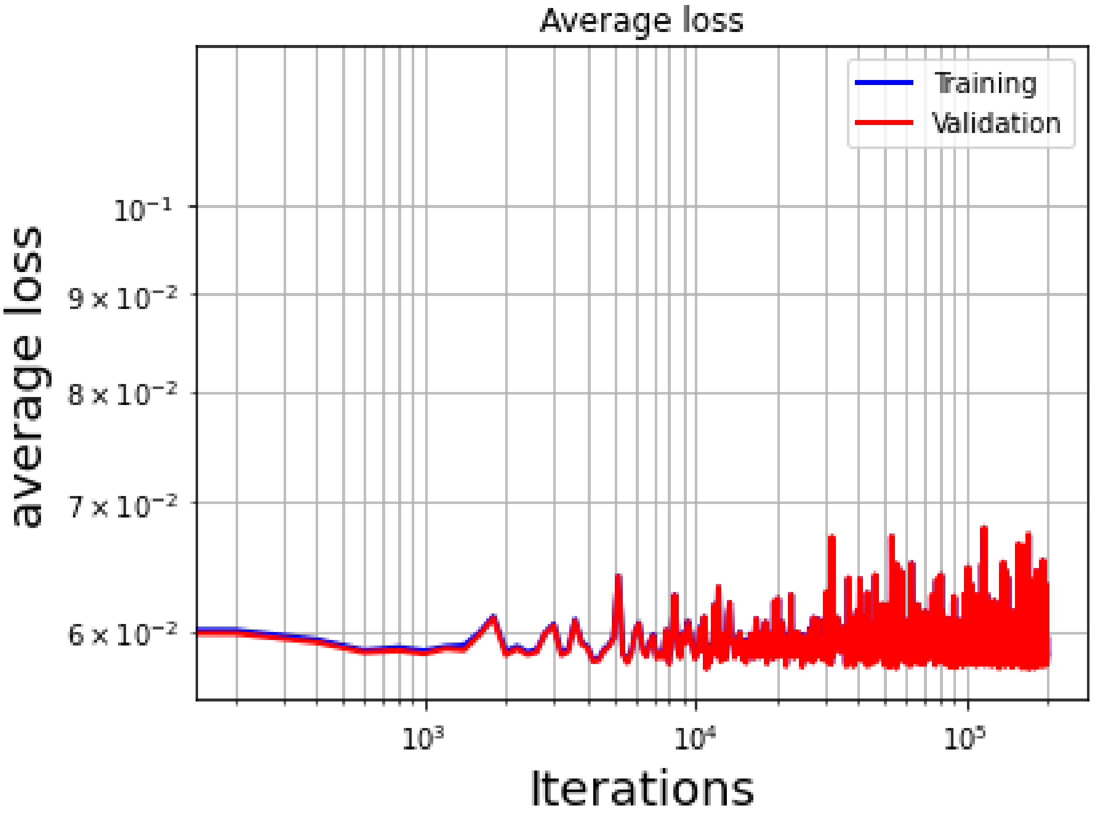


Train non-MLE model

```
BATCHSIZE=batch_size
traces_nonMLE = ([], [], [], [])
traces_step = 200


n_iterations=200000
traces_nonMLE= train(model=model_nonMLE,
              optimizer=optimizer_nonMLE,
              avloss=average_quadratic_loss,
              batch_size=BATCHSIZE,
              n_iterations=n_iterations,
              traces=traces_nonMLE,
              step=traces_step,
              window=200,
                MLE=False)
plot_average_loss(traces_nonMLE)
```

```
train_t shape =  (800000,)
```

```
train_x shape =  (800000, 4)

Iteration vs average loss
 iteration  train-set  valid-set
         0   0.116824   0.115104
    199800   0.058369   0.058304   0.059388
```



