

Becs-114.1100 Computational Science – exercise round 9

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November 24, 2015

1 Solution 1

1.1 Pencil and Paper Problem

Assuming that we are using the Monte Carlo method to estimate the value of a given quantity A where One simulation run gives a single numerical value denoted by A_i and by running the simulation n times we get the set $\{A_i\}_{i=1}^n$

1.1.1 Obtaining a reliable estimate of the true value of A

We can get a reliable estimate of the value of A by drawing more samples A_i . In other words, as we keep increasing the value of n our precision keeps on increasing.

This is an extension of the fact that, if you run m simulations k times to get an estimate E_1 . Or if you run k simulations m times to get an estimate E_2

The precision of E_1 and E_2 remains the same.

1.1.2 How to calculate an estimate of the error?

We can calculate the statistical error

$$\sigma \approx \frac{\sigma_n}{\sqrt{N}} \quad (1)$$

where σ_n is the standard deviation over n samples calculated by using the formula

$$\sigma_N^2 = (\text{Second Moment}) - (\text{First Moment})^2 \quad (2)$$

In the equation above we are calculating the moments of the sequence of $\{A_i\}$ s

1.1.3 How is the central limit theorem related to the estimation ?

According to the Central limit theorem:

For any independently measured values M_1, M_2, \dots, M_m which come from the same (sufficiently short-ranged) distribution $p(x)$, the average

$$\langle M \rangle = \frac{1}{m} \sum_{i=1}^m M_i \quad (3)$$

will asymptotically follow a **Gaussian distribution** (normal distribution) whose mean is $\langle M \rangle$ (equal to the mean of the parent distribution $p(x)$) and variance is $\frac{1}{\sqrt{N}}$ times that of $p(x)$.

In our estimation problem each A_i can be thought of as an independent measurement from a distribution around A . (i.e. $A \pm \text{noise}$)

Then according to the central limit theorem the mean of the samples asymptotically would be the mean of the parent distribution, which is the mean of the distribution around A which is almost equal to A (asymptotically).

Also from the central limit theorem, the variance would be $\frac{1}{\sqrt{N}}$ times that of the parent distribution. We can use this to measure the statistical error in our measure and identify the value of A with a desired precision.

