lab05_student

October 11, 2021

1 Lab 5: Linear Models, Confidence Intervals and Credible Intervals, Bootstrap and Hypothesis Testing

Welcome to the Data 102 Fall 201 Lab 5. In this lab, we are going to look at a variety of topics including Linear Models, Confidence Intervals and Credible Intervals, Bootstrap and Hypothesis Testing. The lab assignment may seem long,. but there are only a few simple lines of code to fill in in this lab assignment. There are a lot of texts in this assignment. Please make sure you carefully read through them.

The code and responses you need to write are commented out with a message `TODO: fill in`. There is additional documentation for each part as you go along.

Please read carefully the introduction and the instructions to each problem.

1.1 Collaboration Policy

Data science is a collaborative activity. While you may talk with others about the labs, we ask that you **write your solutions individually**. If you do discuss the assignments with others please **include their names** in the cell below.

Collaborators:

1.2 Gradescope Submission

To submit this assignment, rerun the notebook from scratch (by selecting Kernel > Restart & Run all), and then print as a pdf (File > download as > pdf) and submit it to Gradescope.

This assignment should be completed and submitted before Wednesday, October 13, 2021 at 11:59 PM. PST

[1]:
```
%matplotlib inline
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import seaborn as sns
from ipywidgets import interact, interactive
import itertools
import hashlib
from scipy.stats import poisson, norm, gamma
```

```
#!pip install pymc3
import statsmodels.api as sm

sns.set(style="dark")
plt.style.use("ggplot")

try:
    from pymc3 import *
    import pymc3 as pm
except:
    ! pip install pymc3
    from pymc3 import *
    import pymc3 as pm

import arviz as az

def get_hash(num, significance = 4):
    num = round(num, significance)
    """Helper function for assessing correctness"""
    return hashlib.md5(str(num).encode()).hexdigest()
```

2 Part I: GLM

3 Question 1: Poisson Regression

4 Atlantic Hurricane Season

With 30 named storms, the 2020 Atlantic hurricane season was the most active on record. Climate scientists argue that the culprit is human induced global warming. There is a an evergrowing body of research linking increased average temperatures and rising sea levels to more frequent, more intense and more destructive storms.

In this lab we will investigate the number of named storms recorded since 1880, and we will argue that there is a statistically significant relationship between rising Sea Surface Temperature (SST) and the frequency of named storms.

For this lab we extracted the number of tropical storms from the HURDAT Database. We also extracted data on Sea Surface Temperatures from the National Center for Atmosferic Research.

4.0.1 Load the data

[2]:
```
# No need to modify: Just run the code to load the data
data_source = "hurricane_data.csv"
df = pd.read_csv(data_source)
df = df[["Year", "Num_Storms", "Temp_Anomaly"]]
df.tail()
```

[2]:

	Year	Num_Storms	Temp_Anomaly
135	2015	11	1.28
136	2016	15	1.12
137	2017	17	1.10
138	2018	15	1.07
139	2019	18	1.24

The `Num_Storms` column contains the number of named storms recorded each year between 1880 and 2019. The `Temp_Anomaly` column contains the deviation in yearly SST from the mean of 1951-1980.

In this question we will model the number of named storms in Year i as: $C_i \sim Poisson(\lambda_i)$, where $\lambda_i = exp(q_0 + q_1 X_i)$, and X_i is the SST deviation in Year i.

This isn't something that we can easily solve from scratch, so we have to use software packages. For Frequentist Poisson Regression we will use `statsmodels.api` and for the Bayesian counterpart we will use `PYMC3`.

4.1 1.a Frequentist Regression

[3]:
```
# Fit Poisson GLM model where Temp_Anomaly is a covariate (exogenous variable):␣
↪No need to modify
freq_model = sm.GLM(df.Num_Storms, exog = sm.add_constant(df.Temp_Anomaly),
                    family=sm.families.Poisson())
freq_res = freq_model.fit()
print(freq_res.summary())
```

```
                 Generalized Linear Model Regression Results
==============================================================================
Dep. Variable:             Num_Storms   No. Observations:                  140
Model:                            GLM   Df Residuals:                      138
Model Family:                 Poisson   Df Model:                            1
Link Function:                    log   Scale:                          1.0000
Method:                          IRLS   Log-Likelihood:                -376.25
Date:                Mon, 11 Oct 2021   Deviance:                       183.00
Time:                        15:36:44   Pearson chi2:                     186.
No. Iterations:                     4
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          z      P>|z|      [0.025      0.975]
------------------------------------------------------------------------------
const          2.2414      0.029     78.130      0.000       2.185       2.298
Temp_Anomaly   0.4866      0.059      8.180      0.000       0.370       0.603
==============================================================================

/opt/conda/lib/python3.9/site-packages/statsmodels/tsa/tsatools.py:142:
FutureWarning: In a future version of pandas all arguments of concat except for
the argument 'objs' will be keyword-only
  x = pd.concat(x[::order], 1)
```

4.1.1 TODO: Inspecting the results of fitting `freq_model`. Does the model suggest that increased SST relate to more storms? Is the influnce of SST on number of storms statistically significant?

Your answer: I think the model does suggest that increased SST relates to more storms since the coefficient is positive (0.4866). However, this increase seems rather low since the coefficient is low. However, it does seem statistically significant because the Pearson chi2 value is so large.

4.2 1.b Bayesian Regression

[4]:
```
# No need to modify
with pm.Model() as bayes_model:
    glm.GLM.from_formula('Num_Storms ~ Temp_Anomaly', df, family=glm.families.
 ↪Poisson())
    # PYMC3 automatically uses exponential link function and adds an intercept␣
 ↪term
    trace_poisson = pm.sample(1000, cores=2, target_accept=0.95,␣
 ↪init='adapt_diag')
```

