lab04

September 26, 2021

1 Lab 4: Sampling from unknown distributions

Welcome to the 4th Data 102 lab!

The goal of this Lab is to get you familiar with 3 sampling strategies for obtaining samples from unknown distributions: - Rejection Sampling - Gibbs Sampling - Metropolis Hastings

The Lab looks long because we are trying to cover a lot of ground. However there is relatively little code you need to write. The only 'bigish' function you need to write is **2.a**.

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, Sep 29th, 2021 at 11:59 PM. PST

[25]:
```
%matplotlib inline
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import seaborn as sns
from scipy.stats import multivariate_normal, norm, uniform
from ipywidgets import interact, interactive

from mpl_toolkits.mplot3d import axes3d
from matplotlib import cm
```

```python
import hashlib

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

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

1.3 Setup

In this Lab you are given a two dimensional unnormalized density function $f(x, y)$ represented by `target_density` below. The goal of the 3 questions in this lab is to build up a sampler that can output samples from the distribution proportional to $f(x, y)$.

In **Question 1** we will compute samples via *Rejection Sampling*. In part **1.a** we will build a sampler for a 1-dimensional projection of the density. In part **1.b** we will extend the approach to two dimensions.

In **Question 2** we will compute samples via *Gibbs Sampling*. We will use the 1-D rejection sampler as a subroutine.

In **Question 3** we will compute samples via *Metropolis-Hastings*.

Finally we will compare the above methods.

Throughout this lab we will assume that our computers have access only to normal and uniform random variables.

[26]:
```python
# This is the target unnormalized density from which we would like to sample
# Run this to define the function
# No TODOs here
@np.vectorize # <- decorator, makes function run faster
def target_density(x, y):
    mean1 = [1, 1.7]
    mean2 = [2, 1.3]
    mean3 = [1.5, 1.5]
    mean4 = [2, 2.1]
    mean5 = [1, 1.2]
    cov1=0.2*np.array([[0.2, -0.05], [-0.05, 0.1]])
    cov2 = 0.3*np.array([[0.1, 0.07], [0.07, 0.2]])
    cov3= np.array([[0.1, 0], [0, 0.1]])
    cov4 = 0.1*np.array([[0.3, 0.04], [0.04, 0.2]])
    cov5 = 0.1*np.array([[0.4, -0.04], [-0.04, 0.2]])
    return(multivariate_normal.pdf([x, y], mean=mean1, cov=cov1) +
           multivariate_normal.pdf([x, y], mean=mean2, cov=cov2) +
           2*multivariate_normal.pdf([x, y], mean=mean3, cov=cov3) +
           0.5*multivariate_normal.pdf([x, y], mean=mean4, cov=cov4)+
```

```
            0.5*multivariate_normal.pdf([x, y], mean=mean5, cov=cov5))
```

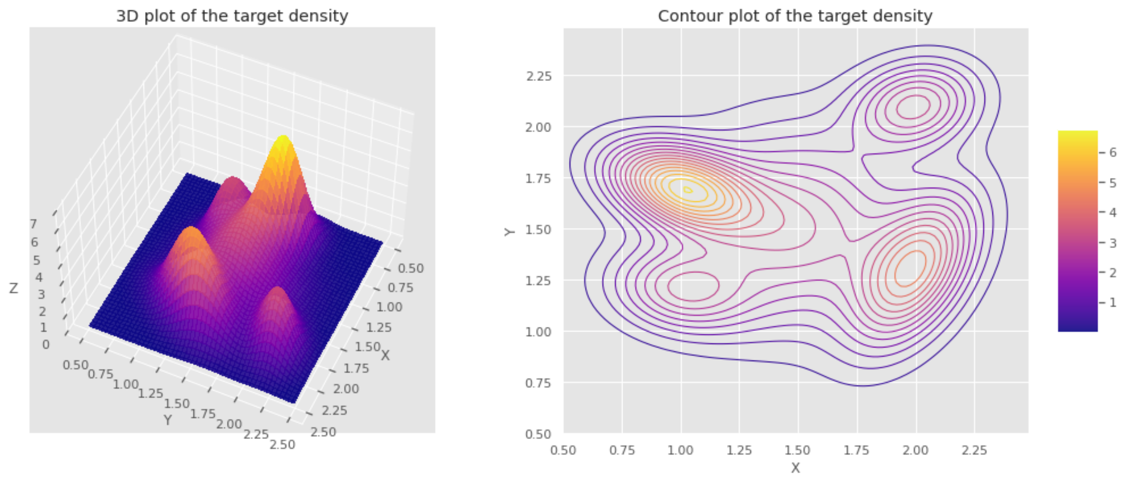
Let's visualize this density. Run the cell below to see a 3D plot of the function along with a contour plot.

[27]:
```
# No TODOs here, just run the cell to make plots
# Create a meshgrid of coordinates
coords = np.arange(0.5, 2.5, 0.02)
X, Y = np.meshgrid(coords, coords)

# Compute the value of the target density at all pairs of (x,y) values
Z = target_density(X,Y)
```

[28]:
```
# Display the 3D plot of the target density
fig = plt.figure(figsize=(15,6))

ax0 = fig.add_subplot(121, projection='3d')
ax1 = fig.add_subplot(122)

surf = ax0.plot_surface(X,Y,Z, cmap=cm.plasma, linewidth=0,␣
 ↪antialiased=False,alpha = 0.9,)

# Customize the z axis.
ax0.set_zlim(0, 7)
ax0.set_xlabel("X")
ax0.set_ylabel("Y")
ax0.set_zlabel("Z")
ax0.set_title("3D plot of the target density")

# Rotate the axes: you can change these numbers in order to see the␣
 ↪distribution from other angles
ax0.view_init(50, 25)

