Basic Monte Carlo

In [1]:

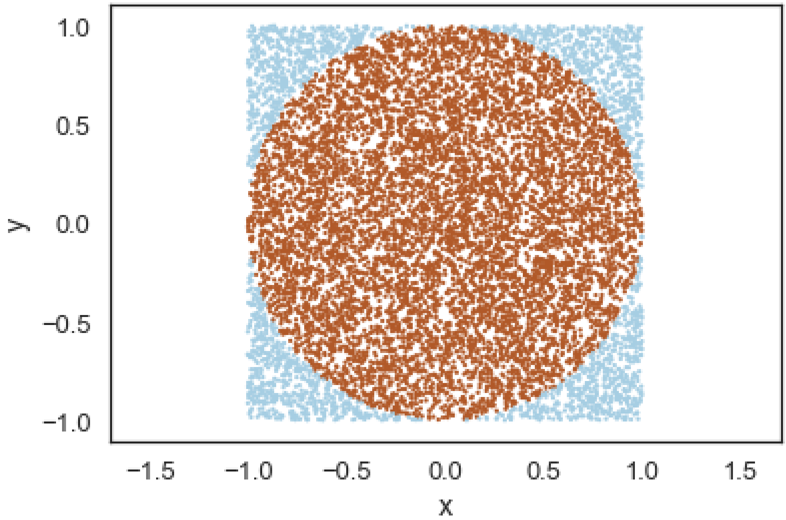
```
%matplotlib inline
import numpy as np
from scipy import stats
from scipy.stats import norm
import matplotlib.pyplot as plt
import seaborn as sns
sns.set_style('white')
sns.set_context('talk')
```

Estimate the area of a unit circle

In [2]:

```
#area of the bounding box
box_area = 4.0

#number of samples
N_total = 10000

#drawing random points uniform between -1 and 1
X = np.random.uniform(low=-1, high=1, size=N_total)
Y = np.random.uniform(low=-1, high=1, size=N_total)

# calculate the distance of the point from the center
distance = np.sqrt(X**2+Y**2);

# check if point is inside the circle
is_point_inside = distance<1.0

# sum up the hits inside the circle
N_inside=np.sum(is_point_inside)

# estimate the circle area
circle_area = box_area * N_inside/N_total

# some nice visualization
plt.scatter(X,Y, c=is_point_inside, s=5.0, edgecolors='none', cmap=plt.cm.Paired
)
plt.axis('equal')
plt.xlabel('x')
plt.ylabel('y')

# text output
print("Area of the circle = ", circle_area)
print("pi = ", np.pi)
```

```
Area of the circle =  3.1448
pi =  3.141592653589793
```



General method of MC

Let $X \sim \phi$ and $\mathbb{E}[X] = \mu$ and $SD(X) = \sigma > 0$, where μ and σ are unknowns.

Our goeal is to eistmiate μ.

In crude MC, suppose computer can generate iid replicates $(X_i : i = 1, 2, \dots)$, then we take the average of the first N replicates as its estimate:

$$\mu_N = \frac{1}{N} \sum_{i=1}^{N} X_i \to \mu, \text{ as } N \to \infty.$$

The above convergence is guranteed by LLN. In other words, if we set the error as

$$e_N = \mu_N - \mu,$$

we have $e_N \to 0$ as $N \to \infty$, which is the most desired property of the estimator.

Another desired property is L^2 convergence, i.e.

$$Var(e_N) = \mathbb{E}e_N^2 \to 0, \text{ as } N \to \infty.$$

This property holds due to the following L^2 error estimation

$$\mathbb{E}e_N^2 = \sigma^2/N.$$

Indeed, by CLT, we also have

$$e_N \Rightarrow \mathcal{N}(0, \sigma/\sqrt{N}).$$

Desired properties of the estimator μ_N

- (unbiasedness) $\lim_N e_N = 0$
- (efficiency) $Var(e_N)$ as small as possible.

Calculate the integral of general form

To calculate $I = \int_D f(x)dx$ for $D \subset \mathbb{R}^d$, we utilize the following identities:

$$I = \frac{1}{|D|} \int_D f(x)\phi(x)dx = \frac{1}{|D|} \mathbb{E}f(X),$$

where $|D|$ is the volume of D, $\phi(x) \equiv |D|^{-1}$, and $X \sim U(D)$ is the uniform distribuiton on D.

Ex. Design a MC for the integral calculation, and prove its convergence.

Ex Calculate $I = \int_2^3 [x^2 + 4\,x\,\sin(x)]\,dx$. by MC. For testing, we can use the anti-derivative $\frac{x^3}{3} + 4\sin(x) - 4x\cos(x)$.

To solve this using MC, we draw N random numbers from 2 to 3 and then take the average of all the values $f(x) = x^2 + 4\,x\,\sin(x)$ and normalized over the volume; in this case the volume is 1 (3-2=1).