1.2 Estimating the value of π using "Hit-or-Miss" method

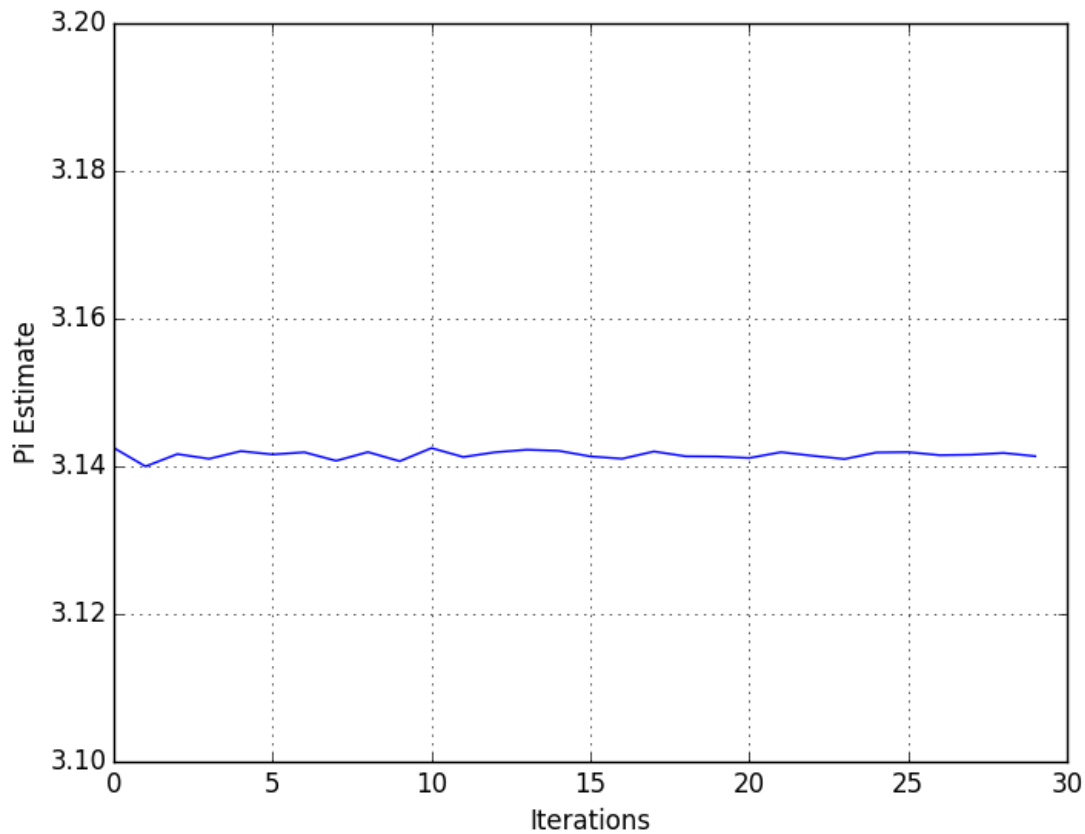


Figure 1: Estimate of the values of π

What relation does the error estimate follow?

It goes down as $\frac{1}{\sqrt{N}}$ with the number of iterations N . As can be seen in 2

What about the absolute error?

The absolute error goes down approximately linearly.

