

Importance-Sampling-and-Metropolis

April 9, 2024

1 Important Sampling

Suppose that we have to evaluate the integral

$$I = \int_0^1 f(x) dx$$

for some f . An alternate method for evaluating the integral would to calculate

$$I \approx \frac{1}{N} \sum_{i=1}^N f(x_i)$$

Here, the average of f is evaluated by considering its values at N values $\{x_i\}$, chosen at random with equal probability anywhere within the interval $[0, 1]$. The error may be estimated as,

$$\frac{1}{N} \sigma_f^2 = \frac{1}{N} \left[\frac{1}{N} \sum_{i=1}^N f^2(x_i) - \left(\frac{1}{N} \sum_{i=1}^N f(x_i) \right)^2 \right]$$

which vanishes for constant f .

Let us consider a normalized weight function $w(x)$ given by,

$$\int_0^1 w(x) dx = 1$$

Then the integral can be written as

$$I = \int_0^1 dx w(x) \frac{f(x)}{w(x)}$$

Let us make a change of variable

$$y(x) = \int_0^x dx' w(x')$$

such that,

$$\frac{dy}{dx} = w(x)$$

Then the integral becomes,

$$I = \int_0^1 dy \frac{f(x(y))}{w(x(y))}$$

1.1 Example

Find numerically

$$4 \int_0^1 \frac{dx}{1+x^2} = \pi$$

```
[19]: import numpy as np
import matplotlib.pyplot as plt
```

```
[21]: def f(x):
    return 1/(1+x**2)

Ns = [10, 20, 50, 100, 200, 500, 1000, 2000, 50000]

for N in Ns:
    store = 0.0
    for i in range(N):
        xi = np.random.rand()
        store += f(xi)
    res = 4*store/N
    print(N, "\t", res, "\t", abs(res-np.pi))
```

10	3.216340647679113	0.07474799408932009
20	3.1843031940402957	0.0427105404505026
50	3.184601014359154	0.04300836076936099
100	3.178529074146181	0.036936420556387795
200	3.119225068790803	0.022367584798990148
500	3.1387177546184386	0.0028748989713545114
1000	3.1249157302564594	0.016676923333333704
2000	3.135881910892079	0.0057107426977141
50000	3.1432774846909313	0.0016848311011381512

1.1.1 Find the same integral using the weight function

$$w(x) = \frac{1}{3}(4-2x)$$

```
[24]: def f(x):
    return 1/(1+x**2)

def w(x):
    return (4-2*x)/3

def x(y):
    return 2 - (4 - 3*y)**0.5

Ns = [10, 20, 50, 100, 200, 500, 1000, 2000, 50000]

for N in Ns:
```

```

store = 0.0
for i in range(N):
    yi = np.random.rand()
    xi = x(yi)
    store += f(xi)/w(xi)
res = 4*store/N
print(N, "\t", res, "\t", abs(res-np.pi))

