Assignment_I

December 7, 2022

Aluno: Felipe Adrian Moreno Vera Materia: Estadistica Computacional

Doutorado - EMAp

0.0.1 Setting global variables and Libraries

```
[1]: # !pip install matplotlib

# !pip install numpy

# !pip install scipy

# !pip install gif

# !pip install seaborn

# !pip install pandas

# !pip install sklearn

# !pip install scikit-learn
```

```
[2]: # For plotting Gaussian contours
from utils.plotters import plot_gaussian_from_points
from utils.plotters import plot_gaussian_from_parameters
from utils.plotters import plot_samples
```

```
[3]: import numpy as np
from scipy.stats import t, describe as stat_describe
from sklearn.metrics import mean_squared_error
from scipy.stats import invgamma, invwishart, norm,multivariate_normal

import matplotlib.pyplot as plt
import pandas as pd
import seaborn as sns
import gif
from IPython.display import Image
```

```
[4]:  # Global Variables
R = 10 # Radius
S = 30 # Interval [0, S]
N = 100000 # samples
Range_value = 3
```

0.0.2 Problem

A large portion of the content of this course is concerned with computing high-dimensional integrals via simulation. Today you will be introduced to a simple-looking problem with a complicated closed-form solution and one we can approach using simulation.

Suppose you have a disc C_R of radius R. Take $p=(p_x,p_y)$ and $q=(q_x,q_y)\in C_R$ two points in the disk.

Consider the Euclidean distance between p and q, $||p-q|| = \sqrt{(p_x - q_x)^2 + (p_y - q_y)^2} = |p-q|$.

0.0.3 Problem A:

What is the average distance between pairs of points in C_R if they are picked uniformly at random?

0.0.4 Part I: nuts and bolts

• To start building intuition, let's solve a related but much simpler problem. Consider an interval [0, s], with s > 0 and take $x_1, x_2 \in [0, s]$ uniformly at random. Show that the average distance between x_1 and x_2 is s/3.

sol:

Let X a random variable uniformly distributed over [0, S], i.e., the probability density function of X is the following:

$$f_X(x) = \begin{cases} \frac{1}{S} & \text{if } x \in [0, S] \\ 0 & \text{otherwise.} \end{cases}$$
 (1)

Let us randomly pick two points in [0, S] independently. Let us denote those by X_1 and X_2 , which are random variables distributed according to f_X .

The distance between the two points is a new random variable $Y = |X_1 - X_2|$.

Hence, we want to find the expected value $\mathbb{E}(Y) = \mathbb{E}(|X_1 - X_2|)$. we can define a function g as follows:

$$g(x_1, x_2) = |x_1 - x_2| = \begin{cases} x_1 - x_2 & \text{if } x_1 \ge x_2 \\ x_2 - x_1 & \text{otherwise.} \end{cases}$$
 (2)

Besides, since the two points are picked independently, the joint probability density function is the product of the pdf's of X_1 and X_2 , i.e., $f_{X_1,X_2} = f_{X_1}(x_1)f_{X_2}(x_2) = \frac{1}{S^2}$.

Therefore, the expected value $\mathbb{E}(Y) = \mathbb{E}(g(X_1, X_2))$ is given by:

$$\mathbb{E}(Y) = \int_0^S \int_0^S g(x_1, x_2) f_{X_1, X_2}(x_1, x_2) \, dx_1 \, dx_2 \tag{3}$$

$$\mathbb{E}(Y) = \int_0^S \int_0^S |x_1 - x_2| \frac{1}{S^2} \, dx_1 \, dx_2 \tag{4}$$

$$\mathbb{E}(Y) = \frac{1}{S^2} \int_0^S \int_0^{x_1} (x_1 - x_2) \, dx_2 \, dx_1 + \frac{1}{S^2} \int_0^S \int_{x_1}^S (x_2 - x_1) \, dx_2 \, dx_1 \tag{5}$$

$$\mathbb{E}(Y) = \frac{1}{S^2} \frac{S^3}{6} + \frac{1}{S^2} \frac{S^3}{6} = \frac{S}{3} \tag{6}$$

sol: Numeric

```
[5]: distances_S = []
  errors_S = []
  exact_value_S = S/3

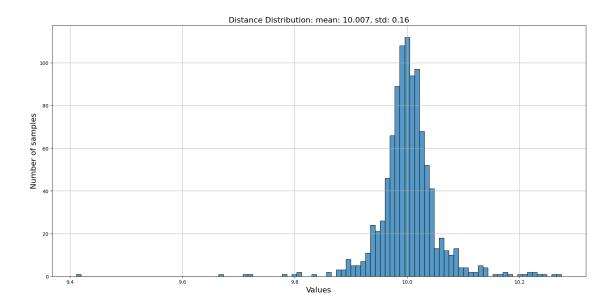
for n in range(1, N, 100):
    x = np.random.uniform(low=0, high=S, size=n)
    y = np.random.uniform(low=0, high=S, size=n)

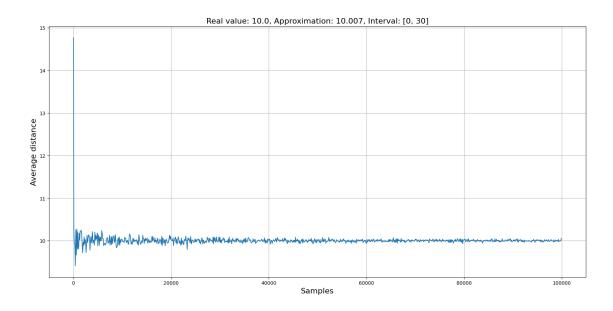
# computing the average
  distance = np.sum(abs(x-y))/n
  distances_S.append(distance)
  errors_S.append(exact_value_S - distance)

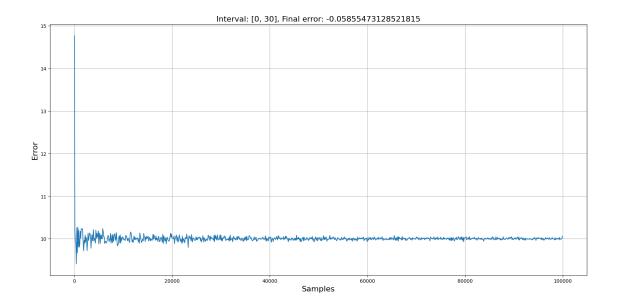
approximation_S = round(np.mean(distances_S), 3)
approximation_S
```

[5]: 10.007

```
[6]: data_plot = pd.DataFrame({"samples": range(1, N, 100), "avg_distance": u odistances_S})
```







• Show that Problem A is equivalent to computing

$$I = \frac{1}{\pi^2 R^4} \int_0^R \int_0^R \int_0^{2\pi} \int_0^{2\pi} \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos \phi(\theta_1, \theta_2)} r_1 r_2 \, d\theta_1 \, d\theta_2 \, dr_1 \, dr_2,$$

where $\phi(\theta_1,\theta_2)$ is the central angle between r_1 and r_2 .