Make sure the train df has the same ranges as the data you want to generate for evaluation

```
def load_train_df(MLE):
    """ returns the dataframe, can be used if the dataframe is saved
in csv format
    of if it is already in dataframe format (e.g. generated in this
notebook). """
    # SUBSAMPLE=int(1e5)
    # if isinstance(df_name,str):
    if MLE:
        train_df =
pd.read_csv('data/two_parameters_theta_0_20_1000k_Examples_MLE_True.cs
v',
                         # nrows=SUBSAMPLE,
                         usecols=['Z','theta','nu', 'N', 'M']
                        )
    else:
        train_df =
pd.read_csv('data/two_parameters_theta_0_20_1000k_Examples_MLE_False.c
sv',
                 # nrows=SUBSAMPLE,
                 usecols=['Z','theta','nu', 'N', 'M']
                )
    return train_df

train_df_MLE = load_train_df(MLE=True)
train_df_MLE.describe()
```

```
                    Z           theta              nu               N
\
count  1000000.000000  1000000.000000  1000000.000000  1000000.000000

mean         0.870055       10.001843       10.000098        4.999642

std          0.336243        5.774806        5.771397        2.581812

min          0.000000        0.000008        0.000020        1.000000

25%          1.000000        4.999020        4.999096        3.000000

50%          1.000000        9.997342       10.002818        5.000000

75%          1.000000       15.006256       14.988187        7.000000

max          1.000000       19.999982       19.999990        9.000000


                    M
count  1000000.000000
mean         4.994021
std          2.581949
min          1.000000
25%          3.000000
50%          5.000000
75%          7.000000
max          9.000000
```

Make "on-the-fly" generated evaluation data

Note that this is one advantage of LFI, where one can always generate more synthetic data (for training as well as evaluation), whereas in traditinoal ML, the raining and evaluation data sets are fixed. Here, we generate binned θ with the same ranges as those of the training set, and constants for $\{\nu ,N ,M\}$.

```
def make_eval_data(Bprime, train_df, nu, N, M, nbins):
    #if MLE true, load the model that was trained on MLE data and vice
versa
    # N, M = D
    # nbins=NBINS
    # thetamin,thetamax=0,20
    thetamin=train_df['theta'].min()
    thetamax=train_df['theta'].max()
    thetastep = (thetamax-thetamin) / nbins
    bb    = np.arange(thetamin, thetamax+thetastep, thetastep)#this is
just making a vector of thetas
    X     = (bb[1:] + bb[:-1])/2
    tensor = torch.Tensor([[x, nu, N, M] for x in X])
    return tensor, X
```

Look at an example of a "on-the-fly" generated evaluation data

```
eval_data_example, eval_bins_example
=make_eval_data(Bprime=100,train_df=train_df_MLE,nu=3, N=1, M=3,
nbins=300)
print(eval_data_example[:5])
```

```
tensor([[0.0333, 3.0000, 1.0000, 3.0000],
        [0.1000, 3.0000, 1.0000, 3.0000],
        [0.1667, 3.0000, 1.0000, 3.0000],
        [0.2333, 3.0000, 1.0000, 3.0000],
        [0.3000, 3.0000, 1.0000, 3.0000]])
```

```
eval_data_example.shape
```

```
torch.Size([300, 4])
```