```

10	3.1334027124404584	0.00818994114933469
20	3.1279395172271194	0.013653136362673735
50	3.1436390726699686	0.0020464190801754434
100	3.134290037337607	0.007302616252186311
200	3.137761950541716	0.0038307030480773108
500	3.1381019013514893	0.0034907522383038625
1000	3.139808443982005	0.0017842096077882452
2000	3.1402017811949174	0.0013908723948756752
50000	3.142042963230884	0.00045030964109082916

```

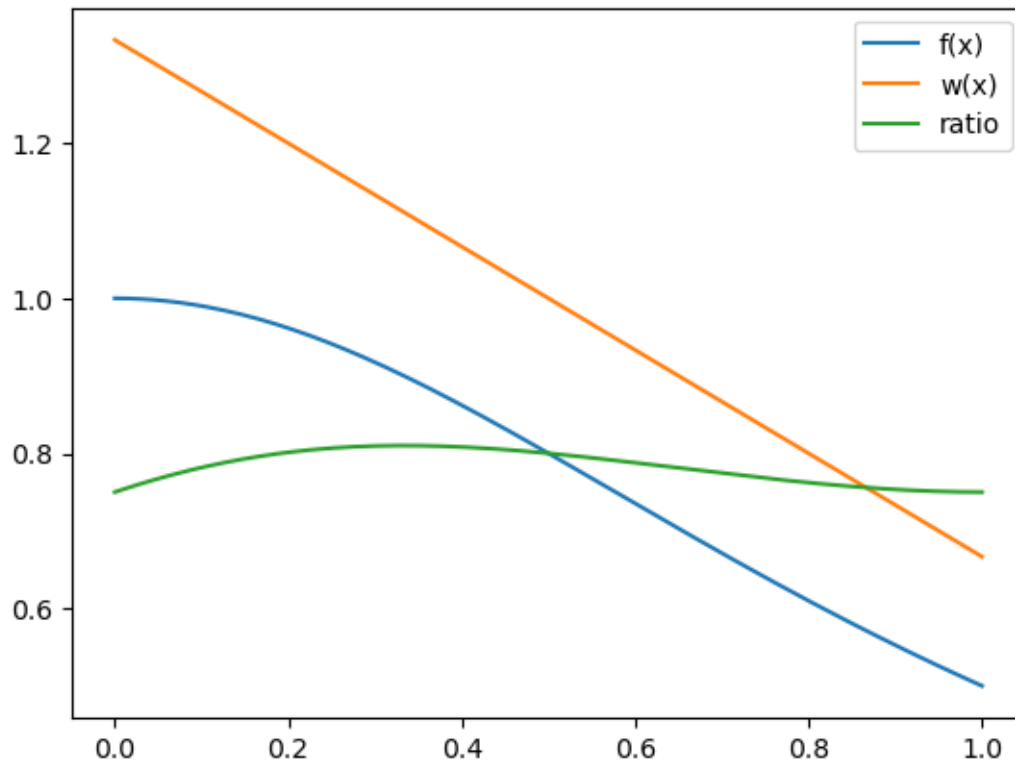
[5]: xs = np.linspace(0.0, 1.0, num=200)
     y1 = [f(x) for x in xs]
     y2 = [w(x) for x in xs]
     y3 = [f(x)/w(x) for x in xs]
     plt.plot(xs, y1, label="f(x)")
     plt.plot(xs, y2, label="w(x)")
     plt.plot(xs, y3, label="ratio")
     plt.legend()

```

```

[5]: <matplotlib.legend.Legend at 0x7f1abc253080>

```



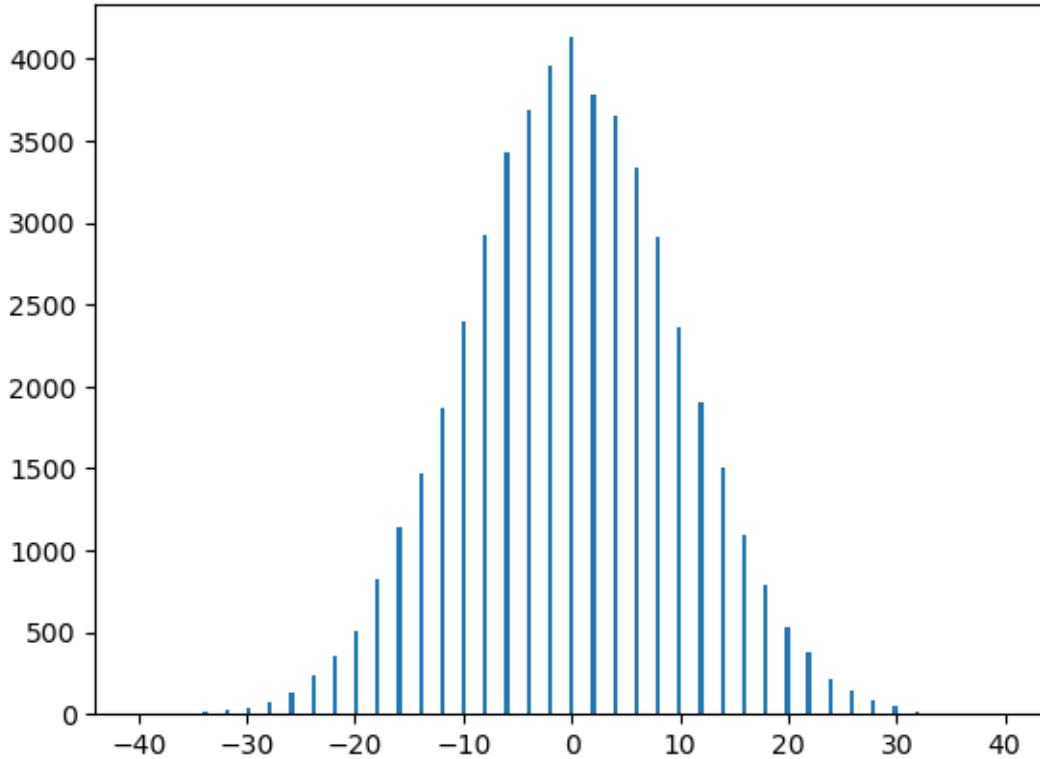
1.2 Random walk

Position of a random walker after N steps form a normal distribution.

```
[6]: def take_a_step():
      if np.random.rand() < 0.5:
          return -1
      return 1

      steps = 100
      walkers = 100000
      finpos = np.zeros(walkers,)
      #finpos = np.zeros((walkers,), dtype=int)
      k = 0
      for w in range(walkers):
          pos = 0
          for s in range(steps):
              pos += take_a_step()
          finpos[k] = pos
          k += 1
```

```
[7]: plt.hist(finpos[0::2], bins=2*steps+1);
```



What if we need a *random walk* with a desired distribution? Markov chain.

