Sheet 1

In [1]:
```
# imports
import random
import math
import matplotlib.pyplot as plt
```

Exercise 1: Random number generators

(a) Generate 100000 uniformly distributed random numbers between 0 and 1 and save the output.

In [2]:
```
xs = [random.random() for _ in range(100000)]
```

(b) Write a program which calculates the average value, the variance and the error of the mean of given data and use it to evaluate the random numbers generated in (a)

In [3]:
```
def mean(xs):
    x_mean = 0.0
    for x in xs:
        x_mean += x
    x_mean /= len(xs)
    return x_mean

def var(xs):
    x_var = 0.0
    x_mean = mean(xs)
    for x in xs:
        x_var += (x - x_mean)**2
    x_err = math.sqrt(x_var / len(xs))
    return x_var, x_err
```

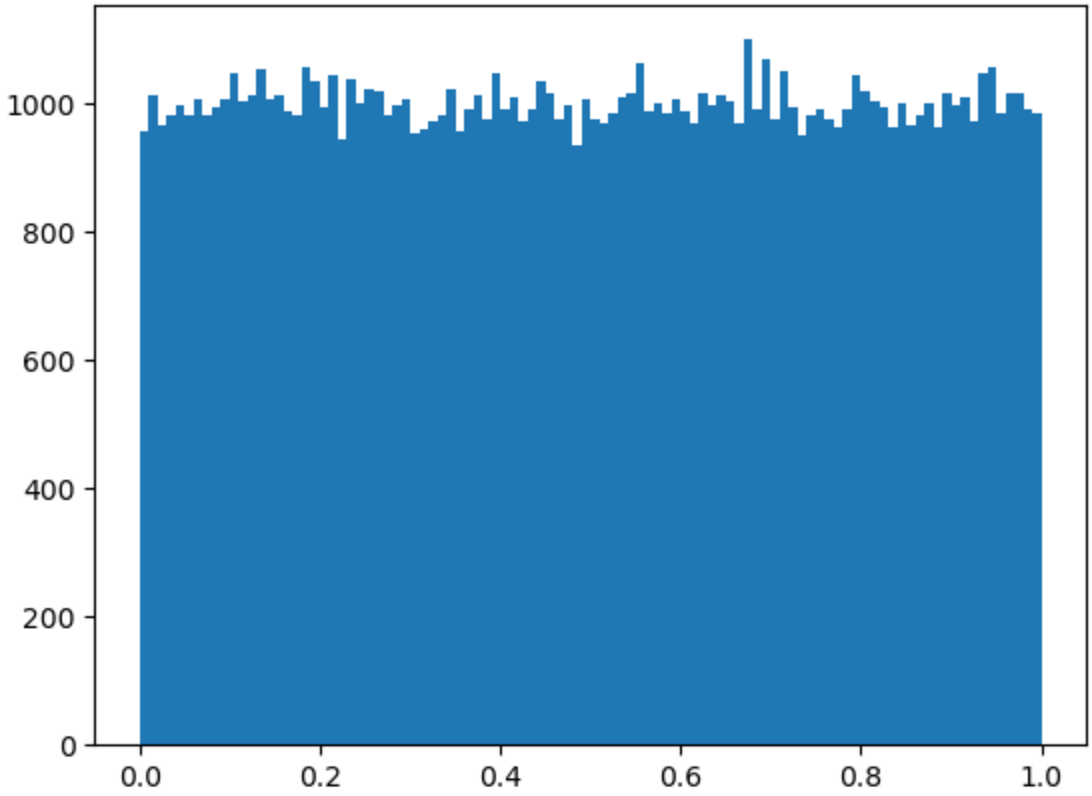
In [4]:
```
x_mean = mean(xs)
x_var, x_err = var(xs)

x_mean, x_var, x_err
```

Out[4]:
```
(0.5000713557629796, 8337.363174492417, 0.2887449250548383)
```

(c) Uniformity Test: Create a histogram of the data with 100 bins and plot it.