# Plot the contour plot of the density
cont = ax1.contour(X,Y,Z, levels = 20, cmap=cm.plasma, linewidths=1)
ax1.set_xlabel("X")
ax1.set_ylabel("Y")
ax1.set_title("Contour plot of the target density")

# Add a color bar which maps values to colors.
fig.colorbar(surf, shrink=0.5, aspect=5)
plt.tight_layout()
plt.show()
```

```
/tmp/ipykernel_45/725971890.py:26: MatplotlibDeprecationWarning: Starting from
Matplotlib 3.6, colorbar() will steal space from the mappable's axes, rather
than from the current axes, to place the colorbar.  To silence this warning,
```

```
explicitly pass the 'ax' argument to colorbar().
  fig.colorbar(surf, shrink=0.5, aspect=5)
```



Take a moment to examine the plots. Make sure you can see correspondances between each peak in the 3D plot on the left; and the "high-altitude" regions in the countour plot on the right.

Next we will plot 1-dimensional projections of the target densities onto the X and Y axis. These correspond to conditional target distributions of the form $f(x, y = y')$ and $f(x = x', y)$.

[29]:
```
# Do not modify
# Run the cell below to define the plotting functions

COORDINATES = np.arange(0, 3, 0.02)
def plot_x_cond(y_val):
    fig, axs = plt.subplots(1, 2)
    fig.set_figheight(5)
    fig.set_figwidth(12)
    axs[0].contour(X,Y,Z, levels = 20, cmap=cm.plasma, alpha = 0.8,␣
 ↪linewidths=0.8)
    axs[0].axhline(y_val,  ls="--", color = 'olive', lw = 2)
    axs[0].set_xlabel("X")
    axs[0].set_ylabel("Y")
    axs[0].set_title("Contour plot of the target density")

    axs[1].plot(COORDINATES, target_density(COORDINATES, y_val), color =␣
 ↪'olive')
    axs[1].set_ylim(0,10)
    axs[1].set_xlim(0,3)
    axs[1].set_xlabel("X")
    axs[1].set_title("Conditional target density: f(x | y={:.1f})".
 ↪format(y_val))
```

```
    plt.show()

def plot_y_cond(x_val):
    fig, axs = plt.subplots(1, 2)
    fig.set_figheight(5)
    fig.set_figwidth(12)
    axs[0].contour(X,Y,Z, levels = 20, cmap=cm.plasma, alpha = 0.8,␣
 ↪linewidths=0.8)
    axs[0].axvline(x_val,  ls="--", color = 'olive', lw = 2)
    axs[0].set_xlabel("X")
    axs[0].set_ylabel("Y")
    axs[0].set_title("Contour plot of the target density")

    axs[1].plot(COORDINATES, target_density(x_val, COORDINATES), color =␣
 ↪'olive')
    axs[1].set_ylim(0,10)
    axs[1].set_xlim(0,3)
    axs[1].set_xlabel("Y")
    axs[1].set_title("Conditional target density: f(y | x={:.1f})".
 ↪format(x_val))
    plt.show()
```

[30]:
```
# Display interactive plot
interactive_plot = interactive(plot_x_cond, y_val=(0, 3, 0.1),␣
 ↪add_proposal=False)
interactive_plot
```

```
interactive(children=(FloatSlider(value=1.0, description='y_val', max=3.0),␣
 ↪Output()), _dom_classes=('widget-i…
```

Set different values of `y_val`, observe the changes in the conditional target density.

[31]:
```
# Display interactive plot
interactive_plot = interactive(plot_y_cond, x_val=(0, 3, 0.1),␣
 ↪add_proposal=False)
interactive_plot
```

```
interactive(children=(FloatSlider(value=1.0, description='x_val', max=3.0),␣
 ↪Output()), _dom_classes=('widget-i…
```

Set different values of `x_val`, observe the changes in the conditional target density.

1.4 Question 1. Rejection Sampling

In this question we will build a rejection sampler. First let's go over the basics of Rejection Sampling.

Assume we want to sample from an unnormalized target density $f(x)$, using a proposal distribution Q, with density $q(x)$. The proposal distribution is chosen such that we have access to samples from it.

Rejection sampling proceeds as follows:

- Find constant c, such that $cf(x) \leq q(x)$ on the support
- At each iteration:
  - Sample $x_i \sim Q$
  - Compute the ratio $r = \frac{c(f(x_i))}{q(x_i)} \leq 1$, `accept` the sample with probability `r`, this is equivalent to:
  - Sample $\gamma_i \sim Uniform(0, 1)$:
    - `accept` the sample if $\gamma_i \leq r$: Add x_i to the list of samples.
    - `reject` the sample otherwise: do nothing

1.4.1 1.a Sample from the one-dimensional density $f(x, y = 1.2)$

Throughout part 1.a we will consider a Uniform(0,3) as our proposal distribution. Meaning that $q(x) = \frac{1}{3}\ \forall x \in [0, 3]$

[32]:
```
# Create the target 1D density f(x, y = 1.2)
def target_1D_density(x):
    return(target_density(x, 1.2))
```

[33]:
```
# TODO: fill in
# Hint: the uniform function in scipy might prove useful here
def sample_1D_proposed_distribution(N):
    """
    Produces N samples from the Uniform(0,3) proposal distribution

    Inputs:
        N : int, desired number of samples

    Outputs:
        proposed_samples : an 1d-array of size N which contains N independent␣
 ↪samples from the proposal
    """

    proposed_samples = uniform.rvs(0, 3, N)
    return(proposed_samples)

# TODO: fill in
@np.vectorize
def compute_ratio_1D(proposed_sample, c):
    """
    Computes the ratio between the scaled target density and proposal density␣
 ↪evaluated at the
    proposed sample point