Hint: Draw a picture.

sol:

From polar coordinates theory, in general any function f(x, y) with area A, we wan calculate the area as follows:

$$A = \iint\limits_{\mathbb{R}} f(x, y) \, dx \, dy \tag{7}$$

So, we can be rewrite that using polar coordinates as $f(r,\theta)$ using x as p and y as q:

$$A = \int_0^\theta \int_0^R f(r,\theta) r \, dr \, d\theta \tag{8}$$

So, lets transform to polars:

Let $p=(r_1\cos(\theta_1),r_1\sin(\theta_1))$ and $q=(r_2\cos(\theta_2),r_2\sin(\theta_2))$ where:

$$r_1 = \sqrt{p_x^2 + p_y^2}$$
 and $r_2 = \sqrt{q_x^2 + q_y^2}$

$$\begin{aligned} ||p-q|| &= \sqrt{(r_1^2\cos(\theta_1)^2 + r_2^2\cos(\theta_2)^2 - 2r_1r_2\cos(\theta_1)\cos(\theta_2)) + (r_1^2\sin(\theta_1)^2 + r_2^2\sin(\theta_2)^2 - 2r_1r_2\sin(\theta_1)\sin(\theta_2))} \\ ||p-q|| &= \sqrt{r_1^2 + r_2^2 - 2r_1r_2(\cos(\theta_1)\cos(\theta_2) + \sin(\theta_1)\sin(\theta_2))} \end{aligned}$$

$$||p-q|| = \sqrt{r_1^2 + r_2^2 - 2r_1r_2\cos(\theta_1 - \theta_2)}$$

So, remplacing results we have two points in \mathbb{R}^2 p and q using euclidean distance:

$$\iint\limits_{\mathbb{R}} ||x-y|| \, dx \, dy = \iint\limits_{r_1,\theta_1} \iint\limits_{r_2,\theta_2} \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\theta_1 - \theta_2)} \, r_1 \, r_2 \, d\theta_1 \, d\theta_2 \, dr_1 \, dr_2, \tag{9}$$

Where the factor r_1r_2 comes from the Jacobian.

Besides, our sampling methods tell us how to calculate the average or expectation as follows:

$$E[||x - y||] = \frac{\iint\limits_{\mathbb{R}} ||x - y|| \, dx \, dy}{\text{Total Area}} = \frac{\iint\limits_{r_1, \theta_1} \iint\limits_{r_2, \theta_2} \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\theta_1 - \theta_2)} \, r_1 \, r_2 \, d\theta_1 \, d\theta_2 \, dr_1 \, dr_2,}{\iint\limits_{r_1, \theta_1} \iint\limits_{r_2, \theta_2} dr_1 \, dr_2, \, d\theta_1 \, d\theta_2}$$

$$(10)$$

Where second term refers all possible points to take, so our final result is:

$$I = E[||x-y||] = \frac{1}{\pi^2 R^4} \iint\limits_{r_1,\theta_1} \iint\limits_{r_2,\theta_2} \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\theta_1 - \theta_2)} \, r_1 \, r_2 \, d\theta_1 \, d\theta_2 \, dr_1 \, dr_2, \tag{11}$$

• Compute I in closed-form.

Hint: Look up Crofton's mean value theorem or Crofton's formula.

sol:

We define a function f(R) as the *average distance* in a disc with radius R. From this, we note that f(R) is proportional to R this means that if we **decrease** the radius R, the *average distance* f(R) also **decrease**.

So, we can define f(R) = kR and if R = 1 we have f(1) = k = f'(R). In order to find k we need to calculate this term:

$$\lim_{\delta R \to 0} \frac{f(R) - f(R - \delta R)}{\delta R} \tag{12}$$

Define as the new distance after apply f() divided by the original distance δR : scaling factor.

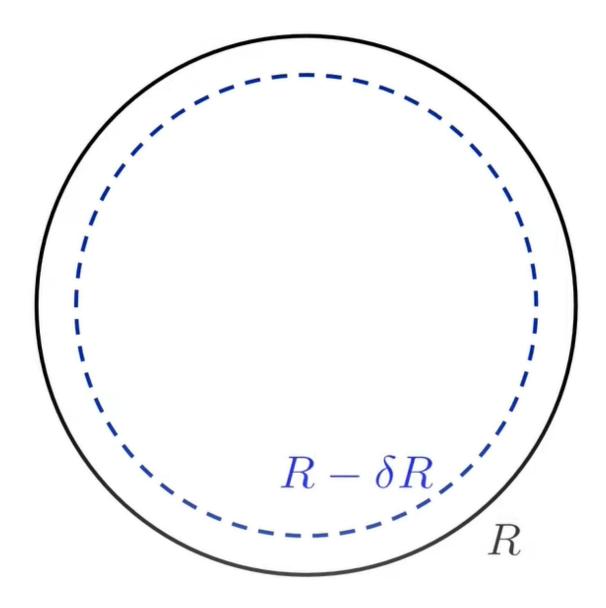
Note: We select the expression $f(R) - f(R - \delta R)$ instead of $f(R + \delta R) - f(R)$ because we want to evaluate the internal region (see Figure below).

```
[13]: from IPython.display import Image from IPython.core.display import HTML

Image(filename= "./images/circle_radius_R.png", height=100, width=100, u

embed=True)
```

[13]:



From Figure, we got 3 different situations: two points inside δR evaluated by f(), one point inside and one out evaluated by other function g(), and two out evaluated by other function h(). See Table to summary the idea:

Using the **Law of total Expectation** our final is the weighted avergae of $f(R) = \alpha \times f(R - \delta R) + \beta \times g(R - \delta R) + \gamma \times h(R, R - \delta R)$.

Let's define our probabilities such as:

$$P(\mathbb{1} \text{ point inside}) = \frac{\text{Area Inner disc } R - \delta R}{\text{Area disc } R} = \frac{\pi (R - \delta R)^2}{\pi R^2} = \frac{(R - \delta R)^2}{R^2}$$
(14)

$$P(1 \text{ point outside}) = 1 - \frac{(R - \delta R)^2}{R^2}$$
 (15)

Since we know that each point is an indepent event, we evaluate for each case defined in Table we have:

First case: Two points inside:

$$P(2 \text{ points inside}) = P(1 \text{ point inside}) \times P(1 \text{ point inside})$$
 (16)

$$P(\text{2 points inside}) = \frac{(R - \delta R)^2}{R^2} \times \frac{(R - \delta R)^2}{R^2}$$
 (17)

$$P(\text{2 points inside}) = \frac{R^4 - 4R^3(\delta R) + 6R^2(\delta R)^2 - 4R(\delta R)^3 + (\delta R)^4}{R^4} \tag{18}$$

$$P(2 \text{ points inside}) \approx 1 - \frac{4\delta R}{R} + o(\delta R)$$
 (19)

$$\alpha = 1 - \frac{4\delta R}{R} \tag{20}$$

Second case: One point inside and one outside:

$$P(1 \text{ point inside and } 1 \text{ point outside}) = P(1 \text{ point inside}) \times P(1 \text{ point outside})$$
 (21)

$$P(\mathbb{1} \text{ point inside and } \mathbb{1} \text{ point outside}) = \frac{(R - \delta R)^2}{R^2} \times (1 - \frac{(R - \delta R)^2}{R^2}) \tag{22}$$

$$P(1 \text{ point inside and } 1 \text{ point outside}) = \left(\frac{(R - \delta R)^2}{R^2} - \left(\frac{(R - \delta R)^2}{R^2}\right)^2\right)$$
 (23)

$$P(\mathbb{1} \text{ point inside and } \mathbb{1} \text{ point outside}) = 1 - 2\frac{\delta R}{R} + \frac{(\delta R)^2}{R^2} - (1 - \frac{4\delta R}{R} + o(\delta R)) \tag{24}$$

$$P(\mathbb{1} \text{ point inside and } \mathbb{1} \text{ point outside}) = 2\frac{\delta R}{R} + \frac{(\delta R)^2}{R^2} + o(\delta R)) \tag{25}$$

$$P(1 \text{ point inside and } 1 \text{ point outside}) \approx \frac{2\delta R}{R} + o(\delta R)$$
 (26)