2 Metropolis-Hastings

Generate a set of random numbers with a desired distribution $w(x)$. Consider a point in the sequence x_i and a new *trial* point x_{i+1} . The trial point can be generated by taking a *random* step from x . The trial point is *accepted* or *rejected* depending on the ratio

$$r = \frac{w(x_{i+1})}{w(x_i)}.$$

If r is 1 or larger, then the step is accepted, else it is *accepted with a probability* r .

So the acceptance probability is

$$a = \min \left[1, \frac{w(x_{i+1})}{w(x_i)} \right]$$

2.0.1 Example 1

You have access to a uniform sampler. Generate a set of random numbers having a distribution

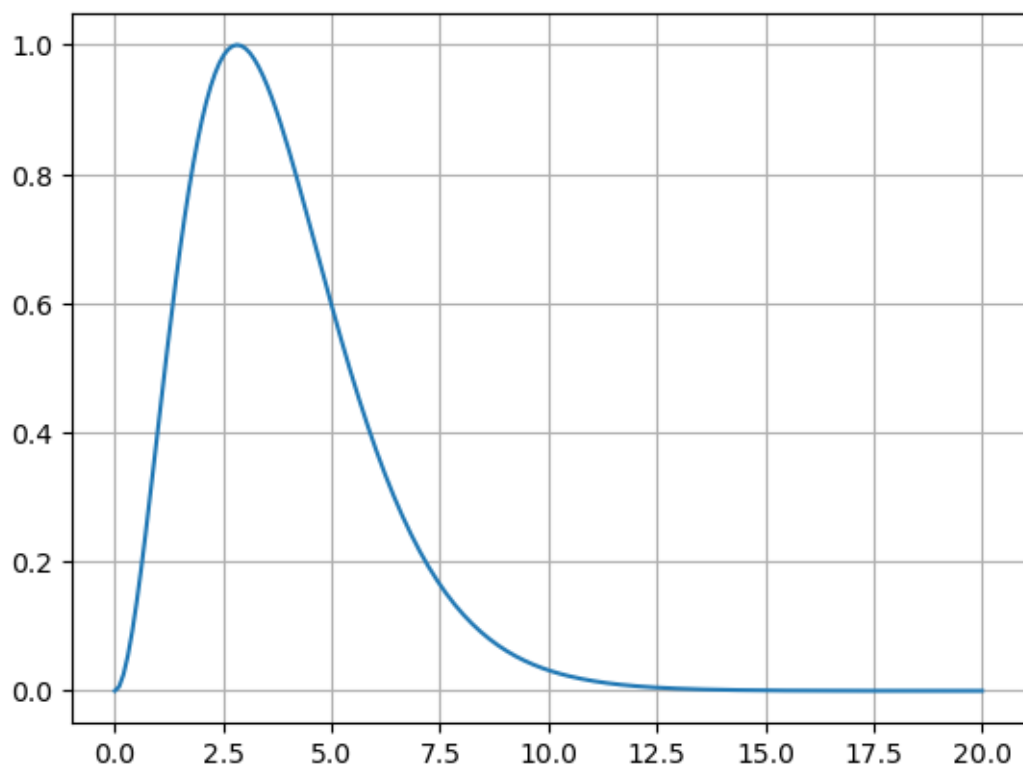
$$\frac{x^3}{e^x - 1}, \forall x \geq 0$$

```
[25]: def target_dist(x):
        if x <= 0.0 :
            return 0.0
        return x**3/(np.exp(x)-1)

xs = np.linspace(0.,20.,num=200)
ys = [target_dist(x) for x in xs]

ys = ys/np.max(ys)

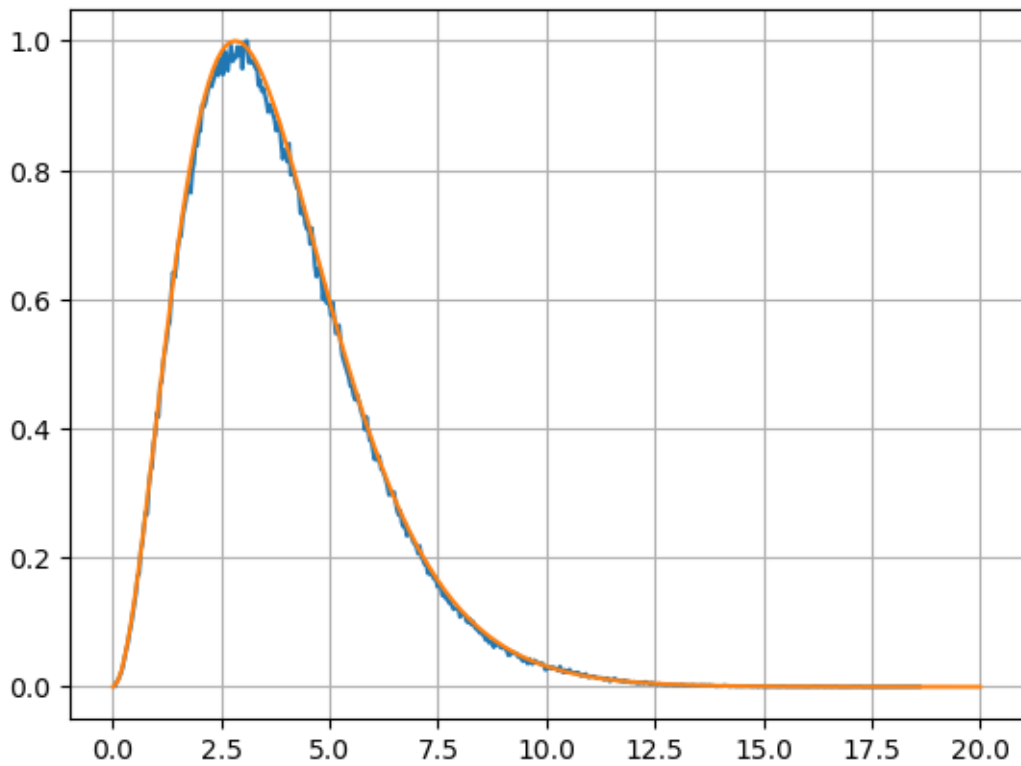
plt.plot(xs, ys);
plt.grid()
```



```
[26]: x = 2.5
N = 1000000
sequence = np.zeros(N)
for i in range(N):
    xt = x + 2.0*(np.random.rand()-0.5)
    a = min([1.0, target_dist(xt)/target_dist(x)])
    if np.random.rand() < a:
        x = xt
    sequence[i] = x
```

```
[27]: freq, edges = np.histogram(sequence, bins=500);
      freq = freq/np.max(freq);
      strip = edges[1]-edges[0];
```

```
[29]: plt.plot(edges[0:-1]+strip/2, freq)
      plt.plot(xs, ys)
      plt.grid()
```