Evaluate Trained model at this generated data

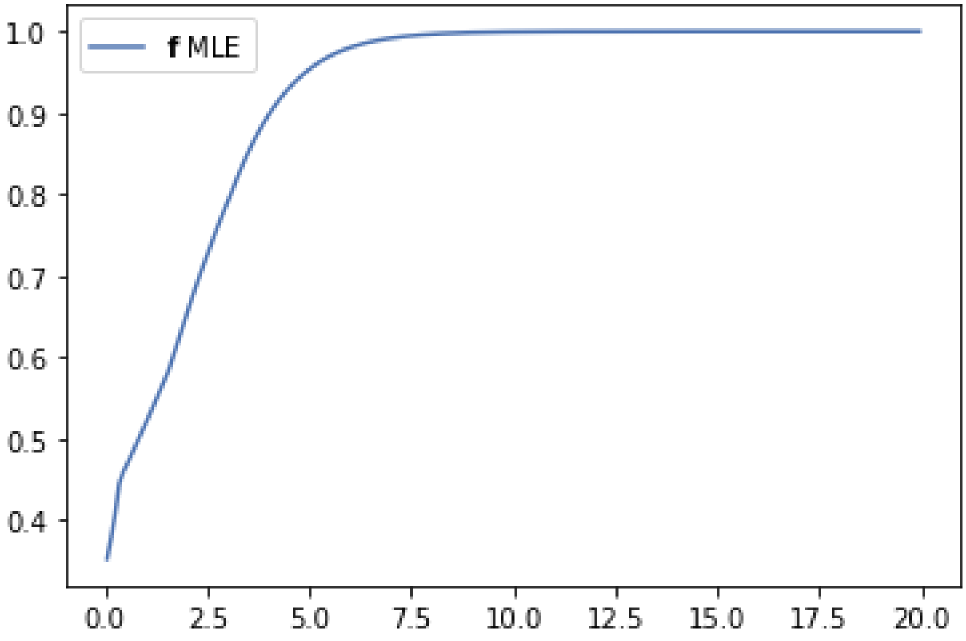
```
def usemodel(Bprime, train_df, nu, N,M, MLE, nbins):
    #make evaluation data at those fixed nu, N, M values
    eval_data, eval_bins =make_eval_data(Bprime,train_df,nu, N,M,
nbins)#eval data is indipendent of MLE, since its just constants witha
theta variable

    # if MLE==True:
    #     model=model
    #else load the model trained on non-MLE data
    # PATH='models/MLE_TRUE_Regressor_200.0K_training_iter.pt'
    if MLE:
        PATH= 'models/MLE_TRUE_Regressor_200.0K_training_iter.pt'
    else:
        PATH= 'models/MLE_False_Regressor_200.0K_training_iter.pt'
    n_layers = int(BEST_PARAMS["n_layers"])
    hidden_size = int(BEST_PARAMS["hidden_size"])
    dropout = float(BEST_PARAMS["dropout"])
    optimizer_name = BEST_PARAMS["optimizer_name"].to_string().split()
[1]
    learning_rate =  float(BEST_PARAMS["learning_rate"])
    batch_size = int(BEST_PARAMS["batch_size"])
    model =  RegularizedRegressionModel(
        nfeatures=train_x.shape[1],
        ntargets=1,
        nlayers=n_layers,
        hidden_size=hidden_size,
        dropout=dropout
        )
    model.load_state_dict(torch.load(PATH) )
    model.eval()
    return model(eval_data).detach().numpy(), eval_bins
```

```
phat_MLE, phatbins_MLE = usemodel(Bprime=1000,train_df=train_df,nu=3,
N=2, M=3, MLE=True, nbins=200)
print(phat[:5])
```

```
[[0.3516053 ]
 [0.37797767]
 [0.40793678]
 [0.44479653]
 [0.4591592 ]]
```

```
plt.plot(phatbins_MLE, phat_MLE, label=r'$\mathbf{f}$ MLE');
plt.legend()
```