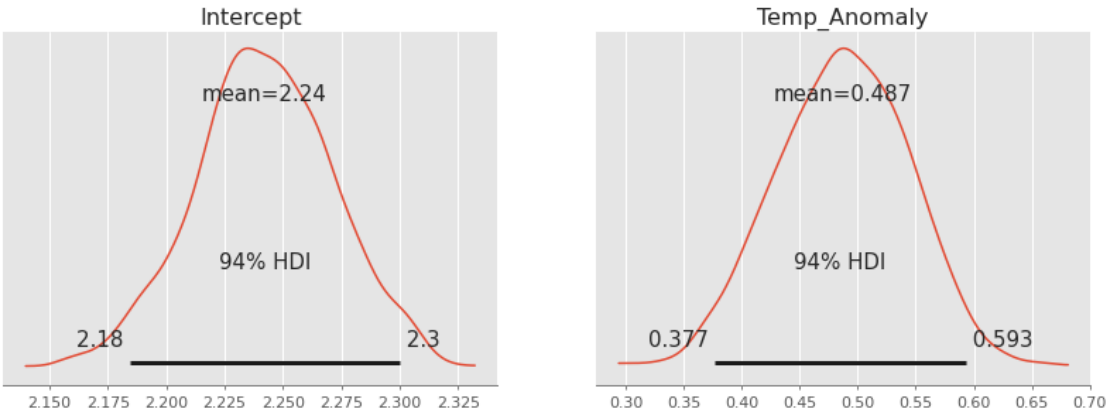
```
/tmp/ipykernel_198/1885856346.py:5: FutureWarning: In v4.0, pm.sample will
return an `arviz.InferenceData` object instead of a `MultiTrace` by default. You
can pass return_inferencedata=True or return_inferencedata=False to be safe and
silence this warning.
  trace_poisson = pm.sample(1000, cores=2, target_accept=0.95,
init='adapt_diag')
Auto-assigning NUTS sampler…
Initializing NUTS using adapt_diag…
Multiprocess sampling (2 chains in 2 jobs)
NUTS: [mu, Temp_Anomaly, Intercept]
```

```
<IPython.core.display.HTML object>
```

```
Sampling 2 chains for 1_000 tune and 1_000 draw iterations (2_000 + 2_000 draws
total) took 4 seconds.
```

[5]:
```
# Plot the posterior distribution for the intercept and Temp_Anomaly␣
 ↪coefficients
az.plot_posterior(trace_poisson, ['Intercept', 'Temp_Anomaly'], round_to = 3)
plt.show()
```

```
Got error No model on context stack. trying to find log_likelihood in
translation.
/opt/conda/lib/python3.9/site-packages/arviz/data/io_pymc3_3x.py:98:
FutureWarning: Using `from_pymc3` without the model will be deprecated in a
future release. Not using the model will return less accurate and less useful
results. Make sure you use the model argument or call from_pymc3 within a model
context.
  warnings.warn(
```



Note: "HDI" in the plots above stands for Highest Density Interval, which is another term for credibal interval.

4.2.1 TODO: Compare the results of `freq_model` in 1.a with the plot above. Are the estimates of Frequentist and Bayesian Regression close to each-other?

Your answer: Yes, they seem to be very close to eachother.

The mean for the intercept is 2.24 in Bayesian Regression, compared to 2.2414 in Linear Regression, which is very similar.

The mean for `Temp_Anomaly` is 0.488 in Bayesian Regression, compared to 0.4866 in Linear Regression, which is very similar.

The 94% Credible Interval for the intercept seems to range from 2.18 to 2.3 for Bayesian Regression, compared to the 95% Confidence Interval ranging from 2.185 to 2.298 for Frequentist Regression, which is very similar.

The 94% Credible Interval for `Temp_Anomaly` seems to range from 0.37 to 0.59 for Bayesian Regression, compared to the 95% Confidence Interval ranging from 0.370 to 0.603 for Frequentist Regression, which is very similar.

4.3 1.c Posterior Predictive Checks

In order to validate our Bayesian model we perform Posterior Predictive Checks (PPC). After performing Bayesian Regression we have access to a generating distribution for counts $C_i'|X_i$. The crux of PPC is to sample such counts and to compare them to the original historical data.

The code below computes PPC samples and plots their distribution. Note that here, C has been renamed y, and the band labeled "Posterior predictive y" is a collection of curves, each of which is the density plot of y for a given draw of the coefficient vector β from the posterior.

[6]:
```
# No need to modify
with pm.Model() as poisson_model:
    glm.GLM.from_formula('Num_Storms ~ Temp_Anomaly', df, family=glm.families.
 ↪Poisson())
```

```
    # PYMC3 automatically uses exponential link function and adds an intercept␣
↪term
    trace_poisson = pm.sample(1000, cores=2, target_accept=0.95,␣
↪init='adapt_diag')
```

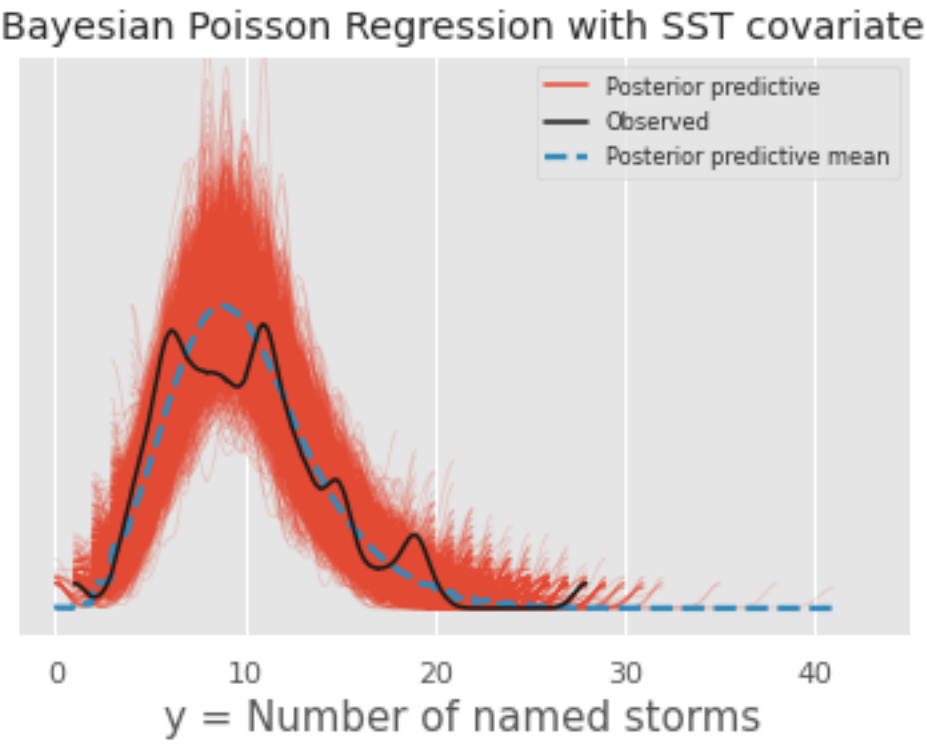
```
/tmp/ipykernel_198/3548577695.py:5: FutureWarning: In v4.0, pm.sample will
return an `arviz.InferenceData` object instead of a `MultiTrace` by default. You
can pass return_inferencedata=True or return_inferencedata=False to be safe and
silence this warning.
  trace_poisson = pm.sample(1000, cores=2, target_accept=0.95,
init='adapt_diag')
Auto-assigning NUTS sampler…
Initializing NUTS using adapt_diag…
Multiprocess sampling (2 chains in 2 jobs)
NUTS: [mu, Temp_Anomaly, Intercept]
```

```
<IPython.core.display.HTML object>
```

```
Sampling 2 chains for 1_000 tune and 1_000 draw iterations (2_000 + 2_000 draws
total) took 4 seconds.
```