In [3]:

```
# define f(x) for our integral
def f(x):
    return x**2 + 4*x*np.sin(x)

# and the anti-derivative for testing
def anti_derivative_f(x):
    return x**3/3.0+4.0*np.sin(x) - 4.0*x*np.cos(x)
```

In [4]:

```
#sage
#plot(f, xmin = -1., xmax = 4.)
```

In [5]:

```
# upper and lower limits:
a = 2;
b = 3;

# use N draws
N= 10000

#1. N values uniformly drawn from a to b
X = np.random.uniform(low=a, high=b, size=N)

#2. Compute f(X)
Y = f(X)
# and the average
f_average = np.sum(Y)/ N

#3. estimate value of integral
estimate = (b-a) * f_average;

#we compute the exact value for testing
exact_val = anti_derivative_f(b) - anti_derivative_f(a)

print("Monte Carlo estimate = ",estimate)
print("Exact value = ", exact_val)
```

```
Monte Carlo estimate =  11.80977006827323
Exact value =  11.811358925098283
```

Mutlidimensional example:

Calculate the integral $I = \int \int f(x, y) dxdy$

where $f(x, y) = x^2 + y^2$

over the region defined by the condition $x^2 + y^2 \leq 1$.

The steps are the same as above, but we need an additional check that the region condition is fulfilled by our random samples. In particular, we transform the problem into $I = \int_D f(x) dx$ with

$$D = [-1, 1]^2, \quad f(x, y) = (x^2 + y^2) \cdot I_{[0,1]}(x^2 + y^2).$$

In [6]:

```
#define our f(x,y)
f_circle = lambda x,y: x**2 + y**2

# use N draws
N= 10000

#sample X and Y
X= np.random.uniform(low=-1, high=1, size=N)
Y= np.random.uniform(low=-1, high=1, size=N)

# calculate f(x)
f_value = f_circle(X, Y)

# reject all samples that do not satisfy our region condition
N = np.sum(f_value<1)

f_average = np.sum(f_value[f_value<1]) / N

print("Monte Carlo estimate = ", np.pi*f_average)
print("Exact value", np.pi/2.0)
```

```
Monte Carlo estimate =  1.585025597585936
Exact value 1.5707963267948966
```

In [7]:

```
#sage
#f_circle_sage (x, y) = x^2 + y^2
#plot3d(f_circle_sage, (x,-2,2), (y,-2,2))
```

Error estimate

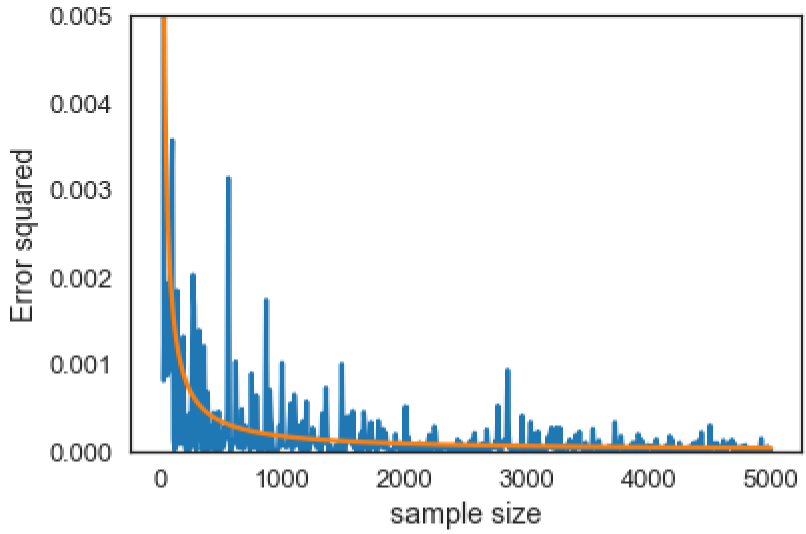
How does the accuracy depend on the number of points(samples)? Let's try the same 1-D integral $I = \int_2^3 [x^2 + 4\,x\,\sin(x)]\,dx$ as a function of the number of points.

ex

Let $X \sim U(2, 3)$ and $Y = X^2 + 4Xsin(X)$. Find the variance of Y.

In [8]:

```
simN = 500 #simulation number
estimates = np.zeros(simN)

# upper and lower limits:
a = 2;
b = 3;

exactval= anti_derivative_f(b)-anti_derivative_f(a)


for N in np.arange(simN):
    sampleN = 10*N + 10 #sample number
    X = np.random.uniform(low = a, high = b, size = sampleN)
    Y = f(X)
    estimates[N] = (b-a)*np.sum(Y)/sampleN;
errors_sq = np.square(estimates - exactval)
x_cd = 10*np.arange(simN)+10 #sample numbers

plt.plot(x_cd, errors_sq)
sigma_sq = 0.1702
plt.plot(x_cd, sigma_sq/x_cd)

plt.xlabel("sample size")
plt.ylabel("Error squared")
plt.ylim(0, 0.005);
```



Our errors follow a normal distribution, and the variance of this distribution can be seen by plotting the histogram:

In [9]:

```
# multiple MC estimations
m=1000
N=1000

estimates = np.zeros(m)


for i in np.arange(0,m):
    X = np.random.uniform(low=a, high=b, size=N) # N values uniformly drawn from
 a to b
    Y =f(X)   # calculate f(x)

    estimates[i]= (b-a) * np.sum(Y)/ N;


plt.hist(estimates)
plt.xlabel("Estimate")
plt.ylabel("Counts")
print("Mean: ", np.mean(estimates))
print("Variance: ", np.var(estimates))
print("Theoretical variance is:", sigma_sq/N)
```

```
Mean:  11.811037937288562
Variance:  0.00017002372428973325
Theoretical variance is: 0.0001702
```