    Inputs:
```

```
        proposed_sample : float, proposed sample
        c : float, constant scaling factor that ensures that the proposal␣
 ↪density is above the target density

    Outputs:
        ratio : float
    """
    ratio = c * target_1D_density(proposed_sample) / (1/3)
    assert(ratio <= 1)
    return(ratio)

# TODO: fill in
@np.vectorize
def accept_proposal(ratio):
    """
    Accepts or rejects a proposal with probability equal to ratio

    Inputs:
        ratio: float, probability of acceptance

    Outputs:
        accept: True/False, if True, accept the proposal
    """
    accept = uniform.rvs(0, 1) <= ratio
    return(accept)
```

Now we have all the ingredients for making a sampler:

[34]:
```
# TODO: complete the function
def get_1D_samples(N, c):
    """
    Produces samples from target_1D_density

    Inputs:
        N : int, number of proposed_samples
        c : float, constant scaling factor that ensures that the proposal␣
 ↪density is above the target density

    Outputs:
        rejection_samples : an 1d-array of which contains independent samples␣
 ↪from the target
    """

    proposed_samples = sample_1D_proposed_distribution(N)
    ratios = compute_ratio_1D(proposed_samples, c)
    accept_array = accept_proposal(ratios)

```

```
    rejection_samples = proposed_samples[accept_array]
    return(rejection_samples)
```

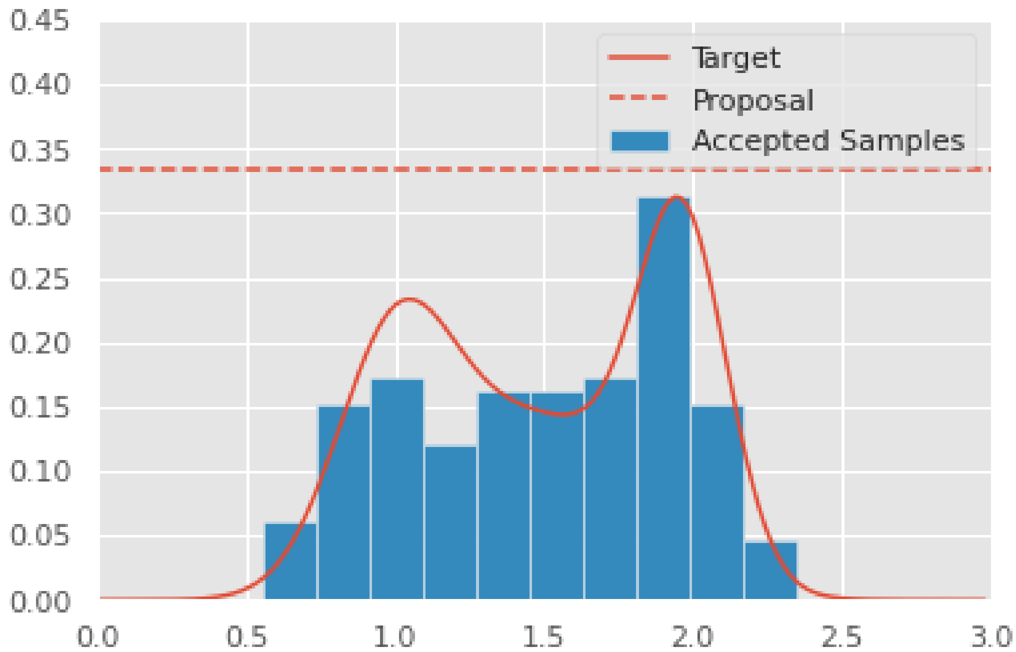
[35]:
```
# Validation tests: do not modify
N = 1000
assert(np.abs(1.5-np.mean(get_1D_samples(N, 1/15))) < 0.1)
assert(np.abs(0.3-len(get_1D_samples(N, 1/15))/N) < 0.05)
assert(np.abs(0.23-len(get_1D_samples(N, 1/20))/N) < 0.05)
assert(np.abs(0.18-len(get_1D_samples(N, 1/25))/N) < 0.05)
print('Test passed!')
```

```
Test passed!
```

From the interactive plot above we can see that $f(x, y = 1.2)$ is allways smaller than 5. Hence to make it smaller than $q(x) = 1/3$ we need to scale the target density by a factor $c \leq \frac{1}{3} \cdot \frac{1}{5} = 1/15$.

Let's use $c = 1/15$, compute target samples and plot their histogram

[36]:
```
# No TODOs here
# Just run it once you passed the assertion tests above

fig = plt.figure(figsize = (6, 4))
c = 1/15
target_samples = get_1D_samples(1000, c)
density_values =  target_1D_density(COORDINATES)*c
plt.plot(COORDINATES, density_values, label='Target')
plt.axhline(1/3, ls = '--', label = 'Proposal')
n, bins, rects = plt.hist(target_samples, density = True, label="Accepted␣
↪Samples")
max_height = np.max([r.get_height() for r in rects])
for r in rects:
    r.set_height(r.get_height()*np.max(density_values)/max_height)
plt.legend()
plt.xlim(0,3)
plt.ylim(0,0.45)
plt.show()
```



Computing the acceptance ratio for varying scaling constants c

[37]:
```
# No TODOs here
# Just run it and comment in the section below

N = 1000
c_values = [0.06, 0.05, 0.04, 0.03, 0.02, 0.01]
for c in c_values:
    # compute target samples
    target_samples = get_1D_samples(N, c)
    acceptance_percentage = 100*len(target_samples)/N
    print("For c = {:.2f}, the acceptance percentage is {:.1f}%".format(c,␣
 ↪acceptance_percentage))
```