[7]:
```
# Do not modify
# Sample C'_i|X_i
with poisson_model:
    poisson_ppc = pm.sample_posterior_predictive(trace_poisson)
    poisson_ppc['y'] = poisson_ppc['y'] + 0.0
    ppc_poisson = az.from_pymc3(trace_poisson, posterior_predictive=poisson_ppc)

# Plot PPC samples

az.plot_ppc(ppc_poisson)
plt.xlabel('y = Number of named storms')
plt.title('Bayesian Poisson Regression with SST covariate')
plt.axis([-2, 45, -0.01, 0.2])

plt.show()
```

```
<IPython.core.display.HTML object>
```



We can also estimate by employing a Bayesian perspective without using the covariate $X_i's$.

Following this perspective, the model is implemented below.

[8]:
```
# No need to modify
with pm.Model() as simple_poisson_model:
    glm.GLM.from_formula('Num_Storms ~ 1', df, family=glm.families.Poisson())
    # PYMC3 automatically uses exponential link function and adds an intercept␣
 ↪term
    trace_simple_poisson = pm.sample(1000, cores=2, target_accept=0.95,␣
 ↪init='adapt_diag')
```

```
/tmp/ipykernel_198/312990582.py:5: FutureWarning: In v4.0, pm.sample will return
an `arviz.InferenceData` object instead of a `MultiTrace` by default. You can
pass return_inferencedata=True or return_inferencedata=False to be safe and
silence this warning.
  trace_simple_poisson = pm.sample(1000, cores=2, target_accept=0.95,
init='adapt_diag')
Auto-assigning NUTS sampler…
Initializing NUTS using adapt_diag…
Multiprocess sampling (2 chains in 2 jobs)
NUTS: [mu, Intercept]
```

```
<IPython.core.display.HTML object>
```

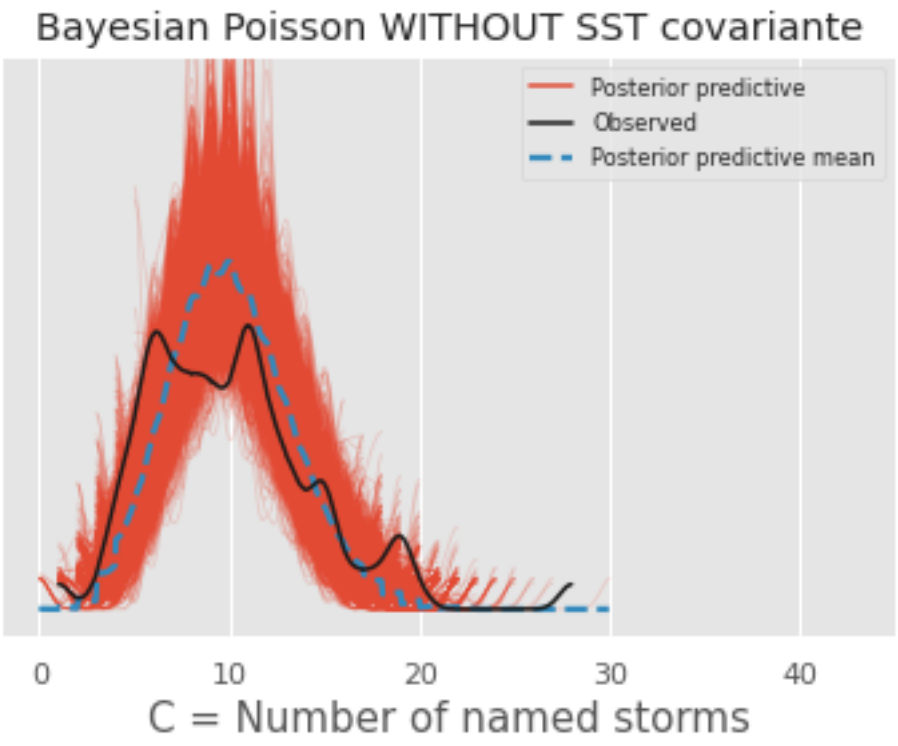
```
Sampling 2 chains for 1_000 tune and 1_000 draw iterations (2_000 + 2_000 draws
total) took 4 seconds.
```

Similarly perform Predictive Posterior Checks

[9]:
```
# Do not modify
# Sample C'_i|X_i
with simple_poisson_model:
    simple_poisson_ppc = pm.sample_posterior_predictive(trace_simple_poisson)
    simple_poisson_ppc['y'] = simple_poisson_ppc['y'] + 0.0
    ppc_simple_poisson = az.from_pymc3(trace_simple_poisson,␣
 ↪posterior_predictive=simple_poisson_ppc)

# Plot PPC samples
#ppc_simple_poisson = az.from_pymc3(trace_simple_poisson,␣
 ↪posterior_predictive=simple_poisson_ppc)
az.plot_ppc(ppc_simple_poisson)
plt.xlabel('C = Number of named storms')
plt.title('Bayesian Poisson WITHOUT SST covariante')
plt.axis([-2, 45, -0.01, 0.2])
print(plt.axis())
plt.show()
```

```
<IPython.core.display.HTML object>
```

```
(-2.0, 45.0, -0.01, 0.2)
```



4.3.1 TODO: Compare the two plots above. In your opinion, which model is a better fit for the observed data?

Your answer: I think the Bayesian Poisson WITH SST covariate is a better fit for the observed data, as all points of the observed lies within the orange curve (the posterior predictive), as opposed to the Bayesian Poisson WITHOUT SST covariate where the bottom part of the curve lies outside the orange region.

5 Part II: Bootstrap and Hypothesis Testing

In the following questions, we are going to experiment with bootstrap and hypothesis testing.

5.1 Goal: testing for multimodality

Suppose that $X_1, ..., X_n$ are i.i.d. samples from a distribution with continuous density $p(x)$. One important property of the density $p(x)$ is the number of modes it has. Multimodality of the density indicates a heterogeneity in the data. In this lab, we will demonstrate how to perform a hypothesis test to determine whether a distribution is multimodal. We'll use the Bootstrap Method to perform this hypothesis test.