The corresponding python code can be found at 3

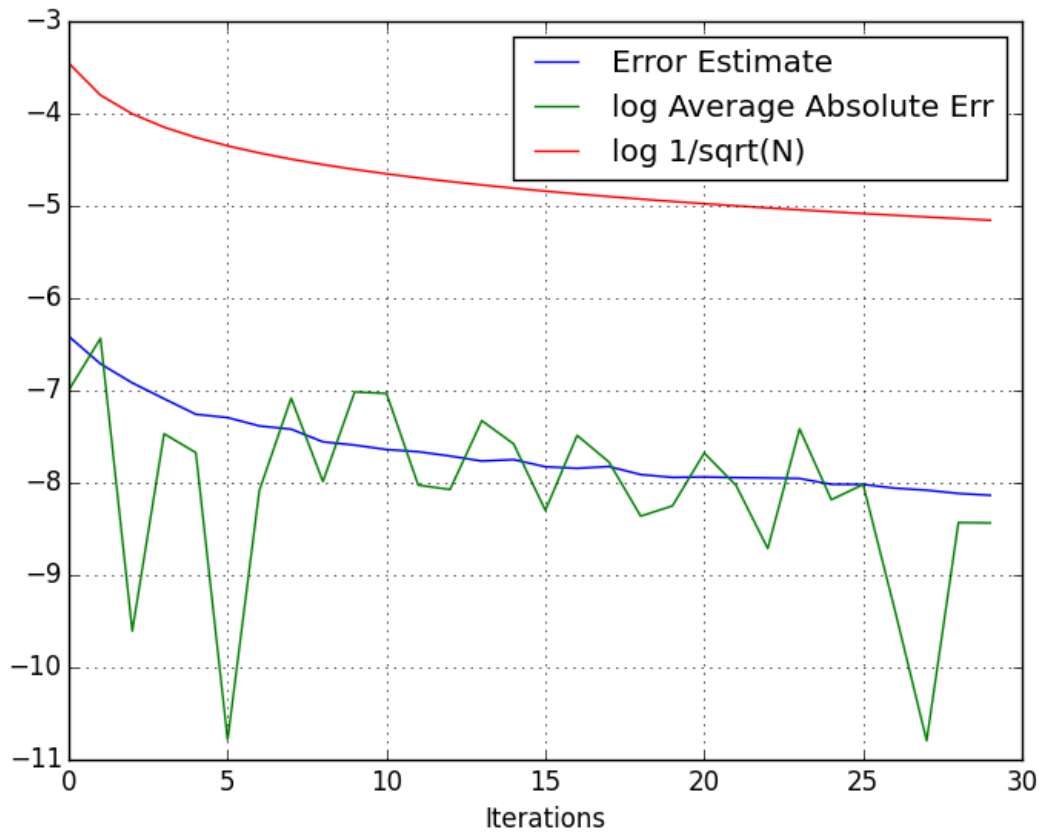


Figure 2: change of error estimate and absolute error with increasing values of N . Here $\log(\frac{1}{\sqrt{N}})$ has been plotted for reference.

N	Pi Estimate	$\log(\frac{\sigma}{\sqrt{N}})$	Average Absolute Error
1000	3.142508	-6.41348792121	-6.99620842209
2000	3.139988	-6.71147219026	-6.43484712196
3000	3.14166	-6.91763448245	-9.60566704811
4000	3.141022	-7.08901447367	-7.46872748644
5000	3.1420576	-7.25796392872	-7.67358928815
6000	3.14161333333	-7.2936121459	-10.7863757461
7000	3.14190171429	-7.38430359819	-8.0819742007
8000	3.1407535	-7.41917293679	-7.08311631649
9000	3.14193244444	-7.55625404967	-7.98718147024
10000	3.1406948	-7.59155617352	-7.0155030864
11000	3.14247527273	-7.63964380553	-7.03261724305
12000	3.14126566667	-7.66343122719	-8.0255891238
13000	3.14190461538	-7.71002347021	-8.07263114507
14000	3.14225	-7.7644752777	-7.32730004188
15000	3.142104	-7.74859962632	-7.57846409317
16000	3.14134375	-7.82647958467	-8.29844327801
17000	3.14103223529	-7.8432896092	-7.48682636454
18000	3.14201311111	-7.82393930635	-7.77416807873
19000	3.14135894737	-7.91094478818	-8.36144394036
20000	3.1413314	-7.94131111675	-8.2500174438
21000	3.14112952381	-7.93669418525	-7.67750235447
22000	3.14191890909	-7.94388132238	-8.02783099513
23000	3.141428	-7.94778029614	-8.71166425548
24000	3.14099083333	-7.95348895198	-7.41555105294
25000	3.14187184	-8.01644609615	-8.1836323316
26000	3.141922	-8.01782795101	-8.01840168809
27000	3.1415082963	-8.05814633533	-9.38044442293
28000	3.14157214286	-8.0804222317	-10.7945422655
29000	3.14181075862	-8.11554628555	-8.43053569888
30000	3.14137533333	-8.13521894018	-8.43413656861

Table 1: Table of Values for the π estimate using Monte Carlo Simulations.

2 Solution Q3

In this problem we are trying to Identify which meathod, Importance Sampling or Sample Mean method, we should choose for the task of identifying integrals given a function and its limits. To choose between them, we use each of the methods to perform a definite integral $\int_1^2 (2x^8 - 1)dx$. After executing both the methods, we plot their respective absolute error with the analytically calculated exact integral value of 112.5555 We then state our conclusion below.