```
For c = 0.06, the acceptance percentage is 27.3%
For c = 0.05, the acceptance percentage is 23.2%
For c = 0.04, the acceptance percentage is 17.7%
For c = 0.03, the acceptance percentage is 13.0%
For c = 0.02, the acceptance percentage is 9.3%
For c = 0.01, the acceptance percentage is 3.8%
```

TODO: in the cell below explain why the accepted percentage decreases as c decreases: As c decreases, the ratio r also decreases since c is in the numerator of the ratio. Since the ratio decreases and we only accept the sample if it is less than the ratio, fewer samples fall under that threshold so more samples are rejected. Hence, the acceptance percentage decreases as c decreases.

1.4.2 1.b Sample from the two-dimensional density $f(x, y)$

In two dimensions Rejection Sampling is nearly identical to the 1-dimension case:

- Find constant c, such that $cf(x, y) \leq q(x, y)$ on the support
- At each iteration:
  - Sample $(x_i, y_i) \sim Q$
  - Compute the ratio $r = \frac{c(f(x_i,y_i))}{q(x_i,y_i)} \leq 1$, `accept` the sample with probability `r`, this is equivalent to:
  - Sample $\gamma_i \sim Uniform(0, 1)$:
    * `accept` the sample if $\gamma_i \leq r$: add (x_i, y_i) to the list of samples.
    * `reject` the sample otherwise: do nothing

Throughout part 1.b we will consider $(x, y) \sim Uniform(0, 3) \times Uniform(0, 3)$ as our proposal distribution. Meaning that $q(x, y) = \frac{1}{9}$ $\forall x, y \in [0, 3]$

`TODO` complete the function below

[41]:
```
# TODO: fill in
@np.vectorize
def compute_ratio_2D(proposed_sample_x, proposed_sample_y, c):
    """
    Computes the ratio between the scaled target density and proposal density␣
 ↪evaluated at the
    proposed sample point

    Inputs:
        proposed_sample_x : float, x components of the proposed sample point
        proposed_sample_y : float, y components of the proposed sample point
        c : float, constant scaling factor that ensures that the proposal␣
 ↪density is above the target density

    Outputs:
        ratio : float
    """
    ratio = (c*target_density(proposed_sample_x, proposed_sample_y)) / (1/9)
    assert(ratio <= 1)
    return(ratio)
```

Now we have all the ingredients for making a sampler.

[42]:
```
# No TODOs here, just run the 2D version of the functions we built in 1.a
def get_2D_samples(N, c):
    """
    Produces samples from target_density

    Inputs:
        N : int, number of proposed_samples
```

```
        c : float, constant scaling factor that ensures that the proposal␣
↪density is above the target density

    Outputs:
        rejection_samples : ndarray of which contains independent samples from␣
↪the target
    """
    proposed_samples_x = sample_1D_proposed_distribution(N)
    proposed_samples_y = sample_1D_proposed_distribution(N)
    ratios = compute_ratio_2D(proposed_samples_x, proposed_samples_y, c)
    accept_array = accept_proposal(ratios)
    proposed_samples = np.concatenate((proposed_samples_x.reshape(N,1),␣
↪proposed_samples_y.reshape(N,1)), axis = 1)
    rejection_samples = proposed_samples[accept_array]
    return(rejection_samples)
```

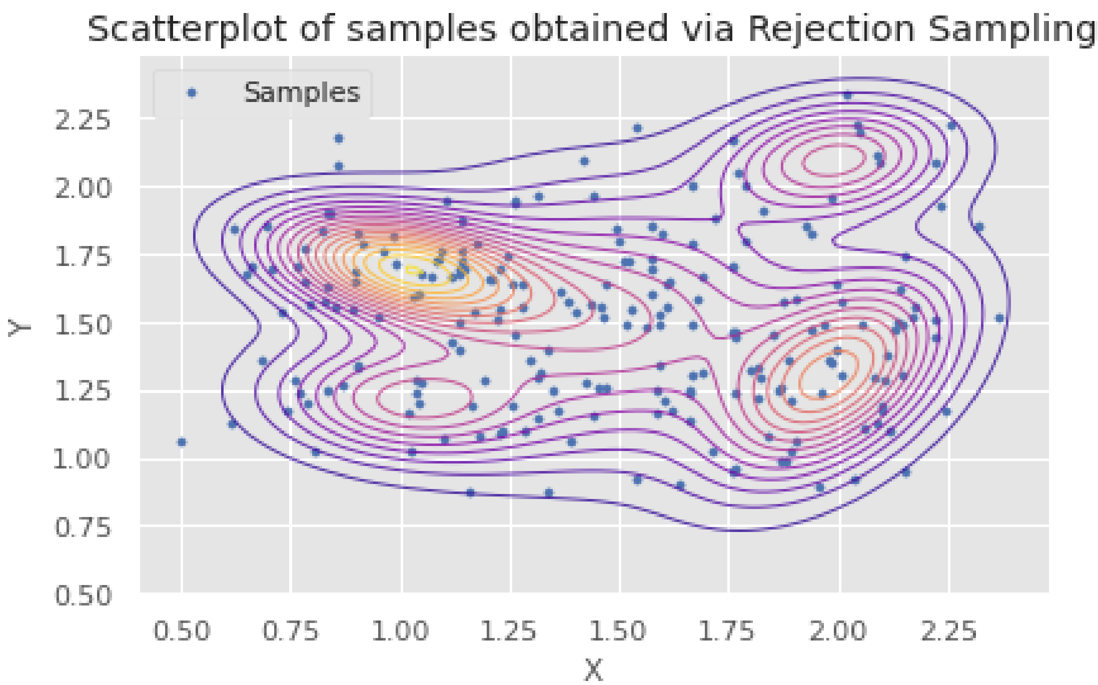
[43]:
```
# Validation tests: Do not modify
N = 5000
assert(np.abs(0.075-len(get_2D_samples(N, 0.015))/N) < 0.015)
assert(np.abs(0.045-len(get_2D_samples(N, 0.01))/N) < 0.015)
print('Test passed!')
```