5.2 Galaxy data

We will be working with galaxy data. The dataset contains velocities in km/sec of 82 galaxies from 6 well-separated conic sections of an unfilled survey of the Corona Borealis region. The distribution of galaxy velocities provides information about the structure of the far universe—in particular, a multimodal distribution of velocities is seen as evidence for the existence of voids and superclusters (links to wikipedia pages on voids and superclusters).

Let $X_1, ..., X_n$ be the velocities of each galaxy, where X_i is the velocity of the ith galaxy and we observe $n = 82$ galaxies.

We want to test whether or not the distribution that the X_i's are drawn from is multimodal. Let the null and alternative hypotheses be defined as follows:

$$H_0 : m(p) = 1$$
$$H_A : m(p) > 1$$

where p is the distribution of galaxy velocities, and $m(p)$ is the number of modes of a distribution p.

5.3 Load the data

First, we'll load the data and see what the histogram looks like.

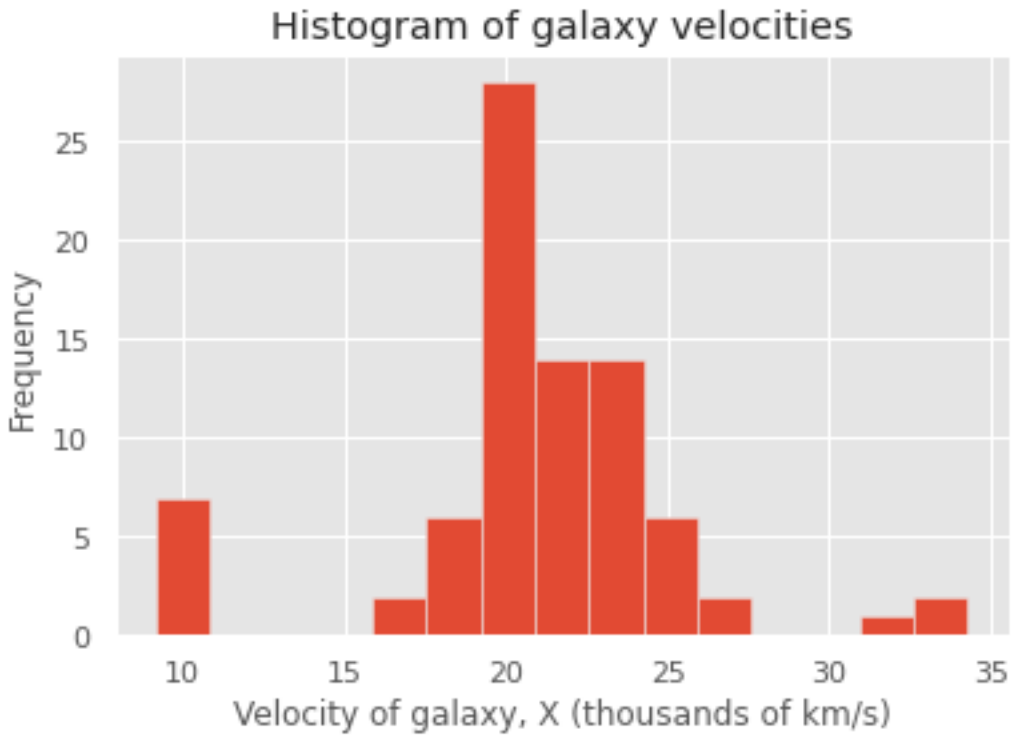
[10]:

```
galaxies_df = pd.read_csv('galaxies.csv', index_col=0, header=0,␣
 ↪names=['velocity'])
# Divide all entries by 1000 for ease of reading.
galaxies_df['velocity'] = galaxies_df['velocity'] / 1000
X_observed = np.array(galaxies_df['velocity'])
galaxies_df.head()
```

[10]:

	velocity
1	9.172
2	9.350
3	9.483
4	9.558
5	9.775

[11]:
```
plt.hist(X_observed, bins=15)
plt.title("Histogram of galaxy velocities")
plt.xlabel("Velocity of galaxy, X (thousands of km/s)")
plt.ylabel("Frequency")
plt.show()
```



6 Question 2. Estimating the density and test statistic

In order to infer whether or not the $X_1, ..., X_n$ were drawn from a multimodal distribution, we need to come up with a test statistic that reflects how suitable a unimodal distribution is for modeling this data.

To do this, we first need to come up with a model for the density function itself. In this lab you will have the chance to learn about a non-parametric density estimatation technique called *kernel density estimation*. This was also covered briefly in Data 100. To revisit the concept, see data 100 textbook.

Kernel Density Estimation Given a set of points $X_1, X_2, \ldots, X_n \sim p(x)$. The goal of Kernel Density Estimation is to estimate the density $p(x)$ via a function $\hat{p}_h(x)$ of the form:

$$\hat{p}_h(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right) \tag{1}$$

The function K is a non-increasing function that takes only non-negative values. These functions are known as kernel functions. They are often used to capture the influence of each data point X_i on the density of an arbitrary point x. A common choice of kernel is the Gaussian kernel, which is what we will use in this lab:

$$K(x) = \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)$$

In addition, the parameter $h > 0$ is a bandwidth parameter that captures how close data points X_i must be to x to influence its density: for larger values of h, more data points have an influence on the density at x, whereas for smaller values of h, only data points very close to x influence it.

It can be shown that the number of modes of $\hat{p}_h(x)$ (a.k.a. $m(\hat{p}_h(x))$) decreases monotonically as h increases. Therefore, h will be an important tool in our hypothesis test.

6.1 2.a. Plot the density estimates $\hat{p}_h(x)$

Using the kernel function $K(x) = \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)$, we will first plot $\hat{p}_h(x)$ to get a sense of what these density estimates look like for different values of h.

$$\begin{aligned}
\hat{p}_h(x) &= \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right) \\
&= \frac{1}{nh} \sum_{i=1}^{n} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x - X_i)^2}{2h^2}\right) \\
&= \frac{1}{nh\sqrt{2\pi}} \sum_{i=1}^{n} \exp\left(-\frac{(x - X_i)^2}{2h^2}\right)
\end{aligned}$$

Using the final simplified form above, implement a function that calculates $\hat{p}_h(x)$ at a given point x.