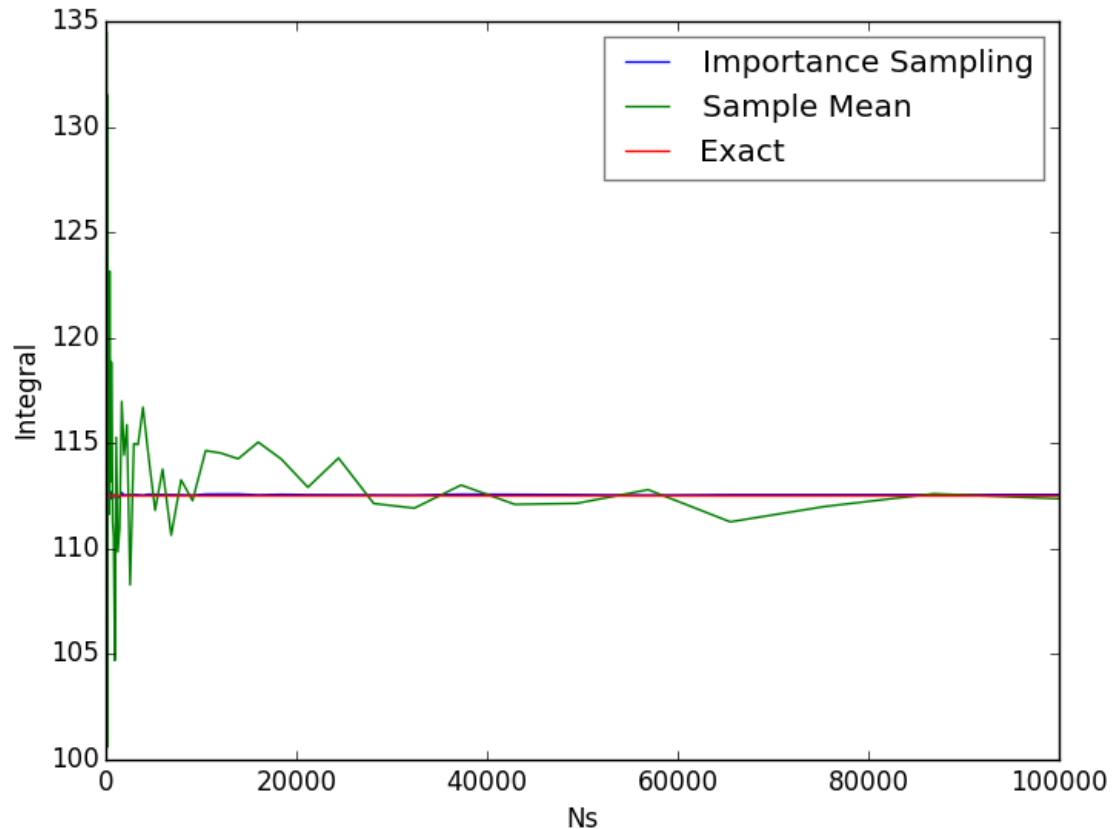


Figure 3: Value of Integral calculated using Importance sampling and Sample Mean method as a function of the Number of random samples. The exact value is plotted in Red for comparison.

Which method is better? It can be seen from the graph above and also from the table of values below, that the absolute error achieved by Importance sampling is much lower than that achieved by sample mean method. Hence **Importance Sampling** method is better.