But this happen twice, so we have:

$$P(1 \text{ point inside and } 1 \text{ point outside}) \approx \frac{4\delta R}{R} + o(\delta R)$$
 (27)

$$\beta = \frac{4\delta R}{R} \tag{28}$$

Third case: Two points outside

$$P(2 \text{ points outside}) = P(1 \text{ point outside}) \times P(1 \text{ point outside})$$
 (29)

$$P(\text{2 points outside}) = \left(1 - \frac{(R - \delta R)^2}{R^2}\right) \times \left(1 - \frac{(R - \delta R)^2}{R^2}\right) \tag{30}$$

$$P(2 \text{ points outside}) \approx 4 \frac{(\delta R)^2}{R^2} + o(\delta R) \approx 0$$
 (31)

$$\gamma = 0 \tag{32}$$

As you note, for powers of δR we assume 0, because in our limit $\delta R \to 0$.

Finally, we calculate our f(R) (eliminating all o(R)) as:

$$f(R) \approx (1 - \frac{4\delta R}{R}) \times f(R - \delta R) + \frac{4\delta R}{R} \times g(R, R - \delta R) \tag{33} \label{eq:33}$$

$$f(R) - f(R - \delta R) \approx -\frac{4\delta R}{R} \times f(R - \delta R) + \frac{4\delta R}{R} \times g(R, R - \delta R) \tag{34}$$

$$f(R) - f(R - \delta R) \approx \delta R \times \frac{4}{R} (g(R, R - \delta R) - f(R - \delta R)) \tag{35}$$

$$\frac{f(R) - f(R - \delta R)}{\delta R} \approx \frac{4}{R} (g(R, R - \delta R) - f(R - \delta R)) \tag{36} \label{eq:36}$$

This expression is similar to our derivate, so doing $\lim_{\delta R \to 0}$ we have:

$$f'(R) = \frac{4}{R}(g(R,R) - f(R)) \tag{37}$$

$$f'(R) = -\frac{4}{R}f(R) + \frac{4}{R}g(R,R)$$
 (38)

This is the Crofton's differential equation formula.

Finally, we need to calculate the value of the function g(R,R). Since we define a g() as the distance between one point inside and one outside, when $\delta R \to 0$ the second point $R - \delta R$ goes to the disc

contour (edge). This means to calculate the average distance between a random point inside the disc and the edge.

We can do this calculating the average distance ρ using polar coordinates:

$$g(R,R) = \text{Distance of random point inner to the edge}$$
 (39)

$$g(R,R) = \frac{1}{\pi R^2} \int_{-\pi/2}^{\pi/2} \int_0^{2R\cos(\theta)} \rho \, \rho \, d\rho \, d\theta \tag{40}$$

$$g(R,R) = \frac{32R}{9\pi} \tag{41}$$

Then, replacing in the Crofton's differential equation formula:

$$f'(R) = -\frac{4}{R}f(R) + \frac{4}{R}g(R,R)$$
 (42)

$$k = -\frac{4}{R}kR + \frac{4}{R}\frac{32R}{9\pi} \tag{43}$$

$$k = \frac{128}{45\pi} \tag{44}$$

Finally, we find that:

$$I = \frac{1}{\pi^2 R^4} \iint_{r_1,\theta_1} \iint_{r_2,\theta_2} \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\theta_1 - \theta_2)} \, r_1 \, r_2 \, d\theta_1 \, d\theta_2 \, dr_1 \, dr_2, \tag{45}$$

$$I = \frac{128R}{45\pi} \tag{46}$$

[10]: | 128*R/(45*np.pi)

[10]: 9.054147873672267

0.0.5 Part II – getting your hands dirty

Now we will move on to implementation.

Problem B:

Employ a simulation algorithm to approximate I. Provide point and interval estimates and give theoretical guarantees about them (consistency, coverage, etc).

• Represent I as $\int_{\mathcal{X}} \phi(x)\pi(x) dx$ and justify your choice of ϕ , π and \mathcal{X} . Recall that these choices are arbitrary up to a point, but they might lead to wildly different empirical performances and theoretical properties for estimators of I.

Justify your choices in light of the method you have been given to work with. Choose wisely and be rigorous in your justifications.

sol:

We start from $I = \int_{\mathcal{X}} f(x) dx = \int_{\mathcal{X}} \phi(x) \pi(x) dx$ where π is the probability density function on \mathcal{X} and:

$$\phi: x \to f(x)/\pi(x) \tag{47}$$

We need to think about our data:

- We have two points p and q within a circle, e.g. let p = (x,y) with $x^2 + y^2 \le R^2$.
- We want to simulate the average distance between them: ||p-q||
- We want to construct a good estimator for this experiment.
- We want to use polar coordinates (R,θ) to simulate them, where $R \geq \sqrt{x^2 + y^2}$ and $\theta = \arctan(x/y)$.

From this insights, we need to define the density function of R and θ :

$$f_{\Theta}(\theta) = \frac{1}{2\pi} \sim \mathcal{U}_{[0,2\pi]} \tag{48}$$

$$F_{\Theta}(\theta) = P_{\Theta}(\Theta < \theta) = \frac{\theta}{2\pi} \tag{49}$$

For θ we can pick any value from $[0, 2\pi]$ uniformly, in the case of the redius R, we kow that $0 < R < \infty$ and they are **independent**.