```
Test passed!
```

From the contour plot above we can see that $f(x, y = 1.2)$ is allways smaller than 7.4. Hence to make it smaller than $q(x) = 1/9$ we need to scale the target density by a factor $c \leq \frac{1}{7.4} \cdot \frac{1}{8} = 0.015$.

Let's use $c = 0.015$, compute target samples and plot them on top the contour lines

[44]:
```
fig = plt.figure(figsize=(6,4))

# Plot the contour plot of the density
cont = plt.contour(X,Y,Z, levels = 20, cmap=cm.plasma, linewidths=1, alpha = 0.
↪8)
plt.xlabel("X")
plt.ylabel("Y")
plt.title("Scatterplot of samples obtained via Rejection Sampling")

# Add sample points obtained via rejection sampling
c = 1/72
target_samples = get_2D_samples(3000, c)
plt.scatter(target_samples[:,0], target_samples[:,1], c='b', alpha = 1, s = 10,␣
↪label = 'Samples')

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



[45]:
```
# No need to modify this
# just run it and comment in the section below

N = 3000
c_values = [0.015, 0.01, 0.005, 0.001]
for c in c_values:
    # compute target samples
    target_samples = get_2D_samples(N, c)
    acceptance_percentage = 100*len(target_samples)/N
    print("For c = {:.3f}, the acceptance percentage is {:.1f}%".format(c,␣
 ↪acceptance_percentage))
```

```
For c = 0.015, the acceptance percentage is 7.7%
For c = 0.010, the acceptance percentage is 4.4%
For c = 0.005, the acceptance percentage is 2.5%
For c = 0.001, the acceptance percentage is 0.6%
```

TODO: in the cell below explain why the accepted percentage when sampling from 2D distribution is so much smaller than sampling from the 1D version in 1.a. In 1a, we used a c value of 1/15 i.e. 0.067. Here, in 1b, we are using a c value of 0.015. As a result, the c value from part a is more than 4 times larger than what we have used here. This means that the ratio from part a was larger, and the ratio here is much smaller. As a result, fewer samples fall under the threshold to be accepted, so there is a smaller acceptance percentage.

1.5 Question 2. Gibbs Sampling

In this question we will build a Gibbs sampler. First let's go over the basics of Gibbs Sampling.

Assume we want to sample from an unnormalized target density $f(x, y)$.

Gibbs Sampling proceeds as follows:

- Start at an initial point (x_0, y_0)
- For `i` in `number of iterations`:
  - Condition on $y = y_{i-1}$: Sample $x_i \sim f(x|y = y_{i-1})$
    - Add (x_i, y_{i-1}) to the list of samples
  - Condition on $x = x_i$: : Sample $y_i \sim f(y|x = x_i)$
    - Add (x_i, y_i) to the list of samples

In many problems we can sample the univariate distributions directly. In this case we don't know how to sample them directly, but we can use the 1-D rejection sampler that we computed in 1.a.

In the cell below we wrote for you helper functions that sample from the conditionals aboves. They are essentially the same function you wrote in 1.a, just slightly modified such that we perform rejection sampling until we get one valid sample.

[46]:
```
# No TODOs here:
# Just look at these helper functions and make sure you understand the syntax

def sample_x_cond(fixed_y_val):
    """
    Produces one sample from x_i ~ f(x | y=fixed_y_val)

    Inputs:
        fixed_y_val : float, current value of y, on which we condition

    Outputs:
        x_sample: float, one sample from x_i ~ f(x, y=fixed_y_val)
        num_samples : int, number of tries until we accepted a sample

    """
    def conditional_density(x):
        return(target_density(x, fixed_y_val))
    x_sample = None
    num_samples = 0
    c = 0.33/(0.2+max(conditional_density(np.arange(0.5, 2.5, 0.05)))) # <- we␣
↪are cheating a bit here by
                                                                          #␣
↪looking for a tight c value
    while x_sample is None:
        proposed_sample = sample_1D_proposed_distribution(1)
        num_samples += 1
        ratio = conditional_density(proposed_sample)*3*c
        assert(ratio <= 1)
```

```
        accept = accept_proposal(ratio)
        if accept:
            x_sample = proposed_sample[0]
    return(x_sample, num_samples)


def sample_y_cond(fixed_x_val):
    """
    Produces one sample from y_i ~ f(y | x=fixed_x_val)

    Inputs:
        fixed_x_val : float, current value of y, on which we condition

    Outputs:
        y_sample: float, one sample from y_i ~ f(y | x=fixed_x_val)
        num_samples : int, number of tries until we accepted a sample

    """
    def conditional_density(y):
        return(target_density(fixed_x_val, y))
    y_sample = None
    num_samples = 0
    c = 0.33/(0.2+max(conditional_density(np.arange(0.5, 2.5, 0.05))))
    while y_sample is None:
        proposed_sample = sample_1D_proposed_distribution(1)
        num_samples += 1
        ratio = conditional_density(proposed_sample)*3*c
        assert(ratio <= 1)
        accept = accept_proposal(ratio)
        if accept:
            y_sample = proposed_sample[0]
    return(y_sample, num_samples)
```

1.5.1 2.a `TODO`: Build a Gibbs sampler using the helper functions above

`Note`: Don't forget that at each iteration the Gibbs sampler adds two samples to the list of samples: (x_i, y_{i-1}) and (x_i, y_i)

[49]:
```
# TODO: fill in
def get_2D_Gibbs_samples(N, x_0, y_0):
    """
    Produces N samples from the target density using Gibbs Sampling

    Inputs:
        N : desired number of samples
        x_0, y_0 : floats, the coordinates of the starting point