[12]:
```
#  TODO: fill in.
from math import pi, exp, sqrt
def p_hat(x, h, X):
    """Calculates p_hat(x) at a single point x, where the bandwidth of the␣
 ↪kernel function is h.

    Inputs:
      x : float, point at which to evaluate the function p_hat.
      h : float, bandwidth parameter in kernel function.
      X : array of floats of length n containing the observed galaxy velocities.

    Outputs:
      y: float, the value of p_hat(x) at the given point x.
    """

    n = len(X)

    summation_value = 0
    for i in range(n):
        summation_value += np.exp((-(x-X[i])**2) / (2*h**2))

    y = (1/(n*h*np.sqrt(2*np.pi))) * summation_value # TODO: fill in
    return(y)
```

[13]:
```
# Validation tests: Do not modify
x_values = [10, 15, 20, 25, 30, 35]
h_values = [0.5, 1, 2, 5, 10]
inputs = list(itertools.product(x_values, h_values))
outputs = [p_hat(*inp, X_observed) for inp in inputs]
hash_list = ['bfde2cf30f9e9ce79408d99cab3e8bc8',␣
 ↪'0574a27738923dd052ed0b873c176afc', '78b6d148d48bbea1345c899ca9e46909',
 'f4ee6417f4b3ac1be9eb6568e73144b6', '3ffdc10d8a61ad159f223313dfbc03e2',␣
 ↪'605849c8f83de4da7c6fd144d7f58826',
 '3f372d09d37f32da442cb9ee0ac460f0', '5b3bc4848902c9a21de80767f9e339b8',␣
 ↪'71c61135ff01aa84ee86864b86711f5b',
 '04d8f0e70a01305f62dbadaa76a8f7cb', '45bd1e472af7b3bc57dc9312833c17a0',␣
 ↪'45367152f5d7346868703d4980f60e03',
 '27e795eb0f314edf0479737480ab0f2a', 'd16aea76e1e1217b7eb5f7395948d364',␣
 ↪'d9cd4af75fe14d77a6faa0335f83b8c0',
 '2f6f54bd4207339ea29d730563c34b14', '2e0bfa827d51449a197fae6ab9f4804c',␣
 ↪'e0e4a546725d40f259b552ae41932f38',
 'ee15c394e25320ba6ce793eeaef72cdb', '9740966b3dc9d6fd0efba0313c963536',␣
 ↪'30565a8911a6bb487e3745c0ea3c8224',
```

```
 '7f77a1b9954bf3ae6f43c6298871aeda', 'e5b43ca16f1f9cf6cbcfa71cdc7220ae',␣
 ↪'83441ddfbbdcf553b5efe63b81eb1832',
 '2a6b856fad8c51aed13cfd58c948b380', '3b15219be5ebd7c0831dc46746a52d3c',␣
 ↪'870b8425c55942fe40463327364cb546',
 'a2eb92865432da0c58cef552428f4ed1', 'dfff58ed1f9b7657068b28b69b62d70e',␣
 ↪'ee217454afa3c02cb3f1799b5aad3608']
for i, inp in enumerate(inputs):
    assert(get_hash(outputs[i])==hash_list[i])
print('Test passed!')
```

```
Test passed!
```

[14]:
```
# No need to modify: Just run this cell after you pass the validation tests␣
 ↪above
def plot_density_estimate(h):
    x_values = np.arange(0, 45, 0.5)
    y_values = [p_hat(x, h, X_observed) for x in x_values]
    fig = plt.figure(figsize=(9,6))
    plt.hist(X_observed, bins=15, density=True, label="Histogram of observed␣
 ↪values")
    plt.plot(x_values, y_values, label = "Estimated kernel density")
    plt.title("Density $\hat{p}_h(x)$")
    plt.ylabel("Density $\hat{p}_h(x)$")
    plt.xlabel("Velocity, x")
    plt.legend()
    plt.show()
```

[15]:
```
# Visualize interactive plot: Do not modify
interactive_plot = interactive(plot_density_estimate, h=(0.1, 4, 0.1))
interactive_plot
```

```
interactive(children=(FloatSlider(value=2.0, description='h', max=4.0, min=0.1),␣
 ↪Output()), _dom_classes=('wid…
```

6.2 2.b. Questions:

6.2.1 (i) Start with a small value of $h = 0.1$, then slide the value of h, what do you observe?

6.2.2 (ii) Does the density estimate $\hat{p}_h(x)$ seem to contain more modes for higher values of h or lower values of h?

6.2.3 (iii) For what values of h (small or large), does $\hat{p}_h(x)$ fit the current data more closely? Would this value generalize well to other unseen data?

TODO: fill in your answer.

Your Answer:

(i) At h = 0.1, the estimated kernel density fits the histogram of observed values very closely. As

I increase the value of h, it seems to lose all its noise and jagged peaks and becomes seemingly unimodal.

(ii) Lower values of h. Modes = "peaks" of the data. There are more peaks for smaller values of h.

(iii) Values of h near 0.4 seem to fit the data the closest. So small values of h fit the current data more closely. This value would generalize well to unseen data.

7 Question 3. Count the modes of $\hat{p}_h(x)$

7.0.1 There are no todo's in this question except for a simple fill-in-the-blank question at the end. Make sure you read through the questions and understand the solutions before you move on.

Now we will write a function that counts the number of modes of a given density estimate $\hat{p}_h(x)$. This is the $m(p)$ function mentioned above.

To do this, we say that a density function p has a mode everywhere the function $p(x)$ has an increase followed by a decrease. That is, $p(x)$ has an additional mode for each time the derivative of the function $p(x)$ transitions from non-negative to negative.

Following the above definition, to count the number of modes in $\hat{p}_h(x)$, first we will take the derivative,

$$\frac{d}{dx}\hat{p}_h(x).$$

Then, we will count the number of times that the derivative transitions from positive (or 0) to negative over a grid of x's.

7.1 3.a. Calculate the derivative $\frac{d}{dx}\hat{p}_h(x)$.

Using the kernel function $K(x) = \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)$, we will now calculate the derivative $\frac{d}{dx}\hat{p}_h(x)$ by applying the chain rule.

$$\begin{aligned}
\frac{d}{dx}\hat{p}_h(x) &= \frac{d}{dx}\frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x-X_i}{h}\right) \\
&= \frac{1}{nh}\sum_{i=1}^{n} \frac{d}{dx} K\left(\frac{x-X_i}{h}\right) \\
&= \frac{1}{nh}\sum_{i=1}^{n} \frac{1}{h} K'\left(\frac{x-X_i}{h}\right) \\
&= \frac{1}{nh^2}\sum_{i=1}^{n} \frac{1}{\sqrt{2\pi}} \frac{-(x-X_i)}{h} \exp\left(-\frac{\left(\frac{x-X_i}{h}\right)^2}{2}\right) \\
&= \frac{1}{nh^3\sqrt{2\pi}}\sum_{i=1}^{n} (X_i - x) \exp\left(-\frac{(x-X_i)^2}{2h^2}\right)
\end{aligned}$$

7.1.1 Using the final simplified form of the derivative above, implement a function that calculates $\frac{d}{dx}\hat{p}_h(x)$ at a given point x.