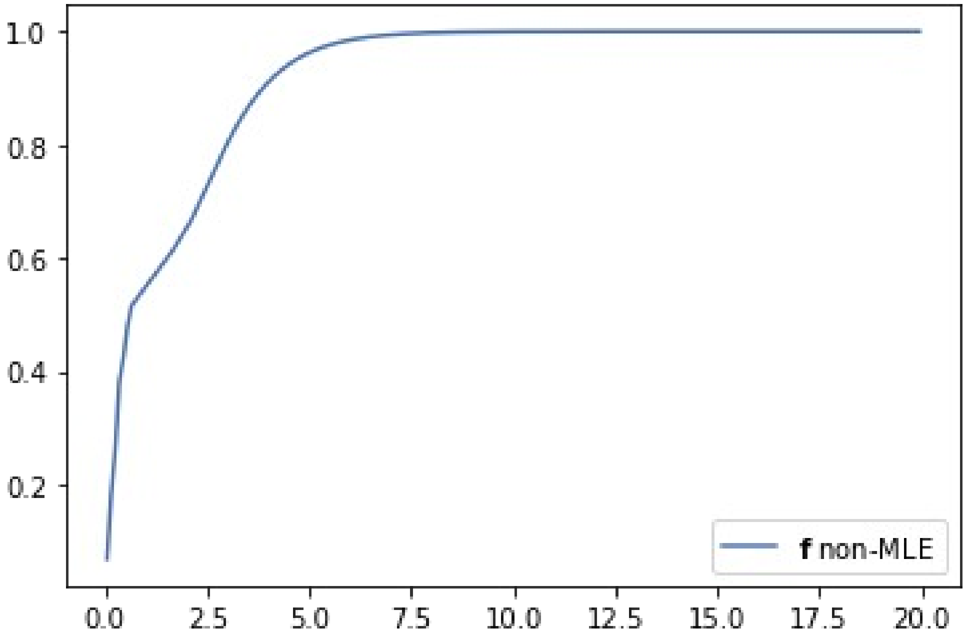
```
<matplotlib.legend.Legend at 0x7f1e92f43e10>
```



```
phat_nonMLE, phatbins_nonMLE =
usemodel(Bprime=1000,train_df=train_df,nu=3, N=2, M=3, MLE=False,
nbins=200)
print(phat[:5])
plt.plot(phatbins_nonMLE, phat_nonMLE, label=r'$\mathbf{f}$ non-MLE');
plt.legend()
```

```
[[0.3516053 ]
 [0.37797767]
 [0.40793678]
 [0.44479653]
 [0.4591592 ]]
```

```
<matplotlib.legend.Legend at 0x7f1e92e22990>
```



SAVE TRAINED MODEL (if it's good)

```
def save_model(MLE):
    if MLE:
        model = model_MLE
    else:
        model = model_nonMLE
    PATH='models/MLE_%s_Regressor_%sK_training_iter.pt' % ( str(MLE),
str(n_iterations/1000) )
    torch.save(model.state_dict(),  PATH)

save_model(MLE=False)
```

This is how you load a trained model

```
#load
PATH='models/MLE_TRUE_Regressor_20.0K_training_iter.pt'
n_layers = int(BEST_PARAMS["n_layers"])
hidden_size = int(BEST_PARAMS["hidden_size"])
dropout = float(BEST_PARAMS["dropout"])
optimizer_name = BEST_PARAMS["optimizer_name"].to_string().split()[1]
learning_rate =  float(BEST_PARAMS["learning_rate"])
batch_size = int(BEST_PARAMS["batch_size"])
model =  RegularizedRegressionModel(
    nfeatures=train_x.shape[1],
    ntargets=1,
    nlayers=n_layers,
    hidden_size=hidden_size,
    dropout=dropout
    )
model.load_state_dict(torch.load(PATH) )
#OR
#model=torch.load(PATH)#BUT HERE IT WILL BE A DICT (CANT BE EVALUATED RIGHT AWAY) DISCOURAGED!
model.eval()
print(model)
```

```
RegularizedRegressionModel(
  (model): Sequential(
    (0): Linear(in_features=4, out_features=11, bias=True)
    (1): Dropout(p=0.1320798105984151, inplace=False)
    (2): ReLU()
    (3): Linear(in_features=11, out_features=11, bias=True)
    (4): Dropout(p=0.1320798105984151, inplace=False)
    (5): ReLU()
    (6): Linear(in_features=11, out_features=11, bias=True)
    (7): Dropout(p=0.1320798105984151, inplace=False)
    (8): ReLU()
    (9): Linear(in_features=11, out_features=11, bias=True)
    (10): Dropout(p=0.1320798105984151, inplace=False)
    (11): ReLU()
    (12): Linear(in_features=11, out_features=1, bias=True)
    (13): Sigmoid()
  )
)
```