```

```
    Outputs:
        gibbs_samples : array of dimension (N, 2) where each row is a sample␣
↪from the target distribution
                        of the form (x_i, y_i)
        num_samples : total number of samples required
    """

    gibbs_samples = [] # Each entry corresponds to a (x_i, y_i)
    num_samples = 0 # Add the number of samples to this variable, note this is␣
↪not equal to N since rejection sampling
                    # does not accept every sample
    x_curr = x_0 # Current value of x, initialized to x_0
    y_curr = y_0 # Current value of y, initialized to y_0

    for i in range(N//2): # The range is N//2 since we are generating two gibbs␣
↪samples in one iteration
        # TODO: fill in
        x_new, x_num = sample_x_cond(y_curr)
        y_new, y_num = sample_y_cond(x_new)
        num_samples += (x_num + y_num)

        gibbs_samples.append([x_new, y_curr])
        gibbs_samples.append([x_new, y_new])

        y_curr = y_new

    return(gibbs_samples, num_samples)
```

[50]:
```
# Validation tests: Do not modify
N = 100
output = get_2D_Gibbs_samples(N, 1, 1)
assert(get_hash(len(output)) == 'c81e728d9d4c2f636f067f89cc14862c')
assert(get_hash(len(output[0])) == 'f899139df5e1059396431415e770c6dd')
assert(get_hash(len(output[0][0])) == 'c81e728d9d4c2f636f067f89cc14862c')
assert(np.abs(410-output[1]) < 100)
print('Test passed!')
```

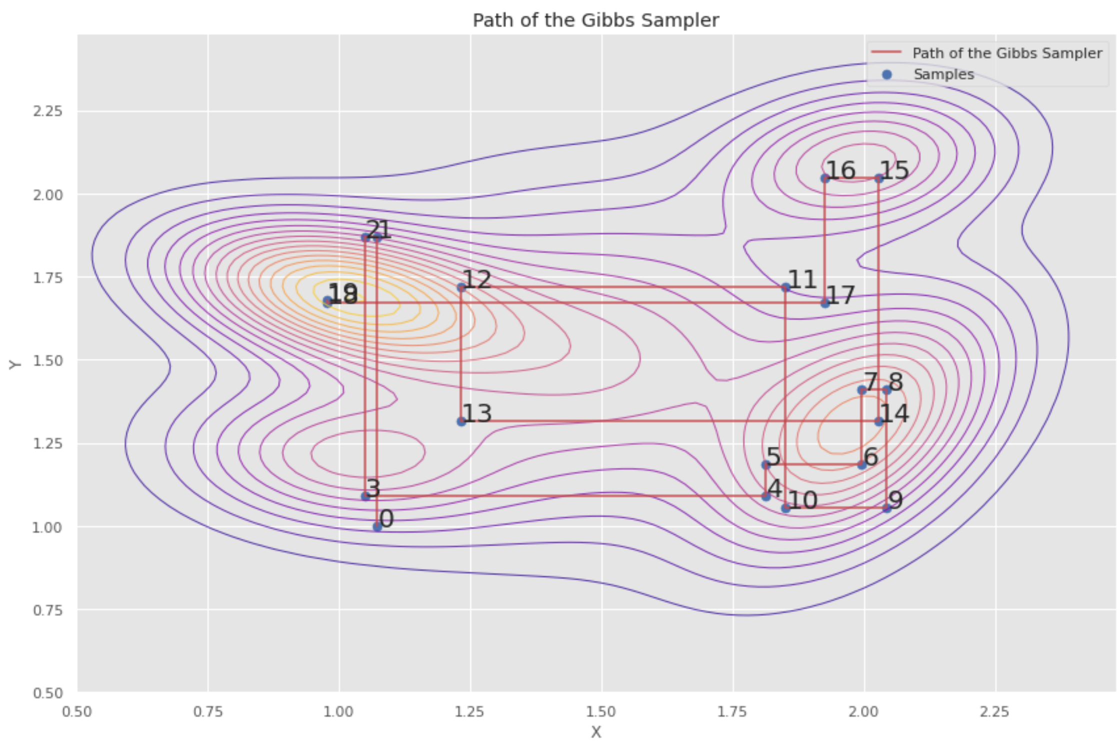
```
Test passed!
```

1.5.2 2.b : Path traced by the Gibbs sampler

Run the code below to overlay the path traced by the Gibbs Sampler

[51]:
```
# No TODOs here
# Just run this once you've passed the validation tests above
N = 20
target_samples, total_samples = get_2D_Gibbs_samples(N, 1, 1)
```

```
target_samples = np.array(target_samples)

fig = plt.figure(figsize=(12,8))

# Plot the contour plot of the density
cont = plt.contour(X,Y,Z, levels = 20, cmap=cm.plasma, linewidths=1, alpha = 0.
 ↪8)
plt.xlabel("X")
plt.ylabel("Y")
plt.title("Path of the Gibbs Sampler")

# Add sample points obtained via Gibbs sampling
plt.scatter(target_samples[:,0], target_samples[:,1], c='b', alpha = 1, s=50,␣
 ↪label = 'Samples')
for i in range(N):
    plt.annotate(i, (target_samples[i,0], target_samples[i,1]), fontsize = 20)
plt.plot(target_samples[:,0], target_samples[:,1], c='r', alpha = 1, label =␣
 ↪'Path of the Gibbs Sampler')

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



TODO: Inspect the scatter plot above. Trace the Gibbs sampler path from the initial point (labeled 0) to the final point. What do you observe? Why do you think that's the case. All the points seem to occur near the high-density regions of the contour ports i.e. the "peaks". I think this is because this is where the majority of the points from the target distribution lie, so the peaks need to be visited pretty often.

1.5.3 2.c: 'Efficiency' of Gibbs Sampling

[53]:
```python
# Let's compute 1000 Gibbs samples and compute how many times the rejection␣
↪sampling subroutine
# accepted the proposed sample (running this might take a little while)
N = 1000
target_samples, total_samples = get_2D_Gibbs_samples(N, 1, 1)
acceptance_rate = N/total_samples*100
print("The acceptance rate for Gibbs Sampling is {:.1f}%".
↪format(acceptance_rate))
```