Since we know circumference of a disc ir $2\pi r$ and it grows linearly with r, let's say f(r) = Cr should be a probability density. Then, integrating f(r) over the interval [0, R] we have $F(r) = 1 = \frac{C}{2}R^2$. Just replacing and we get that $C = 2/R^2$. So:

$$f_R(r) = 2\frac{r}{R^2} \tag{50}$$

$$F_R(r) = P_R(R < r) = \frac{r^2}{R^2} \tag{51}$$

In order to simulate them, let's apply the inverse transformation for each, taking $u \sim \mathcal{U}_{[0,1]}$:

$$F_{\Theta}^{-1}(u) = 2\pi u \sim \mathcal{U}_{[0,2\pi]} \tag{52}$$

$$F_R^{-1}(u) = R\sqrt{u} \sim \mathcal{U}_{[0,R]} \tag{53}$$

So, let's construct a joined pdf $\pi(r,\theta)=f_{R,\Theta}(r,\theta)=f_R(r)f_{\Theta}(\theta)$ we have:

$$\pi(r,\theta) = \frac{2r}{R^2} \frac{1}{2\pi} \tag{54}$$

$$\pi(r,\theta) = \frac{r}{\pi R^2} \tag{55}$$

So, for the two points $p=(r_1\cos(\theta_1),r_1\sin(\theta_1))$ and $q=(r_2\cos(\theta_2),r_2\sin(\theta_2))$ we have

$$\pi(x_p, y_p) = \frac{1}{\pi R^2} r_1 \tag{56}$$

$$\pi(x_q, y_q) = \frac{1}{\pi R^2} r_2 \tag{57}$$

So, the points p and q can be chosen independently each one, we have:

$$P(||p-q||) = \pi(x_p, y_p) \times \pi(x_q, y_q) \tag{58}$$

$$P(||p-q||) = \frac{1}{\pi R^2} r_1 \times \frac{1}{\pi R^2} r_2 \tag{59}$$

$$P(||p-q||) = \frac{1}{\pi^2 R^4} r_1 r_2 \tag{60}$$

In summary, we have our f, ϕ , and π evaluated in our points p and q in polar coordinates:

$$f(p,q) = \frac{1}{\pi^2 R^4} \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\theta_1 - \theta_2)} r_1 r_2$$
(61)

$$\pi(p,q) = \frac{1}{\pi^2 R^4} r_1 r_2 \tag{62}$$

$$\phi(p,q) = \frac{f(p,q)}{\pi(p,q)} \tag{63}$$

$$\phi(p,q) = \sqrt{r_1^2 + r_2^2 - 2r_1r_2\cos(\theta_1 - \theta_2)}$$
 (64)

Finally, in order to simulate each point $\mathcal{X}_1, \mathcal{X}_2, \dots, \mathcal{X}_n$, each $\mathcal{X}_i = (r_i \cos(\theta_i), r_i \sin(\theta_i))$ where $r_i \in [0, R]$ and $\theta_i \in [0, 2\pi]$.

We will use the *uniform distribution* as follows:

- For each sample \mathcal{X}_i we define two numbers $u_1, u_2 \sim \mathcal{U}_{[0,1]}$
- Assign values to $r_i = R\sqrt{u_1}$ and $\theta_i = 2\pi u_2$
- We have $r_i \sim \mathcal{U}_{[0,R]}$ and $\theta_i \sim \mathcal{U}_{[0,2\pi]}$
- $\mathcal{X}_i = (r_i \cos(\theta_i), r_i \sin(\theta_i))$

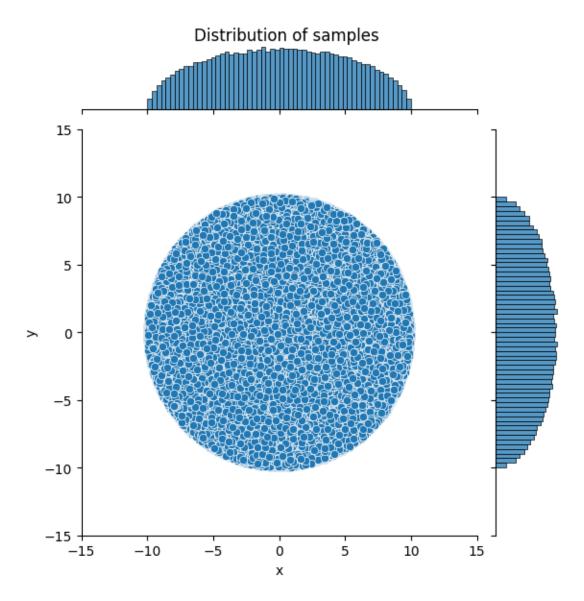
MonteCarlo example:

```
[11]: def polar_distance(r_1, theta_1, r_2, theta_2):
    return np.sqrt( r_1**2 + r_2**2 - 2*r_1*r_2*np.cos(theta_1 - theta_2) )
```

```
[12]: def polar_coordinates(n, R):
          theta_1 = 2*np.pi* np.random.uniform(low=0, high=1, size=n)
          r_1 = R* np.sqrt(np.random.uniform(low=0, high=1, size=n))
          theta_2 = 2*np.pi* np.random.uniform(low=0, high=1, size=n)
          r_2 = R* np.sqrt(np.random.uniform(low=0, high=1, size=n))
          return r_1, theta_1, r_2, theta_2
[13]: def sample_polar(n, R):
          theta_1 = 2*np.pi* np.random.uniform(low=0, high=1, size=n)
          r_1 = R* np.sqrt(np.random.uniform(low=0, high=1, size=n))
          return np.vstack((r_1*np.cos(theta_1), r_1*np.sin(theta_1))).T
[14]: distances_MC = []
      errors_MC = []
      exact_value_R = 128*R/(45*np.pi)
      X_MC = []
      Y_MC = []
      for n in range(1, N, 100):
          r_1, theta_1, r_2, theta_2 = polar_coordinates(n, R)
          distance = np.mean(polar_distance(r_1, theta_1, r_2, theta_2))
          X_MC.append(r_1*np.cos(theta_1))
          Y_MC.append(r_1*np.sin(theta_1))
          distances_MC.append(distance)
          errors_MC.append(exact_value_R - distance)
      approximation_MC = np.mean(distances_MC)
      approximation_MC
[14]: 9.049445578953408
[15]: data_points = pd.DataFrame({"x": X_MC[-1], "y": Y_MC[-1]})
[16]: sns_fig = sns.jointplot(data=data_points,
                              x="x",
                              v = "v".
      #
                               kind='hex'
      sns_fig.fig.suptitle("Distribution of samples")
```

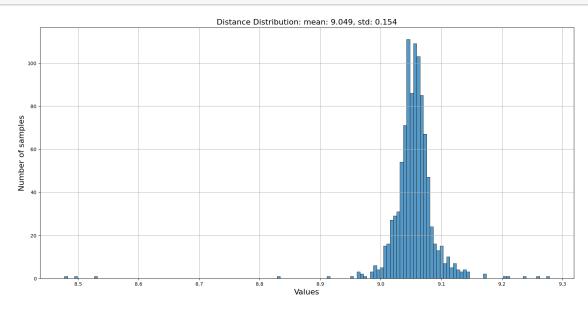
```
sns_fig.fig.tight_layout()
sns_fig.fig.subplots_adjust(top=0.95) # Reduce plot to make room
sns_fig.ax_marg_x.set_xlim(-1.5*R, 1.5*R)
sns_fig.ax_marg_y.set_ylim(-1.5*R, 1.5*R)
# sns_fig.fig.set_figwidth(8)
# sns_fig.fig.set_figheight(16)
```