You could also evaluate the trained model on the validation data

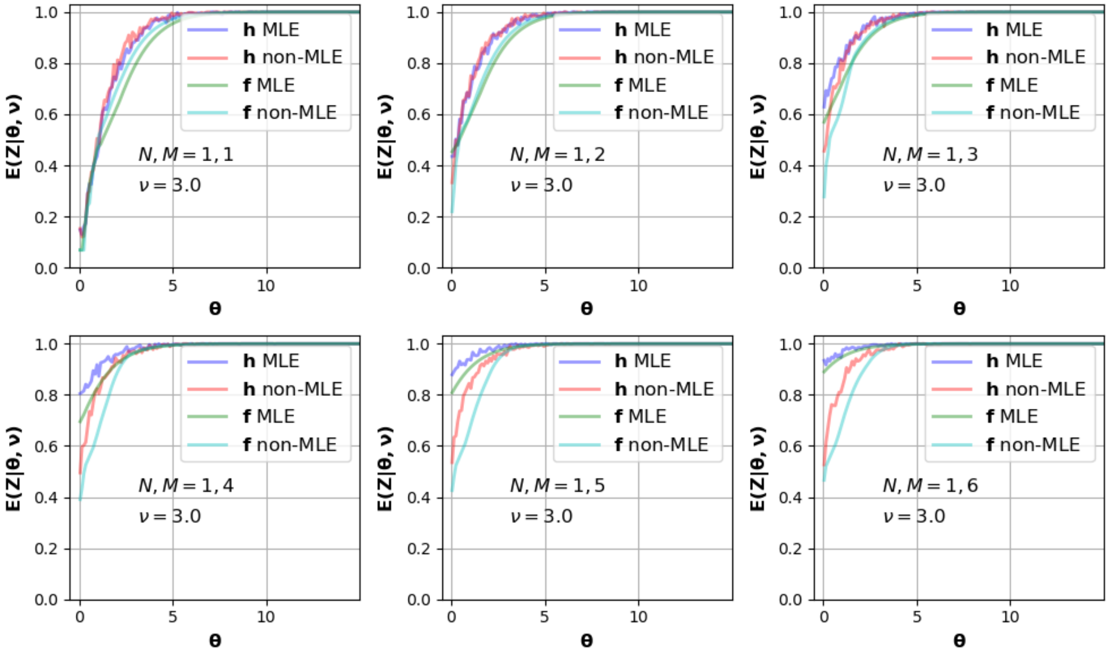
```
# nbins=100
# thetamin=train_df['theta'].min()
# thetamax=train_df['theta'].max()
# thetastep = (thetamax-thetamin) / nbins
# bb    = np.arange(thetamin, thetamax+thetastep, thetastep)#this is just making a vector of thetas
# X     = (bb[1:] + bb[:-1])/2
eval_data=torch.Tensor(valid_x)
model.eval()
phat=model(eval_data).detach().numpy()
```

```
phat
```

```
array([[0.8695913],
       [0.8695913],
       [0.8695913],
       ...,
       [0.8695913],
       [0.8695913],
       [0.8695913]], dtype=float32)

def plot_data_one_nu_with_model(Bprime, thetamin, thetamax, nu, D,
MLE,
                     NBINS,
              FONTSIZE=15,
              func=None,
              fgsize=(10, 6), save_image=False):

    # make room for 6 sub-plots
    fig, ax = plt.subplots(nrows=2,
                           ncols=3,
                           figsize=fgsize)

    # padding
    plt.subplots_adjust(hspace=0.01)
    plt.subplots_adjust(wspace=0.20)

    # use flatten() to convert a numpy array of
    # shape (nrows, ncols) to a 1-d array.
    ax = ax.flatten()

    for j, (N, M) in enumerate(D):

        y, bb = make_hist_data(Bprime,
                              thetamin, thetamax,
                              nu, N, M,
                              nbins=NBINS,
                              MLE=True)

        ax[j].set_xlim(thetamin-0.5, thetamax-5)
        ax[j].set_ylim(0, 1.03)
        ax[j].set_xlabel(r'$\mathbf{\theta}$', fontsize=FONTSIZE-3)
        ax[j].set_ylabel(r'$\mathbf{E(Z|\theta, \nu)}$',
fontsize=FONTSIZE-3)

        x = (bb[1:]+bb[:-1])/2
        ax[j].plot(x, y, 'b', lw=2, label='$\mathbf{h}$ MLE',
alpha=0.4)
        #h is histogram approximation

        y_nonMLE, bb_nonMLE = make_hist_data(Bprime,
                              thetamin, thetamax,
                              nu, N, M,
                              nbins=NBINS,
                              MLE=False)


        x_nonMLE = (bb_nonMLE[1:]+bb_nonMLE[:-1])/2
        ax[j].plot(x_nonMLE, y_nonMLE, 'r', lw=2, label='$\mathbf{h}$
non-MLE',alpha=0.4)


        if func:
            train_df_MLE = load_train_df(MLE=True)
            train_df_nonMLE = load_train_df(MLE=False)

            f_MLE, f_bins_MLE = func(Bprime, train_df_MLE, nu, N, M,
MLE=True, nbins=NBINS)
            ax[j].plot(x, f_MLE, color='g', lw=2, label='$\mathbf{f}$
MLE', alpha=0.4)
            #f is model approximation

            f_nonMLE, f_bins_nonMLE = func(Bprime, train_df_nonMLE,
nu, N, M, MLE=False, nbins=NBINS)
            ax[j].plot(x, f_nonMLE, color='c', lw=2, label='$\
mathbf{f}$ non-MLE', alpha=0.4)

        ax[j].grid(True, which="both", linestyle='-')
        ax[j].text(3.1, 0.42, r'$N, M = %d, %d$' % (N, M),
fontsize=font_legend-3
                   # fontsize=FONTSIZE
                  )

        ax[j].text(3.1, 0.30, r'$\nu = %5.1f$' % nu,
fontsize=font_legend-3
                   # fontsize=FONTSIZE
                  )

        ax[j].legend(loc='upper right',fontsize=font_legend-3)

    # hide unused sub-plots
    for k in range(j+1, len(ax)):
        ax[k].set_visible(False)

    plt.tight_layout()
    if save_image:
        plt.savefig('images/h_MLE_nonMLE_f_MLE_f_nonMLE_one_nu.png')
    plt.show()
```