```
The acceptance rate for Gibbs Sampling is 23.7%
```

TODO: How does Gibbs Sampling compare to vanilla Rejection Sampling from 2b? Is this approach more efficient or less efficient? Why do you think that's the case? The acceptance percentage for Gibbs Sampling seems to be much higher than rejection sampling (~24% compared to a maximum of ~7%). I think this is more efficient because since you're accepting more samples, you need to go back and resample fewer number of times. E.g. if you need a total of N samples, and you get N/3 out of them via Gibbs and N/10 of them via Rejection Sampling, Gibbs is more efficient because you need to perform it a fewer number of times.

1.6 Question 3. Metropolis Hastings

In this final question we will build a Metropolis-Hastings sampler. First let's go over the basics of Metropolis-Hastings Sampling.

Assume we want to sample from an unnormalized target density $f(x, y)$.

In this question we will consider a Random-Walk Metropolis Hasting Algorithm. The algorithm proceeds as follows:

- Start at an initial point (x_0, y_0)
- For `i` in `number of iterations`:
  - Condition on $(x, y) = (x_{i-1}, y_{i-1})$. Define proposal distribution $Q(x, y|x_{i-1}, y_{i-1})$: $\begin{bmatrix} x \\ y \end{bmatrix} \sim Normal\left(\begin{bmatrix} x_{i-1} \\ y_{i-1} \end{bmatrix}, \sigma^2 I\right)$
  - Sample $(x', y') \sim Q(x, y|x_{i-1}, y_{i-1})$
  - Compute the ratio $r = \frac{f(x',y')}{f(x_{i-1},y_{i-1})} \frac{q(x_{i-1},y_{i-1}|x',y')}{q(x',y'|x_{i-1},y_{i-1})} = \frac{f(x',y')}{f(x_{i-1},y_{i-1})}$,
    * If $r \geq 1$: `move` : $(x_i, y_i) = (x', y')$ *(we move to the proposed location)*
    * If $r \leq 1$: `move` with probability r, `stay` with probability $1 - r$, this is equivalent to:
      · Sample $\gamma_i \sim Uniform(0, 1)$: · if $\gamma_i \leq r$, **move:** $(x_i, y_i) = (x', y')$
      · otherwise, **stay:** $(x_i, y_i) = (x_{i-1}, y_{i-1})$

– Add (x_i, y_i) to the list of samples

Note: in step 3, when computing the ratio r we can cancel out the q terms. We can do that because the proposal distribution is symmetric, meaning that $q(x_{i-1}, y_{i-1}|x', y') = q(x', y'|x_{i-1}, y_{i-1})$

[54]:
```
# No TODOs here: we are providing all the functions to you
# Spend some time examining the code and the algorithm described above

def sample_proposed_normal_distribution(mean, sigma_squared):
    """
    Produces a sample from the Uniform(0,3) proposal distribution

    Inputs:
        mean : array of length 2, containing the mean of the proposal␣
 ↪distributions
        sigma_squared : float, the variance of the proposal distribution

    Outputs:
        proposed_sample : array of size 2 which contains a sample (x, y) from␣
 ↪the proposal
    """

    proposed_sample = multivariate_normal.rvs(mean = mean, cov = sigma_squared)
    return(proposed_sample)

def compute_ratio(proposed_sample, current_sample):
    """
    Computes the ratio r:

    Inputs:
        proposed_sample : array of size 2 which contains sample (x, y) from the␣
 ↪proposal
        current_sample : array of size 2 which contains the current (x, y)␣
 ↪sample

    Outputs:
        ratio : float
    """
    ratio = target_density(*proposed_sample)/target_density(*current_sample)
    return(ratio)

def move_now(ratio):
    """
    Decides to move to the proposed location, or stay at the current location

    Inputs:
        ratio: float
```

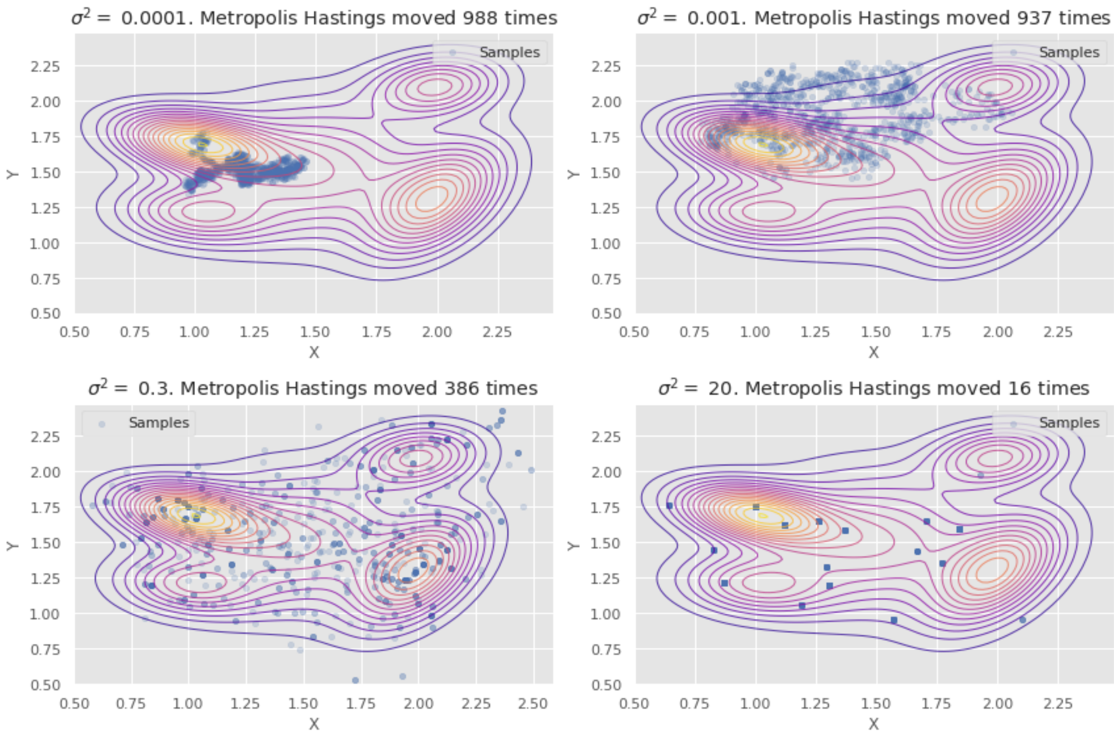
```
    Outputs:
        move: True/False, if True, move to the proposed locatio,
                          if False, stay at the current location
    """
    if ratio >= 1:
        move = True
        return(move)
    else:
        gamma = uniform.rvs(0, 1)
        move = gamma <= ratio
        return(move)
```

[55]:
```
# No TODOs here: Just run the cell to define the function