[16]:
```
def p_hat_derivative(x, h, X):
    """Calculates the derivative d/dx p_hat(x) at a single point x.

    Inputs:
      x : float, point at which to evaluate the derivative.
      h : float, bandwidth parameter in p_hat.
      X : array of floats of length n containing the observed galaxy velocities.

    Outputs:
      y_prime : float, the derivative d/dx phat_h(x) at the given point x.
    """
    n = len(X)
    total = np.sum((X - x) * np.exp(-((x - X)**2) / (2 * h**2)))
    y_prime = total / (n * h**3 * sqrt(2 * pi))
    return(y_prime)
```

[17]:
```
# No need to modify: Just run this cell after you pass the validation tests␣
↪above
def plot_density_derivative(h):
    x_values = np.arange(4, 36, 0.5)
    y_values = [p_hat_derivative(x, h, X_observed) for x in x_values]
    fig = plt.figure(figsize=(9,6))
    plt.plot(x_values, y_values)
    plt.axhline(0, c = 'k', ls = "--")
    plt.title("Derivative of the density $\hat{p}_h(x)$")
    plt.xlabel("Velocity, x")
    plt.show()
```

[18]:
```
# Visualize interactive plot: Do not modify
interactive_plot = interactive(plot_density_derivative, h=(0.1, 4, 0.1))
interactive_plot
```

```
interactive(children=(FloatSlider(value=2.0, description='h', max=4.0, min=0.1),␣
↪Output()), _dom_classes=('wid…
```

We notice that when h is really small the derivative is very 'wiggly' and it frequently crosses the 0 line. As h increases, it crosses the 0 line less frequently.

7.2 3.b. Count the number of modes in $\hat{p}_h(x)$

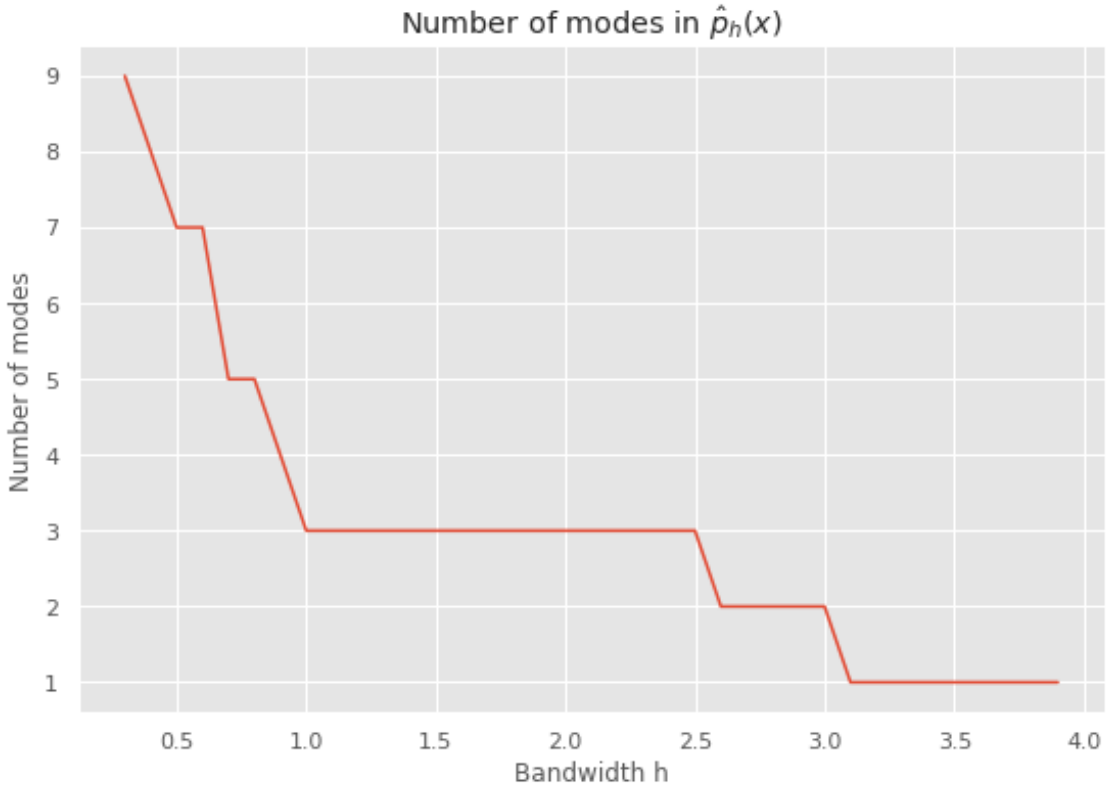
Using the derivative calculated above, we will now count the number of modes in $\hat{p}_h(x)$.

To do this, we will evaluate the derivative $\frac{d}{dx}\hat{p}_h(x)$ at a grid of points $x_1, ..., x_m$ evenly spaced between 5 and 35 (the lower and upper bounds on the velocities in the data), and count the number of times that the derivative crosses from positive to negative. The use of a grid of x's isn't a perfect measurement of the mode count, since if we don't evaluate the derivative at enough points that are close enough together, we may miss some modes. In this lab, we will make sure that the grid we use is fine enough to accurately count the number of modes.

[19]:
```
# Count the modes of phat using the derivative implemented above.
def count_modes(x_values, h, X):
    """Counts the number of modes in p_hat(x), approximated over the given grid␣
↪of x_valies.

    Counts a mode every time the derivative of p_hat(x) crosses from positive␣
↪(or 0)
    to negative over the given grid of x_values.

    Inputs:
      x_values : array of floats of length m
      containing points at which to evaluate the derivative.
      h: float, bandwidth parameter in phat_h.
      X: array of floats of length n containing the observed galaxy velocities.

    Outputs:
      num_modes : int, the number of modes in p_hat(x).
    """
    # First calculate the derivative at all points in x_values.
    all_derivatives = [p_hat_derivative(x, h, X) for x in x_values]

    # Iterate through all of the calculated derivatives,
    # and add a mode every time the derivative crosses from positive (or 0) to␣
↪negative.
    num_modes = 0
    for i in range(0, len(all_derivatives)-1):
        if (all_derivatives[i] >= 0) and (all_derivatives[i + 1] < 0):
            num_modes += 1
```

```
    return num_modes
```

[20]:
```
# No need to modify: Plot the number of modes for different values of h.
# This cell may take a few seconds to run.
x_values = np.arange(5,35,0.05)
h_values = np.arange(0.3,4,0.1)
mode_counts = [count_modes(x_values, h, X_observed) for h in h_values]

fig = plt.figure(figsize=(9,6))
plt.plot(h_values, mode_counts)
plt.title("Number of modes in $\hat{p}_h(x)$")
plt.ylabel("Number of modes")
plt.xlabel("Bandwidth h")
plt.show()
```



7.3 3.c. (To-do) Fill-in-the-blanks

Based on your observation above, we can develop a stategy to find the number of modes. Fill in the blanks below.