Compare the histogrammed function $h(\theta, \nu, N, M)$ to the ML prediction functino $f(\theta, \nu, N, M)$ (which is trained to regress Z).

```
def make_D(train_df):
    Nmin = train_df['N'].min()
    Nmax = train_df['N'].max()
    Mmin = train_df['M'].min()
    Mmax = train_df['M'].max()
    D = [ (N, M) for N in range(Nmin, Nmax) for M in range(Mmin,
Mmax)]
    return D[:6]

D = make_D(train_df)
D

[(1, 1), (1, 2), (1, 3), (1, 4), (1, 5), (1, 6)]

thetamin = train_df['theta'].min()
thetamax = train_df['theta'].max()
plot_data_one_nu_with_model(Bprime=100000, thetamin=thetamin,
thetamax=thetamax,
                  nu=3, D=D, MLE=True, NBINS=200, func=usemodel,
save_image=True)
```



E(Z|θ, ν)
θ
0
5
10
0.0
0.2
0.4
0.6
0.8
1.0
h MLE
h non-MLE
f MLE
f non-MLE
$N, M = 1, 1$
$N, M = 1, 2$
$N, M = 1, 3$
$N, M = 1, 4$
$N, M = 1, 5$
$N, M = 1, 6$
$\nu = 3.0$