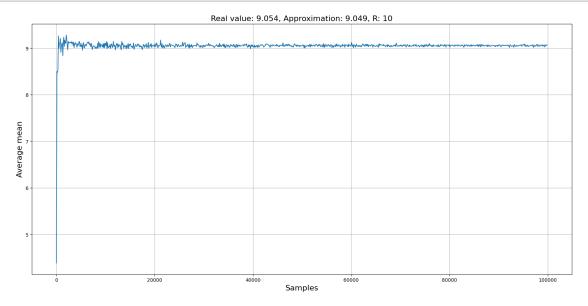
[16]: (-15.0, 15.0)



```
[17]: data_plot = pd.DataFrame({"samples": range(1, N, 100), "avg_distance": ___

¬distances_MC})
[18]: _, ax = plt.subplots(figsize=(16,8),sharex=True, sharey=False,__
       ⇔constrained_layout=True)
      sns.
       Shistplot(data=data_plot[(data_plot["avg_distance"]>=exact_value_R-Range_value)_⊔
       →& (data_plot["avg_distance"] <= exact_value_R+Range_value)],
                   x="avg distance",
                   ax=ax )
      # sns fiq = sns.
       \hookrightarrow displot(data=data\_plot[(data\_plot["avg\_distance"]>=exact\_value\_R-Range\_value)_{\sqcup})
       ⇔& (data_plot["avg_distance"] <= exact_value_R+Range_value)],
                                x="avq_distance",
      #
                               kde=True)
      ax.yaxis.grid(True)
      ax.xaxis.grid(True)
      ax.set_title(f"Distance Distribution: mean: {round(approximation_MC, 3)}, std:__
       →{round(np.std(distances_MC), 3)}", fontsize=16)
      ax.set_xlabel('Values', fontsize=16)
      ax.set_ylabel(f"Number of samples", fontsize=16)
      plt.show()
```

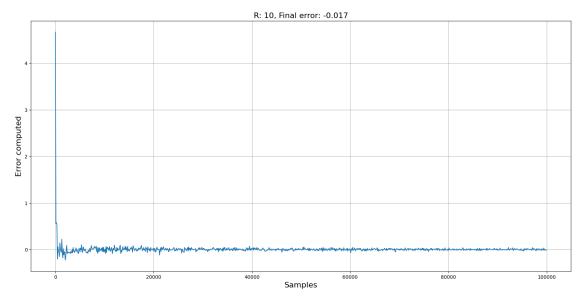




```
ax.yaxis.grid(True)
ax.xaxis.grid(True)

ax.set_title(f"R: {R}, Final error: {round(errors_MC[-1], 3)}", fontsize=16)
ax.set_xlabel('Samples', fontsize=16)
ax.set_ylabel(f"Error computed", fontsize=16)

plt.show()
```



• Again, starting from the eventual samples you will obtain with your method, construct a nonempty family of estimators of *I* and discuss whether it is (strongly) consistent and whether a central limit theorem can be established.

sol:

We want to estimate ϕ by **Gibbs Sampling**. So, in order to sample using Gibbs, we need to sample from a conditional distribution than to marginalize by integrating over a joint distribution.

Suppose we want to obtain k samples of $\mathbf{X}=(x_1,\dots,x_n)$ from a joint distribution $p(x_1,\dots,x_n)$.

Denote the i-th sample by $\mathbf{X}^{(i)} = (x_1^{(i)}, \dots, x_n^{(i)})$. We proceed as follows:

- We begin with some initial value $\mathbf{X}^{(0)}$.
- We want the next sample $\mathbf{X}^{(i+1)} = \left(x_1^{(i+1)}, x_2^{(i+1)}, \dots, x_n^{(i+1)}\right)$ which is a vector, we sample each component of the vector, $x_j^{(i+1)}$, from the distribution of that component conditioned on all other components sampled so far.

But there is a catch: we condition $\mathbf{X}^{(i+1)}$ s components up to $x_{j-1}^{(i+1)}$, and thereafter condition on $\mathbf{X}^{(i)}$, starting from $x_{j+1}^{(i)}$ to x_n^i .

To achieve this, we sample the components in order, starting from the first component.

More formally, to sample $x_{j+1}^{(i)}$, we update it according to the distribution specified by $p(x_j^{(i+1)}|x_1^{(i+1)},\dots,x_{j-1}^{(i+1)},x_{j+1}^{(i)},\dots,x_n^{(i)}).$ We have to evaluate that the (j+1)th component had the ith sample, not the (i+1) sample.

• Repeat the above step k times.

Since we are working in 2-dimensional vectors, we will have each x_i depending on $r_i \sim \mathcal{U}_{[0,R]}$ and $\theta_i \sim \mathcal{U}_{[0,2\pi]}$. So we need to generate our first point $x = (r_i \cos(\theta_i), r_i \sin(\theta_i)) = (x_1^0, x_2^0)$. We define our join probability $p(x_1^0, x_2^0)$ and proceed to calculate next iterations:

$$x_1^1 \sim p(x_1|x_2^0) \tag{65}$$

$$x_2^1 \sim p(x_2|x_1^1) \tag{66}$$

$$x_m^k \sim p(x_m | x_{m=1,2}^{k-1}) \tag{68}$$

In general, in 2-D case we have:

$$p(x_1|x_2) \sim \mathcal{N}(\mu_0 + \frac{\Sigma_{01}}{\Sigma_{11}}(x_1 - \mu_1), \ \Sigma_{00} - \frac{\Sigma_{01}^2}{\Sigma_{11}}) \eqno(69)$$

$$p(x_2|x_1) \sim \mathcal{N}(\mu_1 + \frac{\Sigma_{01}}{\Sigma_{00}}(x_0 - \mu_0), \, \Sigma_{11} - \frac{\Sigma_{01}^2}{\Sigma_{00}}) \tag{70}$$

```
[21]: # Define the posterior for the mean, conditional on the covariance matrix and
     def mult_normal_dist(data, cov):
         return np.random.multivariate_normal(mean = (np.mean(data, axis=0)), cov_
       ⇔=cov/np.size(data, 0))
     # Define the posterior for the covariance matrix, conditional on the mean and
      \hookrightarrow data
     def inv_wishart_dist(data, mean):
         return invwishart.rvs(df = np.size(data, 0), scale = np.matmul(np.
```

In general, we will generate a distribution using a 2-D Gaussian to generate points, first qe calculate the mean μ , variances, and cov of our "original" distribution:

$$P \sim \mathcal{N}(\mu, \Sigma) \tag{71}$$

$$\mu = \begin{bmatrix} \mu_0 \\ \mu_1 \end{bmatrix} \tag{72}$$

$$\Sigma = \begin{bmatrix} \Sigma_{00} & \Sigma_{01} \\ \Sigma_{10} & \Sigma_{11} \end{bmatrix} \tag{73}$$

```
[22]: def gibbs_sampler(R, num_iterations, data, create_gif=False):
          # Starting point, random point inside circle
          mean = sample_polar(1, R)[0]
          cov = np.cov(data.T)
          # How many iterations to sample
          frames = [] # for GIF
          means = list()
          covs = list()
          stds = list()
          cov 1 = list()
          means.append(mean)
          samples = np.zeros([num_iterations+1, 2]) # sampled points
          samples[0] += mean
          tmp_points = np.zeros([num_iterations, 2]) # inbetween points
          # Iteratively sample
          for i in range(0,num_iterations):
              tmp_points[i] += np.random.multivariate_normal(mean, cov, size=1)[0]
              if(create_gif):
                  frames.append(plot_samples(samples, i+1, tmp_points, i+1, mean, ___

cov, title="Num Samples: " + str(i)))
              # Sample the variance conditional on the previous mean and data
              cov = inv_wishart_dist(data, mean)
              covs.append(cov)
              stds.append([cov[0,0], cov[1,1]])
              cov_l.append(cov[1,0])
              # Sample the mean conditional on the previous mean and data
              mean = mult_normal_dist(data, cov)
              means.append(mean)
              # new point
              samples[i+1] += np.random.multivariate_normal(mean, cov, size=1)[0]
              if(create gif):
                  frames.append(plot_samples(samples, i+2, tmp_points, i+1, mean,__
       ⇔cov, title="Num Samples: " + str(i+1)))
```