"*To find the number of modes, we evaluate the (**Blank 1**) on a grid of points, and count the number*

*of times it goes from (**Blank 2**) to (**Blank 3**).”*

Your answer here (one word for each blank):

Blank 1: derivative

Blank 2: positive

Blank 3: negative

8 Question 4. Hypothesis test

Now that we've defined the density estimate $\hat{p}_h(x)$ and figured out how to count the number of modes in $\hat{p}_h(x)$, we will move on to testing whether or not a multimodal distribution can reasonably fit our data $X_1, ..., X_n$.

In the plot in part 2.b. you should have observed that the number of modes in $\hat{p}_h(x)$ decreases monotonically as h increases. Let H_1 be the minimal bandwidth value h for which $\hat{p}_h(x)$ is unimodal.

$$H_1 = \min\{h\colon m(\hat{p}_h) = 1,\ m(\hat{p}_{h'}) > 1 \text{ for all } h' < h\}. \tag{2}$$

Similarly we define H_k to be the minimal bandwidth value h for which $\hat{p}_h(k)$ has k modes:

$$H_k = \min\{h\colon m(\hat{p}_h) = k,\ m(\hat{p}_{h'}) > k \text{ for all } h' < h\}. \tag{3}$$

We will use H_k as the test statistic.

Notice that H_k depends on the data X, because the function $\hat{p}_h(x)$ depends on the data X.

For our particular observed dataset $X_{observed}$, let h_k be the observed minimal bandwidth value h for which $\hat{p}_h(x)$ has k modes.

8.1 Calculate H_k

The first thing we need to do is calculate H_k for a given dataset X. To do this, we will try different values of h until we find the smallest value such that the density estimate $\hat{p}_h$ has k modes. The function below accomplishes that. Take a few minutes to examine it and understand what it is doing.

[21]:
```
# No TODOs here, just understand what this function is doing.
def find_hk(x_values, X, h_min=0.3, h_max=4, h_err = 0.01, k=1):
    """
    Calculates h_k, the minimum bandwidth h such that the density estimate␣
 ↪p_hat has k modes.
    Chooses h_k from within an interval bounded by h_min and h_max, within␣
 ↪error h_err.

    Inputs:
```

```
    x_values: array of floats containing points x to use to count the number␣
↪of modes in p_hat.
    X: array of floats of length n containing the observed galaxy velocities.
    h_min: float, minimum h to try.
    h_max: float, maximum h to try.
    h_err: float, allowed error of h, or step size of hs to try between h_min␣
↪and h_max.
    k: number of modes being tested in the hypothesis test.

  Returns:
    h_k: minimum bandwith h among candidate h_values such that p_hat has k␣
↪modes.
  """
  # Perform a binary search to find the minimum bandwith hk.
  h_opt = 0
  modes_min = count_modes(x_values, h_min, X)
  modes_max = count_modes(x_values, h_max, X)
  while h_max - h_min > h_err:
      h_opt = (h_min + h_max) / 2
      modes_opt = count_modes(x_values, h_opt, X)
      if modes_opt > k:
          h_min = h_opt
          modes_min = modes_opt
      else:
          h_max = h_opt
          modes_max = modes_opt
  return h_max
```

The function above calculates the test statistic H_k. To calculate the value h_1 for the null hypothesis, we apply this same function over the observed data $X_1, ..., X_n$. Run the cell below and compare the outputs with the plot in 2.b.

[22]:
```
# No TODOs here, just run this cell to calculate the value of h_k using the␣
↪function above.
# This cell might take a minute or so to run
x_values = np.arange(5,35,0.05)
for k in range(1,10):
    hk = find_hk(x_values, X_observed, k=k)
    print("For k = {}. Estimate value of h_{}: {:.4f}".format(k, k, hk))
```

```
For k = 1. Estimate value of h_1: 3.0461
For k = 2. Estimate value of h_2: 2.5041
For k = 3. Estimate value of h_3: 0.9359
For k = 4. Estimate value of h_4: 0.8854
For k = 5. Estimate value of h_5: 0.6758
For k = 6. Estimate value of h_6: 0.6686
For k = 7. Estimate value of h_7: 0.4518
```

```
For k = 8. Estimate value of h_8: 0.3650
For k = 9. Estimate value of h_9: 0.3072
```

8.2 Computing the p-value

Let's say we are trying to test if the distribution of galaxies' velocities is unimodal. The corresponding test statistic is H_1 and the observed realization is h_1. Therefore, the p-value for our hypothesis test is:

$$P_0(H_1 \geq h_1)$$

where P_0 is the probability under the null hypothesis that the X_i are drawn from a unimodal distribution. This p-value represents the probability under the null hypothesis that we observe a value as extreme as h_1 for the minimum width parameter.

To perform a hypothesis test at significance level α, we reject the null hypothesis if the p-value is less than α:

$$P_0(H_1 \geq h_1) \leq \alpha.$$

Now, we need to calculate the p-value. Unfortunately, we don't have a closed form for the distribution of the test statistic H_1 under the null hypothesis that the X_i are drawn from a unimodal distribution. In fact, we don't even know what distribution the X_i are drawn from, only that it's unimodal (under the null hypothesis)! Still, to estimate the distribution of the test statistic H_1, we need to pick some distribution to use for the distribution of the X_i's under the null hypothesis.

Among the parameterized densities $\hat{p}_h(x)$, the density $\hat{p}_{h_1}(x)$ is the closest unimodal distribution to the empirical distribution p of the observed data. So, we will use $\hat{p}_{h_1}(x)$ as the distribution of the X_i's under the null hypothesis.

Therefore, the p-value that we will calculate is

$$P_{X_i \sim \hat{p}_{h_1}}(H_1 \geq h_1).$$

More generally, if instead we want to test if the distribution of galaxies' velocities has at most k modes can be calculated as:

$$P_0(H_k \geq h_k) \approx P_{X_i \sim \hat{p}_{h_k}}(H_k \geq h_k)$$

8.3 4.a. Sampling from $\hat{p}_{h_k}$ using the Bootstrap Method

To calculate the p-value, we will first draw i.i.d. samples from $\hat{p}_{h_k}$, and then observe the number of times that the H_k calculated from those samples is greater than or equal to h_k. We will use the bootstrap to draw the i.i.d. samples from $\hat{p}_{h_k}$.