The corresponding python code can be found at 4

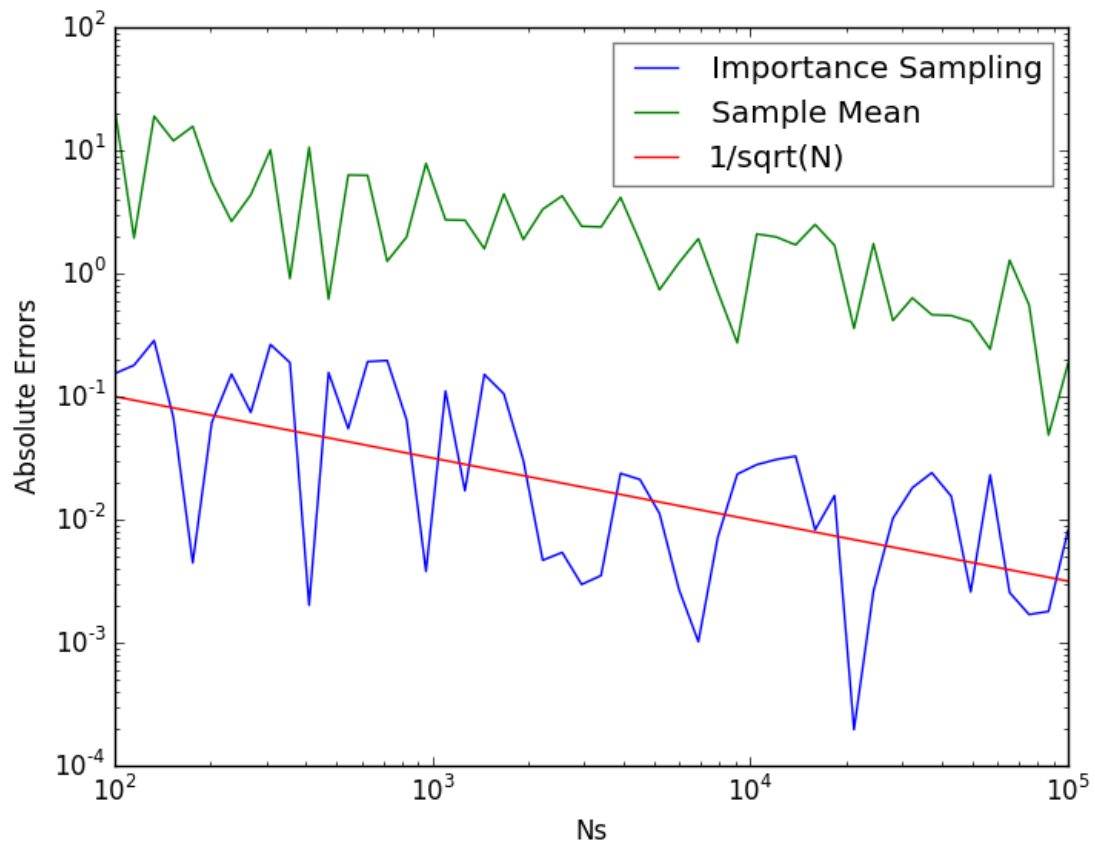


Figure 4: Absolute errors of Integrals calculated using Importance sampling and Sample mean method, when compared to the actual analytic integral. The values have been plotted in the log scale

N	Imp samp est	Abs Err Imp Samp	Sample Mean Est	Abs Err Sample Mean
100	112.817602096	0.262046540193	97.6200018902	14.9355536653
115	112.790934035	0.235378479495	110.387517365	2.1680381906
133	112.862782704	0.307227148659	124.198178589	11.6426230335
153	112.307040131	0.248515424259	116.378833157	3.8232776018
176	112.570447868	0.01489231282	115.172083115	2.6165275593
202	112.807401366	0.251845810884	108.951693299	3.60386225665
233	112.605799413	0.0502438576779	106.077739978	6.47781557707
268	112.727453517	0.171897961599	128.263364923	15.7078093672
...
720	112.425498173	0.130057382117	104.21269517	8.3428603851
7906	112.591896217	0.0363406610969	111.628379791	0.927175764348
9103	112.593672719	0.0381171632268	115.933335012	3.37777945607
10481	112.593388655	0.0378330998116	110.255123721	2.30043183446
12068	112.544424017	0.0111315383437	112.60262766	0.0470721040552
13895	112.578383621	0.0228280654867	112.317530107	0.238025448329
15999	112.57870659	0.0231510344667	114.266579722	1.71102416604
18421	112.584252555	0.0286969996644	113.82109461	1.26553905427
21210	112.567439326	0.011883770476	111.959205762	0.596349793541
24421	112.525425965	0.0301295907316	113.264044066	0.708488510236
28118	112.565090954	0.00953539796538	113.32274423	0.767188674465
32375	112.543195441	0.0123601148601	111.961554588	0.594000967337
37276	112.56452844	0.00897288431986	113.132173579	0.576618023773
42919	112.553776654	0.00177890148414	112.70115021	0.145594654239
49417	112.553603269	0.00195228660451	112.926394176	0.370838620377
56899	112.549206334	0.006349221845	111.432828844	1.12272671195
65513	112.583406579	0.0278510230071	112.367194506	0.188361049716
75431	112.544776726	0.0107788296986	113.524978805	0.969423249651
86851	112.561721621	0.00616606549636	112.540220207	0.0153353481125
100000	112.555043138	0.000512417685144	112.505272248	0.0502833078437

Table 2: Table showing the values of $\int_1^2 (2x^8 - 1)dx$ Estimated using Importance sampling method, its Absolute Error followed by the values using Sample Mean Method and then its Absolute Error in the last column.