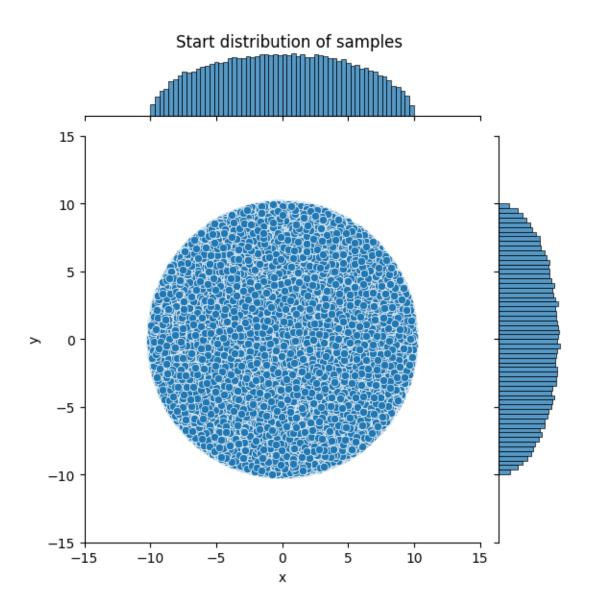
```
return np.array(means), covs, np.array(stds), cov_l, frames
```

We need to generate each initial point $x_i^{(0)} = (r_i \cos(\theta_i), r_i \sin(\theta_i))$, from them we take the mean μ and the variance to generate a Normal distribution.

In addition, we need to calculate estimated mean and variance from our expected data.

```
[23]: original_dist = sample_polar(N, R)
      original_mean = np.mean(original_dist, axis=0)
      original_cov = np.cov(original_dist.T)
      print("True mean: ", np.around(original_mean, decimals=5), "\nTrue CoV:\n", np.
       →around(original_cov, decimals=5))
     True mean: [-0.01294 -0.0202]
     True CoV:
      [[24.98043 -0.11021]
      [-0.11021 24.91393]]
[24]: data_points = pd.DataFrame({"x": original_dist[:,0], "y": original_dist[:,1]})
      sns_fig = sns.jointplot(data=data_points,
                              x = "x"
                              y="y",
      #
                               kind='hex'
      sns_fig.fig.suptitle("Start distribution of samples")
      sns_fig.fig.tight_layout()
      sns_fig.fig.subplots_adjust(top=0.95) # Reduce plot to make room
      sns_fig.ax_marg_x.set_xlim(-1.5*R, 1.5*R)
      sns_fig.ax_marg_y.set_ylim(-1.5*R, 1.5*R)
      # sns_fiq.fiq.set_fiqwidth(8)
      # sns_fig.fig.set_figheight(16)
```

[24]: (-15.0, 15.0)

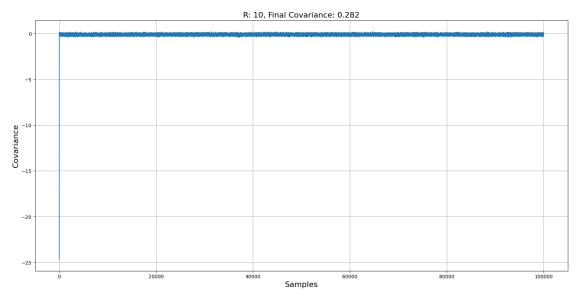


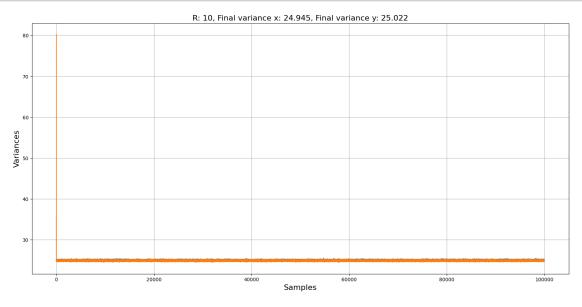
```
ax.yaxis.grid(True)
ax.xaxis.grid(True)

ax.set_title(f"R: {R}, Final Covariance: {abs(round(cov_l[-1], 3))}",
fontsize=16)
ax.set_xlabel('Samples', fontsize=16)
ax.set_ylabel(f"Covariance", fontsize=16)

# ax.set_ylim(-1, 1)
# sns_fig.ax_marg_y.set_ylim(-1.5*R, 1.5*R)

plt.show()
```





Let's see our new sampler:

True mean: [-0.01294 -0.0202]
True CoV:

```
[[24.98043 -0.11021]

[-0.11021 24.91393]]

Estimated mean: [ 0.00744 -0.01065]

Estimated CoV:

[[25.13685 -0.34158]

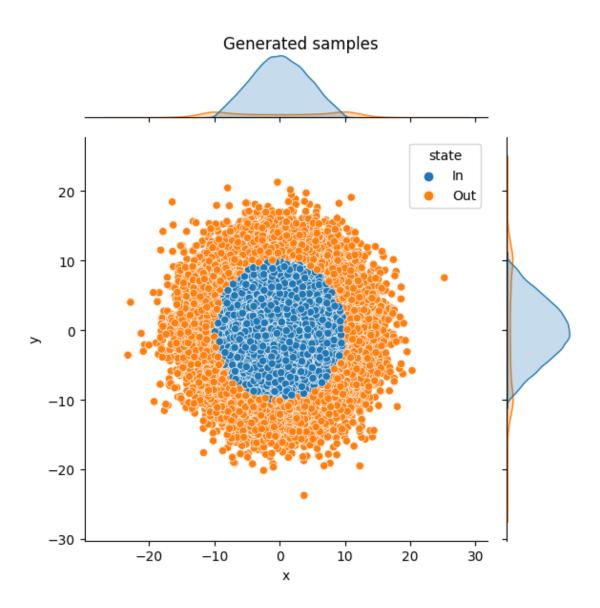
[-0.34158 25.15501]]
```

• Detail a suite of diagnostics that might be employed in your application to detect convergence or performance problems. Extra points for those who design algorithms that exploit the structure of this particular integration problem.

sol:

We show our new data sample. We saw that we obtained samples greater than the radius R = 10, but the distribution of them is close to zero.

```
[30]: data points = pd.DataFrame({"x": samples[:,0], "y": samples[:,1]})
      data_points["state"] = data_points.apply(lambda row: "Out" if row["x"]**2 +__
       →row["y"]**2>100 else "In", axis=1)
      pal = sns.color_palette(n_colors=2)
      sns_fig = sns.jointplot(data=data_points,
                              x = "x"
                              y="y",
                              hue='state',
                              hue_order=['In', 'Out'],
                              palette=pal,
                             )
      sns_fig.fig.suptitle("Generated samples")
      sns_fig.fig.tight_layout()
      sns_fig.fig.subplots_adjust(top=0.95) # Reduce plot to make room
      # sns fig.ax marg x.set xlim(-1.5*R, 1.5*R)
      \# sns_fig.ax_marg_y.set_ylim(-1.5*R, 1.5*R)
      # sns_fig.fig.set_figwidth(8)
      # sns_fig.fig.set_figheight(16)
```



```
# truncate=False,
# ax=sns_fig.ax_joint)

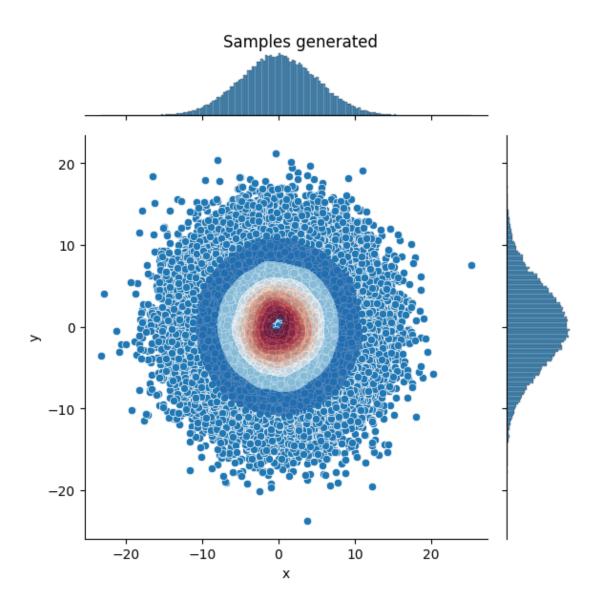
# we select CI: [0.8, 0.85, 0.9, 0.95, 0.99]
sns_fig.plot_joint(sns.kdeplot, cmap="RdBu_r", alpha=0.75, levels = [0.1, 0.3, 0.5, 0.6, 0.7, 0.8, 0.85, 0.9, 0.95, 0.99], fill=True)

#sns_fig.plot_marginals(sns.rugplot, color="r", height=-.15, clip_on=False)

sns_fig.fig.suptitle("Samples generated")
sns_fig.fig.tight_layout()
sns_fig.fig.subplots_adjust(top=0.95) # Reduce plot to make room

# sns_fig.ax_marg_x.set_xlim(-1.5*R, 1.5*R)
# sns_fig.ax_marg_y.set_ylim(-1.5*R, 1.5*R)

# sns_fig.fig.set_figwidth(8)
# sns_fig.fig.set_figwidth(16)
```



Let's see the average distance calculated by our gibbs sampler:

```
[32]: distances_Gibbs = []
errors_Gibbs = []
exact_value_R = 128*R/(45*np.pi)
X_Gibbs = []
Y_Gibbs = []

for n in range(1, N, 100):

    x_1 = np.random.multivariate_normal(sample_mean, sample_cov, size=n)
    x_2 = np.random.multivariate_normal(sample_mean, sample_cov, size=n)
```

```
distance = np.mean(np.linalg.norm(x_1 - x_2, axis=1))
X_Gibbs.append(x_1)
Y_Gibbs.append(x_2)

distances_Gibbs.append(distance)
errors_Gibbs.append(exact_value_R - distance)

approximation_Gibbs = np.mean(distances_Gibbs)
approximation_Gibbs
```

[32]: 8.897217358158036

Now, Let's calculate the CI for this data:

Confidence Interval 95%: in order to calculate this CI we need to apply:

- Let m the average of samples.
- Let N number of samples.
- Let s the standard deviation of samples.

So, we have:

$$CI = (m - t_c \frac{s}{\sqrt{N}}, m + t_c \frac{s}{\sqrt{N}})$$
 (74)

where t_c is the Student- distribution approximated (based on the CLT). This value is calculate as follows for any confidence c:

$$t_c = |I_{N-1}(\frac{1-c}{2})| \tag{75}$$

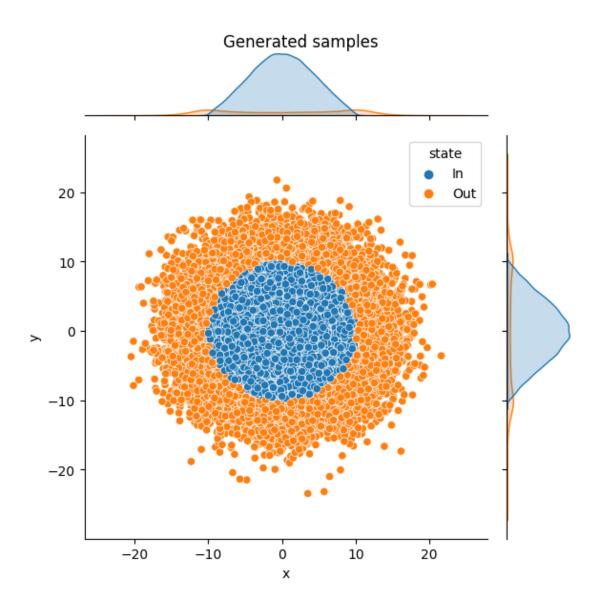
• I_{N-1} is the Student's inverse distribution.