In [5]:
```
plt.hist(xs, bins=100)
plt.plot()
```

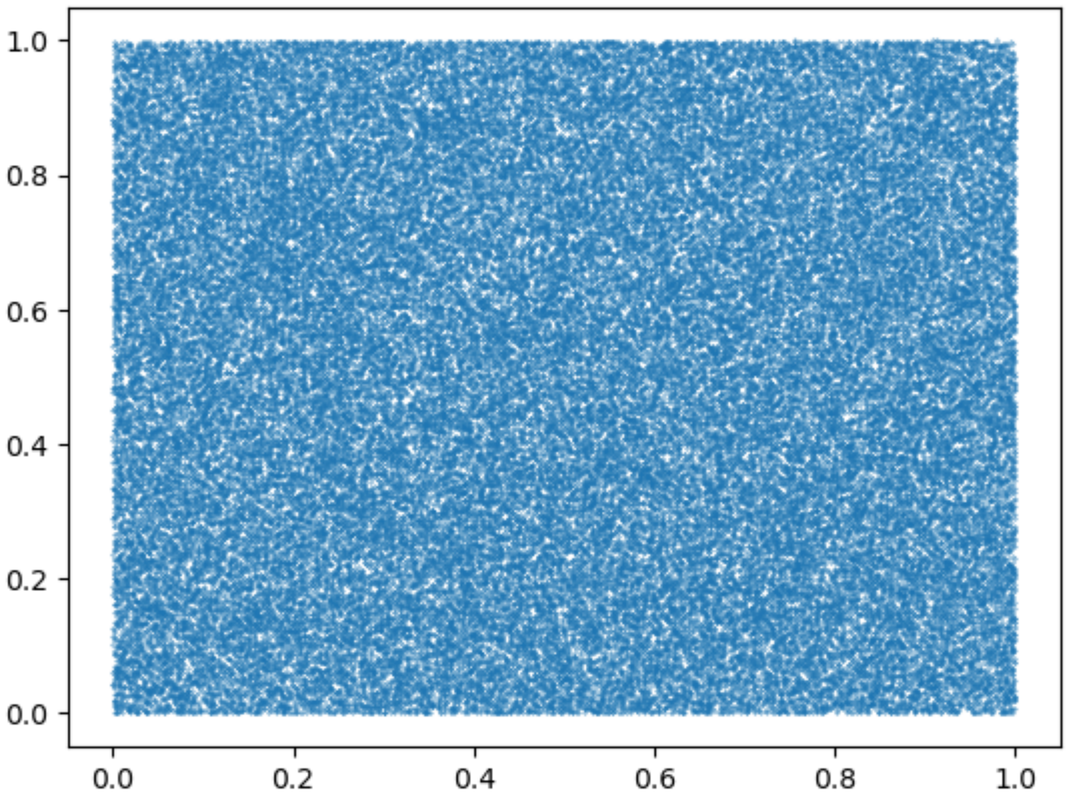
Out[5]:
```
[]
```



(d) Screen Pixel Test

In [6]:
```
xs = [random.random() for _ in range(100000)]
ys = [random.random() for _ in range(100000)]

plt.scatter(xs, ys, 0.1)
plt.plot()
```

Out[6]: []