def get_2D_MH_samples(N, x_0, y_0, sigma_squared):
    """
    Produces N sampled from the target density using Gibbs Sampling

    Inputs:
        N : desired number of samples
        x_0, y_0 : floats, the coordinates of the starting point
        sigma_squared : float, the variance of the proposal distribution

    Outputs:
        MH_samples : array of dimension (N, 2) where each row is a sample from␣
 ↪the target distribution
                     of the form (x_i, y_i)
        num_moves : number of times the MH algorithm moved to a new point
    """
    MH_samples = []
    current_sample = [x_0, y_0]
    num_moves = 0
    for i in range(N):
        proposed_sample = sample_proposed_normal_distribution(current_sample,␣
 ↪sigma_squared)
        ratio = compute_ratio(proposed_sample, current_sample)
        if move_now(ratio):
            current_sample = proposed_sample
            num_moves += 1
        MH_samples.append(current_sample)
    return(MH_samples, num_moves)
```

Run the code below to compute Metropolis Hastings samples for proposal distribution with different variance levels. We overlay the samples on top of the usual contour plots.

[56]:
```
# No TODOs here: Just run the code to create the plots
# Spend some time investigating the code
```

```
N = 1000
sigma_squared_values = [0.0001, 0.001, 0.3, 20]
initial_point = [1, 1.75]

fig, axs = plt.subplots(2, 2)
fig.set_figheight(8)
fig.set_figwidth(12)

itr = 0
for i in range(2):
    for j in range(2):
        sigma_squared = sigma_squared_values[itr]
        target_samples, num_moves = get_2D_MH_samples(N, *initial_point,␣
↪sigma_squared)
        # Convert to numpy array
        target_samples = np.array(target_samples)

        # Plot the contour plot of the density
        cont = axs[i,j].contour(X,Y,Z, levels = 20, cmap=cm.plasma,␣
↪linewidths=1, alpha = 0.8)
        # Add sample points obtained via MH sampling
        axs[i,j].scatter(target_samples[:,0], target_samples[:,1], c='b', alpha␣
↪= 0.2, s=20, label = 'Samples')

        axs[i,j].set_xlabel("X")
        axs[i,j].set_ylabel("Y")
        axs[i,j].set_title("$\\sigma^2 = $ {}. Metropolis Hastings moved {}␣
↪times".format(sigma_squared, num_moves))
        axs[i,j].legend()
        itr += 1
plt.tight_layout()
plt.show()
```



TODO: Examine the 4 plots above. Each plot contains 1000 Metropolis-Hastongs samples, by considering proposal distributions with different variances. What do you observe?

- Why do samples stay clustered close to each-other for small value of σ^2?
- Why does the MH algorithm have so much fewer moves when the value of σ^2?
- Which value of σ^2 would you choose out of the above and why?

I observe that for larger values of σ^2, the samples seem to be more evenly distributed whereas they are clustered for smaller values of σ^2. For larger values of σ^2, Metropolis Hastings moves a fewer number of times.

Smaller values of σ^2 encourage clustering because this means there is less variation in the proposal distribution, so values are closer together, leading to clustering.

The MH algorithm has much fewer moves when the value of σ^2 is large because there is larger variation so samples can "hop around" the proposal distribution with more ease.

The value of σ^2 that I would choose is 0.001. The reason for this is the following:

Choice 1: $\sigma^2 = 0.0001$. This is too clustered around one peak. We want to make sure the sample encompasses all the peaks.

Choice 3: $\sigma^2 = 0.3$. This is too spread out. We want to make sure our sample contains more data points from the peaks, as opposed to being all over the place.

Choice 4: $\sigma^2 = 20$. This is too spread out. We want to make sure our sample contains more data points from the peaks, as opposed to being all over the place.

As a result, $\sigma^2 = 0.001$ is the best option because it doesn't jump around too much, but it also isn't too clustered. In addition, it also fulfills the important condition of containing more samples from the peaks.

[57]:
```
import matplotlib.image as mpimg
img = mpimg.imread('baby_seal.png')
imgplot = plt.imshow(img)
imgplot.axes.get_xaxis().set_visible(False)
imgplot.axes.get_yaxis().set_visible(False)
plt.show()
print('Congrats! You made it to the end of the lab!!!')
```

```
Congrats! You made it to the end of the lab!!!
```

[ ]:
```
```