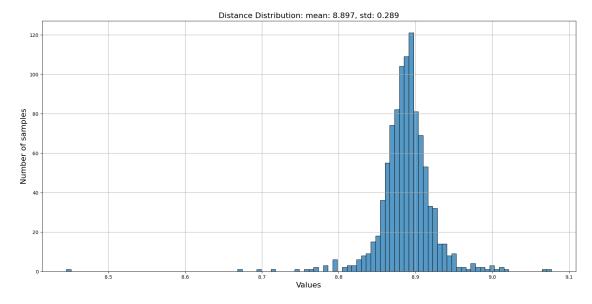
```
[33]: confidence = 0.95
```

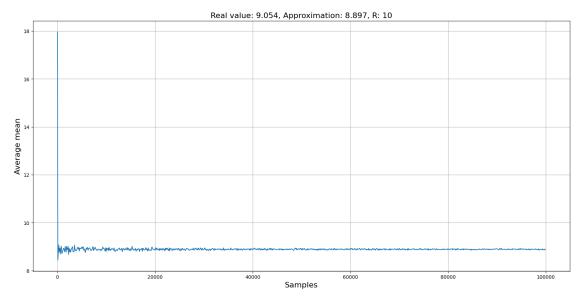
[34]: 1.9599877077718446

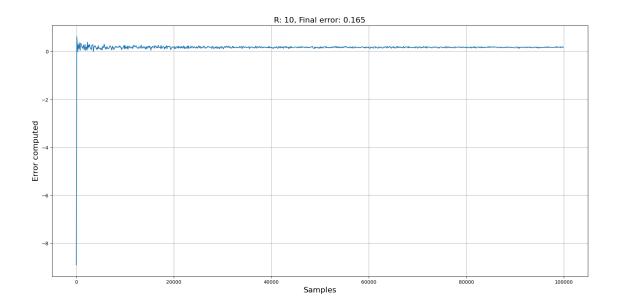
[36]: (8.866137020825409, 8.928297695490663)

```
[37]: data_points = pd.DataFrame({"x": X_Gibbs[-1][:,0], "y": X_Gibbs[-1][:,1]})
      data_points["state"] = data_points.apply(lambda row: "Out" if row["x"]**2 +__
       ⇔row["y"]**2>100 else "In", axis=1)
      pal = sns.color_palette(n_colors=2)
      sns_fig = sns.jointplot(data=data_points,
                              x="x",
                              y="y",
                              hue='state',
                              hue_order=['In', 'Out'],
                              palette=pal,
      sns_fig.fig.suptitle("Generated samples")
      sns_fig.fig.tight_layout()
      sns_fig.fig.subplots_adjust(top=0.95) # Reduce plot to make room
      \# sns\_fig.ax\_marg\_x.set\_xlim(-1.5*R, 1.5*R)
      \# sns\_fig.ax\_marg\_y.set\_ylim(-1.5*R, 1.5*R)
      # sns_fig.fig.set_figwidth(8)
      # sns_fig.fig.set_figheight(16)
```









We note that our gibbs sampler works fine, a little noise generated by the values far from the original disk with radius R (but it doesn't impact too much).

• For each $R \in \{0.01, 0.1, 1, 10, 100, 1000, 10000\}$, perform M = 500 runs from your simulation method and compute: (i) variance (ii) bias (iii) standard deviation of the mean (MCSE).

sol:

```
[42]: R_list = [0.01, 0.1, 1, 10, 100, 1000, 10000]
      M = 500
      N = 10000
      for current_R in R_list:
          mean_list = []
          cov_list = []
          var_list = []
          mcse_list = []
          bias_list = []
          for _ in range(M): # 500 runs for each case
              current_dist = sample_polar(N, current_R) # generating N samples
              current_mean = np.mean(current_dist, axis=0)
              current_cov = np.cov(current_dist.T)
              # N numbers sampling with gibbs
              means, covs, varis, cov_l, frames = gibbs_sampler(current_R, N,__

current_dist, create_gif=False)

              mean_list.append(means[-1])
              cov_list.append(cov_l[-1])
              var_list.append(varis[-1])
```

```
current_samples = np.random.multivariate_normal(means[-1], covs[-1],
⇔size=N)
      # calculating RMSE
     mse = mean squared error(current dist, current samples)
     mcse_list.append(mse)
     bias = np.mean(current_dist - current_samples)
     bias list.append(bias)
     if _==0:
        Ш
oprint("######################")
         print("Current R:", current_R)
         print("True mean: ", np.around(current_mean, decimals=5), "\nTrue_\]
print("Estimated mean: ", np.around(means[-1], decimals=5),

¬"\nEstimated CoV:\n", np.around(covs[-1], decimals=5))

  print("Variance:", np.around(np.mean(np.array(var_list), axis=0), 3))
  print("means:", np.around(np.mean(np.array(mean list), axis=0), 3))
  print("MCSE:", np.around(np.mean(mcse_list), 3))
  print("Bias:", np.around(np.mean(bias list), 3))
```



```
Current R: 0.01
True mean: [-2.e-05 \quad 1.e-05]
True CoV:
[[2.e-05 0.e+00]
[0.e+00 3.e-05]]
Estimated mean: [3.e-05 4.e-05]
Estimated CoV:
[[2.e-05 0.e+00]
[0.e+00 3.e-05]]
Variance: [0. 0.]
means: [0. 0.]
MCSE: 0.0
Bias: 0.0
Current R: 0.1
True mean: [0.00068 0.00044]
True CoV:
[[ 2.49e-03 -4.00e-05]
[-4.00e-05 2.51e-03]]
Estimated mean: [0.00023 0.00077]
Estimated CoV:
[[ 2.50e-03 -4.00e-05]
[-4.00e-05 2.52e-03]]
```

```
Variance: [0.003 0.002]
means: [ 0. -0.]
MCSE: 0.005
Bias: 0.0
Current R: 1
True mean: [-0.00104 -0.0023 ]
True CoV:
[[ 2.4812e-01 -2.2000e-04]
[-2.2000e-04 2.4961e-01]]
Estimated mean: [-0.00986 -0.00132]
Estimated CoV:
[[ 0.25052 -0.00078]
[-0.00078 0.25179]]
Variance: [0.25 0.25]
means: [-0. 0.]
MCSE: 0.5
Bias: 0.0
Current R: 10
True mean: [-0.00343 0.01858]
True CoV:
[[24.64383 0.11291]
[ 0.11291 25.02534]]
Estimated mean: [0.03362 0.00675]
Estimated CoV:
[[25.53651 -0.11972]
[-0.11972 25.01003]]
Variance: [25.032 24.994]
means: [-0.002 0.002]
MCSE: 50.03
Bias: -0.001
Current R: 100
True mean: [ 0.61435 -0.3165 ]
True CoV:
[[2535.04964 5.90567]
   5.90567 2447.41525]]
Estimated mean: [-0.03807 -0.01167]
Estimated CoV:
[[2570.86621 37.27125]
[ 37.27125 2413.49281]]
Variance: [2500.857 2499.677]
means: [ 0.025 -0.058]
MCSE: 4997.819
Bias: 0.011
```

Current R: 1000

36

```
[7.07353 5.8394 ]
True mean:
True CoV:
[[247871.5533
                1788.93049]
[ 1788.93049 247873.74592]]
               [-3.25729 5.26557]
Estimated mean:
Estimated CoV:
[[246533.35045
                6499.80157]
[ 6499.80157 248071.91842]]
Variance: [250546.114 249983.715]
means: [0.103 0.06]
MCSE: 500090.006
Bias: 0.046
Current R: 10000
True mean: [-5.40704 67.95237]
True CoV:
[[24371561.68248
                  132627.06779]
[ 132627.06779 24970727.9736 ]]
Estimated mean: [-18.93856 49.85618]
Estimated CoV:
[[23576569.30895 -134055.31041]
 [ -134055.31041 24789418.27512]]
Variance: [25029254.025 25001708.963]
means: [3.109 1.348]
MCSE: 50046242.315
Bias: -2.805
```

• Can you identify one key quantity missing from the previous item?

Hint: it bears relevance to the real world application of any computational method. estimator.

sol:

I gues some diagnostic of convergence methods such as **burn-in**.

From results, we saw that for a very large radius value the error and bias increase.

In the other hand, radius lower than 100 tends to be more easy to find an estimator.

Finally, we saw the **bias-variance trade-off**, this means that we can achieve a low bias but in contrast we got a high variance which increase the mse also.