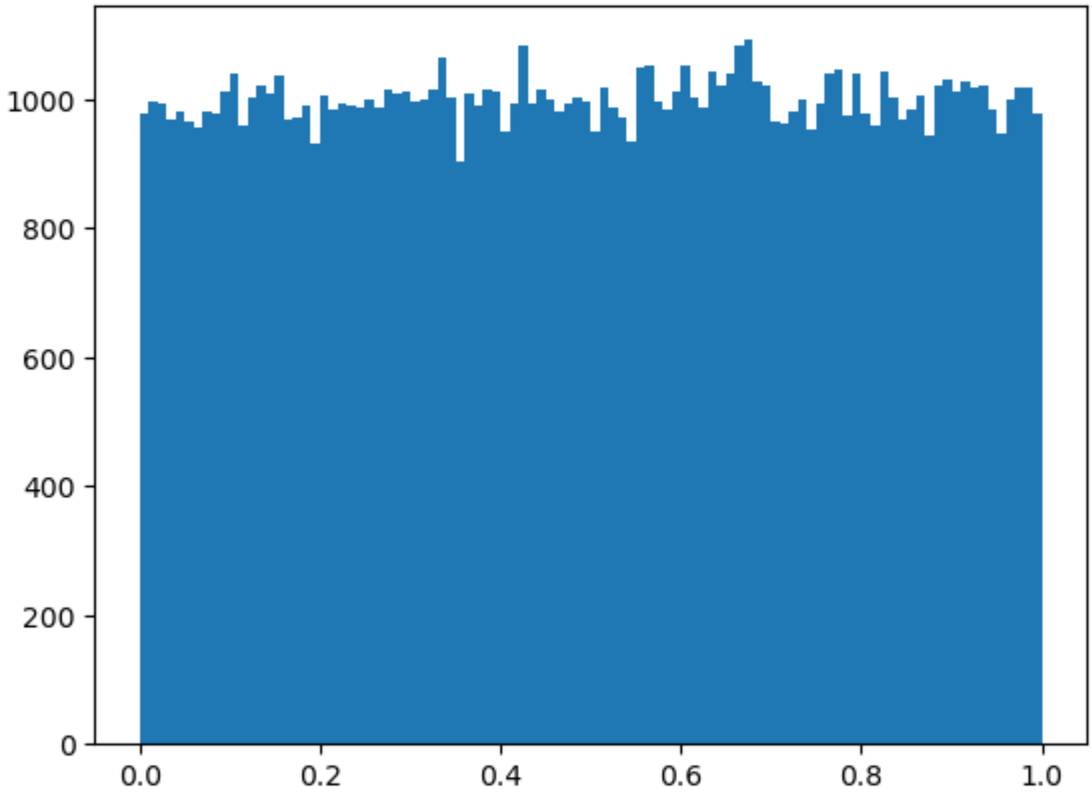


(e) Program your own linear congruential random number generator

In [25]:
```
class MyPRNG:
    def __init__(self, seed = 0):
        self.seed = seed
        self.x_ = seed

    def random(self):
        a = 1664525
        b = 1013904223
        m = 2**32
        x = ((a * self.x_ + b) % m)
        self.x_ = x
        return x / 2**32
```

In [26]:
```
prng = MyPRNG()
xs = [prng.random() for i in range(100000)]
plt.hist(xs, bins=100)
plt.plot()
```

Out[26]: []



Exercise 2: Your first Monte Carlo Simulation

In [33]:
```
n = 1000000

hit = 0
for i in range(n):
    x, y = random.random(), random.random()
    hit += 1 if (x*x + y*y < 1) else 0
pi = 4 * hit / n
pi
```

Out[33]: 3.141644

Exercise 3: Metropolis Criterion

(a)

The Metropolis Criterion states $w_{ij} = min(1, \frac{P_j}{P_i})$. With the Boltzmann Distribution P_i this results in $w_{ij} = min(1, e^{-\beta \Delta E})$.

$\Delta E_{ij} < 0$ results in $w_{ij} = min(1, e^{-\beta \Delta E}) = e^{-\beta \Delta E}$. Additionally $\Delta E_{ij} = -\Delta E_{ji}$ leads to $w_{ji} = min(1, e^{-\beta \Delta E_{ji}}) = 1$ and thus:

$$\frac{\omega_{ij}}{\omega_{ji}} = \frac{e^{-\beta \Delta E_{ij}}}{1} = e^{-\beta \Delta E_{ij}} \tag{1}$$

resulting in ***detailed balance***.

$\Delta E > 0$ results in $w_{ij} = min(1, e^{-\beta \Delta E_{ij}}) = 1$ and $w_{ji} = min(1, e^{-\beta \Delta E_{ji}}) = e^{-\beta \Delta E_{ji}}$ thus:

$$\frac{\omega_{ij}}{\omega_{ji}} = \frac{1}{e^{-\beta \Delta E_{ji}}} = e^{-\beta \Delta E_{ij}} \tag{2}$$

resulting in ***detailed balance***.

□

(b)

$$\begin{gathered} \text{With } \Delta E_{ij} = -\Delta E_{ji} \text{ and} \\ \omega_{ij} = \frac{e^{-\beta \Delta E_{ij}}}{e^{-\beta \Delta E_{ij}} + 1} = \frac{1}{e^{\beta \Delta E_{ij}} + 1} \text{ then:} \\ \frac{\omega_{ij}}{\omega_{ji}} = \frac{e^{-\beta \Delta E_{ij}} + 1}{e^{\beta \Delta E_{ij}} + 1} = e^{-\beta \Delta E_{ij}} \end{gathered} \tag{3}$$

□

(c)

Let the energy difference with be the pair potential $\Delta E_{ij} = V_{ij} = V(\mathbf{r}_i, \mathbf{r}_j)$.

For the Metropolis Criterion we then get:

$$w_{ij} = min(1, e^{-\beta \Delta E}) = min(1, e^{-\beta V_{ij}}) = \begin{cases} 1, & \|\mathbf{r}_{ij}\| \geq \sigma \\ 0, & \|\mathbf{r}_{ij}\| < \sigma \end{cases} \tag{4}$$

Heat bath:

$$w_{ij} = min(1, e^{-\beta \Delta E}) = \frac{e^{-\beta V_{ij}}}{e^{-\beta V_{ij}} + 1} = \begin{cases} 0.5, & \|\mathbf{r}_{ij}\| \geq \sigma \\ 0, & \|\mathbf{r}_{ij}\| < \sigma \end{cases} \tag{5}$$

Exercise 4: Ising model

(a) At low temperatures stable areas form. With the increase of temperature these areas diffuse into noise. This phase transition occurs at approximately $T = 2.5$. For the phase transition the Wolff Algorithm seems appropriate due to critical slowing down while Metropolis is better outside of this "transition zone".

(b)

1. select random cell c
2. calculate energy $E_i = H_i = -J \sum_{j,k \in \mathcal{N}} s_j s_k$
3. flip spin of cell c and calculate E_j
4. calculate energy difference $\Delta E = H_i - H_j$
5. accept flip with $w_i j = min(1, e^{-\beta \Delta E})$ otherwise reject and flip to original spin
6. goto 1.