3 Example 2

Generate a sequence of random numbers that has a normal distribution.

$$e^{-(x-x_o)^2/2\sigma^2} \quad \forall x \in \mathbb{R}$$

```
[12]: def target_dist(x):
      return np.exp(-(x-xo)**2/2/sigma)

      xs = np.linspace(-20.0,20.0,num=200)

      xo = 0.0
      sigma = 4.0
```

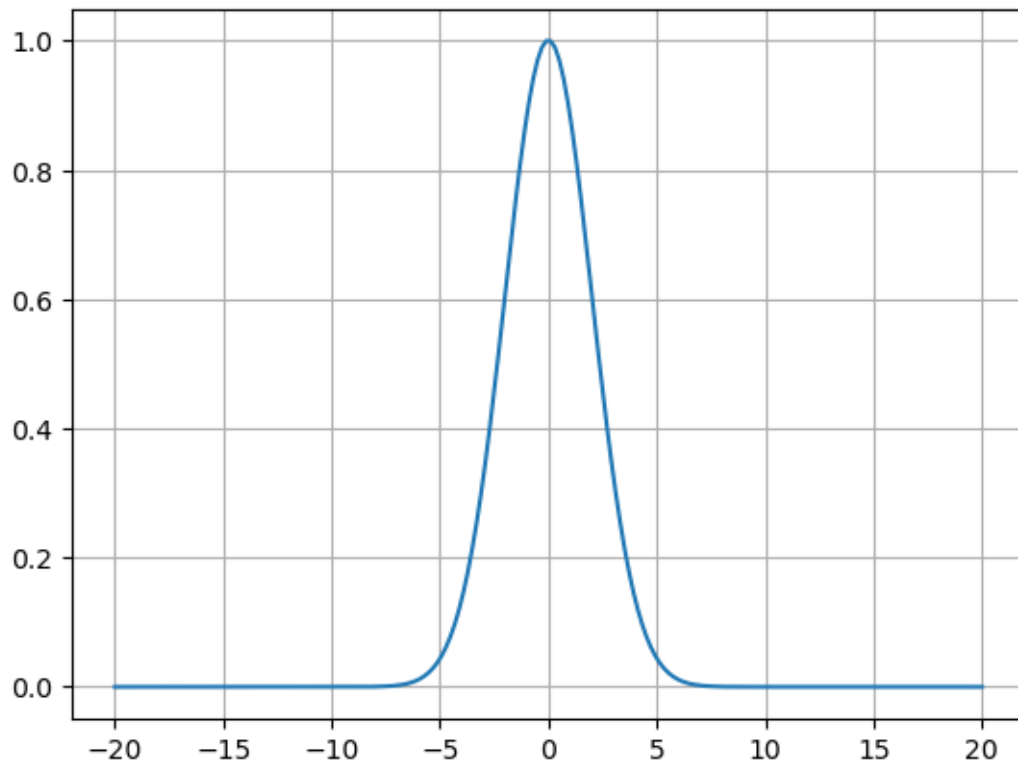
```

ys = [target_dist(x) for x in xs]

ys = ys/np.max(ys)

plt.plot(xs, ys);
plt.grid()

```



```

[16]: x = 0.5
      N = 1000000
      sequence = np.zeros(N)
      for i in range(N):
          xt = x + 2.0*(np.random.rand()-0.5)
          r = min([1.0, target_dist(xt)/target_dist(x)])
          if np.random.rand() < r:
              x = xt
          sequence[i] = x

```

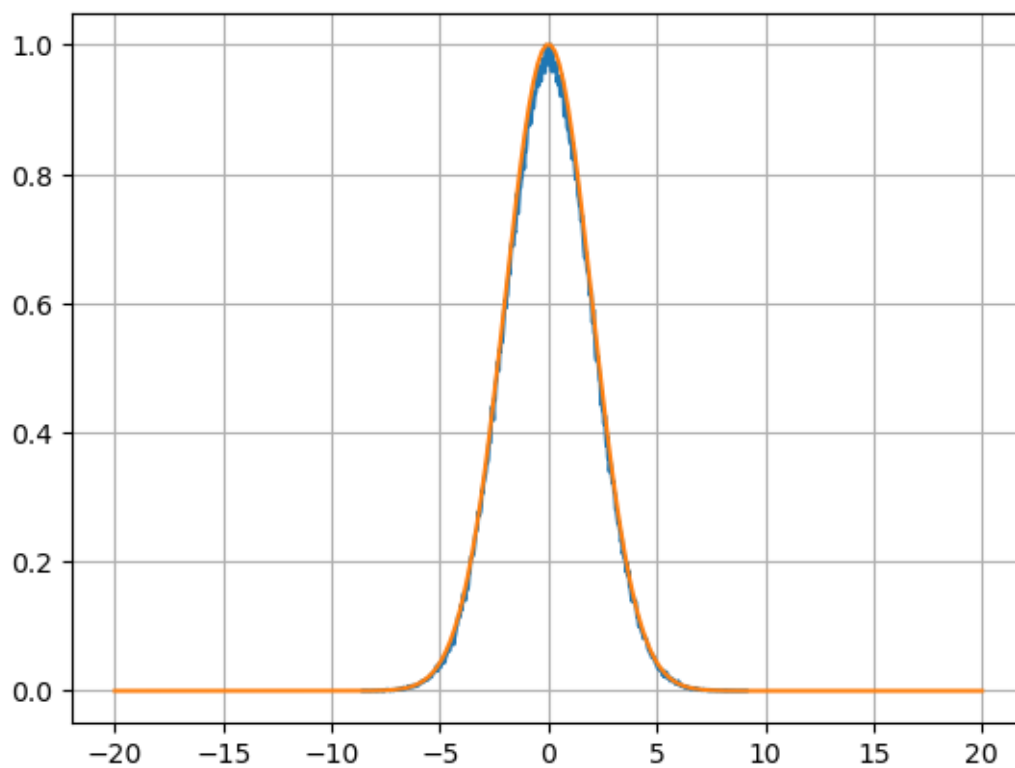
```

[17]: freq, edges = np.histogram(sequence, bins=500);
      freq = freq/np.max(freq);
      strip = edges[1]-edges[0];

```



```
[18]: plt.plot(edges[0:-1]+strip/2, freq)
plt.plot(xs, ys)
plt.grid()
```



```
[ ]:
```