3 Appendix A

Python source code for 1.2.

```
from __future__ import division
import numpy as np
import pylab as pl

def mc_circle_np(n):
    """
    We would be drawing random samples from -1 to 1
    """
    inside = 0
    x = np.random.random(n)*2-1
    y = np.random.random(n)*2-1
    inside = np.sum((np.square(x,out=x) + np.square(y,out=y)) < 1)
    return 4 * (inside/n)

if __name__ == '__main__':
    n = 1000
    pi = 3.141592654
    pi_est = []
    err_est = []
    avg_abs_err = []
    start,end,step = 1000,31000,1000
    for N in xrange(start,end,step):
        pis = np.zeros(n)
        for i in xrange(1000):
            pis[i] = mc_circle_np(N)
        pi_est_m = np.mean(pis)
        pi_est.append(pi_est_m)
        err_est_m = np.log(np.std(pis)/np.sqrt(n)) #Because we always have n (=1000) estimates
        err_est.append(err_est_m)
        avg_abs_err_m = np.log(np.abs(pi_est_m - pi))
        avg_abs_err.append(avg_abs_err_m)
        print("{} & {} & {} & {} \\\\".format(N,pi_est_m,err_est_m,avg_abs_err_m))

    pl.plot(pi_est)
    pl.ylabel("Pi Estimate")
    pl.ylim((3.1,3.2))
    pl.xlabel("Iterations")
    pl.grid()
    pl.savefig("pi_est.png")

    pl.figure()
    pl.plot(err_est)
    pl.plot(avg_abs_err)
    pl.xlabel("Iterations")
    pl.legend(["Error Estimate", "Average Absolute Err"])
    pl.grid()
    pl.savefig("err_est.png")
    pl.show()
```

4 Appendix B

Python source code 2.

```
from __future__ import division
import numpy as np
import pylab as pl

one_by_nine = 1/9.0
nine_by_511 = 9/511.0
def getIest_Imp(N):
    y = np.random.random(N)
    # Inverse function calculated manually
    x = np.power(511*y + 1, one_by_nine)
    f = 2*np.power(x,8) -1
    w = nine_by_511 * np.power(x,8)
    Iest = np.mean(np.true_divide(f,w))
    return Iest

def getIest_Sm(N):
    # b = 2 and a = 1 Hence b-a = 1
    # which doesn't affect the integral
    # has been omitted from the calculations
    x = np.random.random(N)+1 # shift the random values between 1 and 2
    f = 2*np.power(x,8)-1
    Iest = np.mean(f)
    return Iest

if __name__ == '__main__':
    exact = 1013/9.0
    Iest_Imp = []
    absErr_Imp = []
    Iest_Sm = []
    absErr_Sm = []
    Ns = map(lambda x: int(round(x)), np.logspace(2, 5, 50))
    for N in Ns:
        estImp = getIest_Imp(N)
        Iest_Imp.append(estImp)
        errImp = abs(exact-estImp)
        absErr_Imp.append(errImp)

        estSm = getIest_Sm(N)
        Iest_Sm.append(estSm)
        errSm = abs(exact-estSm)
        absErr_Sm.append(errSm)

    print "{} & {} & {} & {} & {} \\\\".format(N,estImp,errImp,estSm,errSm)

    pl.loglog(Ns,absErr_Imp,label="Importance Sampling")
    pl.loglog(Ns,absErr_Sm,label="Sample Mean")
    pl.loglog(Ns,map(lambda x:1/(x**0.5),Ns),label="1/sqrt(N)")
    pl.legend(framealpha=0.5)
    pl.xlabel("Ns")
    pl.ylabel("Absolute Errors")

    pl.savefig("Errors.png")
    pl.show()
```