Let $Z^* = (Z_1^*, \ldots, Z_{82}^*)$ denote a bootstrap sample from the dataset $X_{observed}$. It can be shown that by adding some scaled noise to the bootstrap samples we can obtain samples from the null distribution. More precisely: $Z_i^* + h_k \epsilon_i$ for $\epsilon_i \sim \mathcal{N}(0, 1)$ gives i.i.d. samples from $\hat{p}_{h_k}$.

This leads to the following bootstrap algorithm:

1. Draw B independent bootstrap samples $Z^{*(1)}, \ldots, Z^{*(B)}$ from the observed data. Then add some noise to get samples $X^{*(1)}, \ldots, X^{*(B)}$ from the null distribution $\hat{p}_{h_1}$:

$$X_i^{*(b)} = Z_i^{*(b)} + h_k \epsilon_i^{(b)} \tag{4}$$

$$\epsilon_i^{(b)} \sim \mathcal{N}(0,1) \tag{5}$$

However, since the variance of the bootstrap sample has been increased by adding the normal error term, the data are usually rescaled to have the same sample variance as the original observations. So, we replace the equation above in the algorithm with

$$X_i^{*(b)} = \bar{Z}^{*(b)} + (1 + h_k^2/\hat{\sigma}^2)^{-1/2}(Z_i^{*(b)} - \bar{Z}^{*(b)} + h_k \epsilon_i^{(b)}). \tag{6}$$

We'll use this more complicated variance scaling in the code. In the equation above we have:

- $\bar{Z}^{*(b)}$ is the sample mean of the bootstrap samples $Z^{*(b)}$.
- $\hat{\sigma}$ is the variance of the original observed data.
- h_k is the minimum bandwidth h such that the density estimate for the original observed data has k modes.
- $\epsilon_i^{(b)} \sim \mathcal{N}(0,1)$, iid Gaussian noise

We will call $ X_i^{*(b)}$ **bootstrap replicates**.

2. For each bootstrap replicate X^{*b}, evaluate the value of the test statistic $H_k^{*(b)}$.
3. Estimate the p-value as the fraction of time that the value of the test statistic evaluated on the bootstrap replicates is larger the the test statistic evaluated on the original observed data.

$$\text{estimate of } \mathbb{P}_0(H_k \geq h_k) = \frac{1}{B}\sum_{b=1}^{B} 1[H_k^{*(b)} \geq h_k]. \tag{7}$$

[23]:
```
def estimate_p_value(X, B, k=1):
    """Estimates the p-value for the hypothesis test.

    Inputs:
      X: array of floats containing the observed galaxy velocities.
      B: int, number of bootstrap samples to draw.
      k: int, number of modes we are testing for.

    Outputs:
      p_value: float, an estimate of the p-value.
    """
    # Find hk for the distribution under the null hypothesis.
    x_values = np.arange(5,35,0.05)
    hk = find_hk(x_values, X, k=k)
    # Count of the number of times Hk >= hk.
    Hk_greater_count = 0
    # Variance of the observed data X for rescaling the data.
```

```
    X_var = np.var(X)
    n = len(X)
    for _ in range(B):
        # TODO: obtain the bootstrap sample Z*.
        # Z_star should be an array of n samples drawn from the data array X,␣
↪sampled with replacement.
        # Hint: use np.random.choice.
        Z_star = np.random.choice(X, n) # TODO: fill in

        Z_bar = np.mean(Z_star) # TODO: fill in
        epsilon = np.random.normal(size=n)
        X_star = [Z_bar + (1+(hk**2)/(X_var))**(-0.5) * (Z_star[i] - Z_bar + hk␣
↪* epsilon[i]) for i in np.arange(n)] # TODO: fill in

        # Check if H1 >= h1. Instead of explicitly calculating H1 (which could␣
↪take long),
        # we are using a shortcut where we count the number of modes in X_star␣
↪under bandwidth value h1.
        # If the counted number of modes is greater than the number of modes␣
↪used to find h1
        # for the observed data, then the bandwidth value H1 is greater than or␣
↪equal to the bandwidth value h1.
        # This is true because of number of modes is monotonically decreasing␣
↪in the bandwidth value h.
        modes = count_modes(x_values, hk, X_star)
        if modes > k:
            Hk_greater_count += 1
    p_value = Hk_greater_count / B
    return(p_value)
```

8.4 Try testing for different numbers of modes.

If we reject the hypothesis that the distribution of the data has 1 mode, what about testing if the distribution has more than k modes? We can apply the same techniques to test

$$H_0 : m(p) = k$$
$$H_A : m(p) > k$$

Below, we apply the same techniques to estimate the p-values for $k = 2$ and $k = 3$.

[24]:
```
# No TODOs here, run this cell to calculate the p-value.
p_val_1 = estimate_p_value(X_observed, 100, k=1)
print("p-value for test for more than 1 mode:", p_val_1)
```

```
p-value for test for more than 1 mode: 0.0
```

[25]:
```
# No TODOs here, run this cell to calculate the p-value.
# k = 2
p_val_2 = estimate_p_value(X_observed, 100, k=2)
print("p-value for test for more than 2 modes:", p_val_2)
```

```
p-value for test for more than 2 modes: 0.01
```

[26]:
```
# No TODOs here, run this cell to calculate the p-value.
# k = 3
p_val_3 = estimate_p_value(X_observed, 100, k=3)
print("p-value for test for more than 3 modes:", p_val_3)
```

```
p-value for test for more than 3 modes: 0.42
```

[27]:
```
# Validation tests: Do not modify
assert(np.abs(p_val_1) <= 0.01)
assert(np.abs(p_val_2) <= 0.03)
assert(np.abs(p_val_3 - 0.46) <= 0.15)
print('Test Passed')
```

```
Test Passed
```

8.4.1 4.b. For which values of k were you able to reject the null hypothesis? Did this match your expectation of the number of modes in the data based on looking at the initial histogram?

Your answer here: We reject the null for values k=1 and k=2, and fail to reject for k=3 as the p-value is larger than 0.05. This matches my expectation because the initial histogram had 3 modes (3 peaks) so it makes sense that we didn't reject for k=3 because the null hypothesis was that there were 3 modes.

[28]:
```
print("Great job! You've made it to the end of the lab!")
import matplotlib.image as mpimg
img = mpimg.imread('chinchilla.jpg')
imgplot = plt.imshow(img)
imgplot.axes.get_xaxis().set_visible(False)
imgplot.axes.get_yaxis().set_visible(False)
plt.show()
```

```
Great job! You've made it to the end of the lab!
```

[ ]: