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Monte Carlo - Basics

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**Markov Chain and Master Equation**

*•* Random variables

*•* Concept of errors

*•* Estimation of errors

*•* Markov Chain

*•* Master Equation

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outcomes of such random events *xi*, its variances and so on. PA MonteCarl

**Random variables**

*•* Consider an elementary event with a countable set of random outcomes, *A*1*, A*2*, ....Ak* (e.g. you can consider a rolling dice OR a set of ”Khodkhode”. )

*•* You are data scientist so you need to consider this event occurring repeatedly say N times such that *N >>>* 1 and we count how often the outcome *Ak* is observed (*Nk*).

*•* The probabilities *pk* for outcome *Ak* is

(1)

with *k pk* = 1.

Obviously 0 *≤ pk ≤* 1

*pk* = lim *N→∞*

*Nk N*

You are familiar with conditional probability *P*(*j/i*), average of any 3

error =*σ~~√~~~~n~~*(3) PA MonteCarl

**Statistical errors**

*•* Suppose the quantity *A* is distributed according to a Gaussian with mean value *A* and width *σ*. We consider *n* statistically independent observations *{Ai}* of this quantity *A*.

*•* An unbiased estimator of the mean *A* of this distribution is

*A*¯ =1*nn i*=1

*Ai* (2)

and the standard error of this estimate is 4

(*n*(*n −* 1)) (6) PA MonteCarl

**Statistical errors**

*•* The variance is obtained from mean square deviation

¯*δA*2 =1*nn i*=1

(*δAi*)2 = *A*¯2 *−A*¯2(4)

The expectation value of this quantity is easily related to *σ*2 = *A*2 *− A*2as

¯*δA*2 = *σ*2(1 *−* 1*/n*) (5)

∴ error =¯*δA*2

(*n −* 1) =

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*ni*=1 (*δAi*)2

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**Ingredients of MC**

*•* As mentioned before there are at least four ingredients which are crucial in order to understand the basic MC strategy. (i) Random variables

(ii) Probability distribution functions (PDF),

(iii) Moments of a PDF (iv) and pertinent variance *σ* 6

[ 2*,* 3*,* 4*,* 5*,* 6*,* 7*,* 8*,* 9*,* 10*,* 11*,* 12*.*] (7) PA MonteCarl

**Random Variables**

*•* Let us first demistify the somewhat obscure concept of a random variable. The example we choose is the classic one, the tossing of two dice, its outcome and the corresponding probability. In principle, we could imagine being able to determine exactly the motion of the two dice, and with given initial conditions determine the outcome of the tossing. Alas, we are not capable of pursuing this ideal scheme. However, it does not mean that we do not have a certain knowledge of the outcome. This partial knowledge is given by the probablity of obtaining a certain number when tossing the dice. To be more precise, the tossing of the dice yields the following possible values

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of the final outcome. PA MonteCarl

**Random Variables**

*•* These values are called the domain. To this domain we have the corresponding probabilities

[ 1*/*36*,* 2*/*36*,* 3*/*36*,* 4*/*36*,* 5*/*36*,* 6*/*36*,* 5*/*36*,* 4*/*36*,* 3*/*36*,* 2*/*36*,* 1*/*36] (8)

*•* These values are called the domain. To this domain we have the corresponding probabilities

*•* The numbers in the domain are the outcomes of the physical process tossing the dice. We cannot tell beforehand whether the outcome is 3 or 5 or any other number in this domain. This defines the randomness of the outcome, or unexpectedness or any other synonimous word which encompasses the uncertitude

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random. PA MonteCarl

**Random Variables**

*•* The only thing we can tell beforehand is that say the outcome 2 has a certain probability. If our favorite hobby is to spend an hour every evening throwing dice and registering the sequence of outcomes, we will note that the numbers in the above domain [ 2*,* 3*,* 4*,* 5*,* 6*,* 7*,* 8*,* 9*,* 10*,* 11*,* 12*.*] (9)

appear in a random order.

after (say) 11 throws the results may look like

[ 10*,* 8*,* 6*,* 3*,* 6*,* 9*,* 11*,* 8*,* 12*,* 4*,* 5] (10)

*•* Eleven new attempts may results in a totally different sequence of numbers and so forth. Repeating this exercise the next evening, will most likely never give you the same sequences. Thus, we say that the outcome of this hobby of ours is truely

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**Random Variables**

*• Random variables are hence characterized by a domain which contains all possible values that the random value may take. This domain has a corresponding PDF.*

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*f*(*xi*)*p*(*xi*) (13) PA MonteCarl

**MC Illustration - Integration**

*•* Consider an integration

*I* =

1 0

*N*

*f*(*x*)*dx i*=1

*wif*(*xi*) (11)

where *wi* are the weights determined by specific integration methods like Trapeziod, Simpson etc. In the crudest approach here in MC integration we set up *wi* = 1 then above eq becomes

*I* =

1 0

*f*(*x*)*dx* 1*NN i*=1

*f*(*xi*) (12)

Now introduce the concept of the average of the function *f* for a given PDF *p*(*x*) as

*f* =1*NN*

*i*=1

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*f*2(*xi*) *−* (*f*)2(16) PA MonteCarl

**MC Illustration - Integration**

Now identify *p*(*xi*) = 1 with the uniform distribution when *x ∈* [ 0*,* 1) and zero for all other values of *x*. Then

*I* =

1 0

*f*(*x*)*dx* 1*NN i*=1

*f*(*xi*) *f* (14)

Similarly the variance (which is also important in MC methods) is

*σ*2*f* =1*NN i*=1

(*f*(*xi*) *− f*)2*p*(*xi*) (15)

After inserting value of *p*(*xi*) we get *σ*2*f* =1*NN*

*i*=1

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deviation. PA MonteCarl

**MC Illustration - Integration:Algorithm**

*•* Choose the number of Monte Carlo samples N.

*•* Perform a loop over N and for each step generate a a random number *xi*in the interval [0, 1] through a call to a random number generator. Translate the random numbers to other required interval if it needs.

*•* Use this number to evaluate *f*(*xi*).

*•* Evaluate the contributions to the mean value and the standard deviation for each loop.

*•* After N samples calculate the final mean value and the standard 13

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**MC Illustration - Integration** *•* As an example evaluate following by MC method:

exp(*x*)*dx* (17)

and

*I* =

1 0

3

*I* =

1

exp(*x*)*dx* (18)

Also Compare the final results with the correct and hence estimate the errors.

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**MC Illustration - Integration**

import random

import numpy as np

import math

a = 0.

b = 1.

integral = 0.0

i=0

while i*<*1000:

x=random.random()

integral += math.exp(x)

i=i+1

ans=integral\*(b-a)/float(N)

print (”The value calculated by monte carlo integration is *{ }*”.format(ans))

HW: You also estimate it following above algorithm. Further estimate integral for different set of random numbers and hence estimate *σN* . 15

Also follow the discussion in my lecture PA MonteCarl

**MC Illustration - Estimate** *π*

1. Initialize circle points, square points and interval to 0. 2. Generate random point x.

3. Generate random point y.

4. Calculate d = x\*x + y\*y.

5. If d *<*= 1, increment circle points.

6. Increment square points.

7. Increment interval.

8. If increment *<* NOOFITERATIONS, repeat from 2. 9. Calculate pi = 4\*(circle points/square points). 10. Terminate.

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what you did in 2D is ust a special case of above equation in n=2. PA Mont~~e~~Carl

**HW: Estimate** *π*

1. Estimate value of *π* also from

*π* =

4*dx*

1

1 + *x*2(19) 0

2. What we did in previous slide was to estimate value of *π* from area of a circle in 2 dimensions. Can you think of similar methods for higher dimensions? You may need volume of a hypersphere of radius

R in *n* dimensions:

*Vn*(*R*) = *πn/*2

17

*n*

2

!*Rn*(20)

need to discuss change of variables. PA MonteCarl

**Concept of Importance Sampling**

*•* Till now we discussed about ’simple sampling’ of MC *•* In principle, MC integrations and other simulations can be performed using the simple sampling techniques we discussed till now. Unfortunately most of the saples produced in this fashion will contribute relatively little to the equilibrium (time independent) averages and more sophisticated methods are required if we are to obtain results of sufficient accuracy to be useful.

*•* One of such a methods is ”Importance Sampling”. For this we 18

consideration. PA MonteCarl

**Concept of Importance Sampling**

*•* With improvements we think of a smaller variance and the need for fewer Monte Carlo samples, although each new Monte Carlo sample will most likely be more times consuming than corresponding ones of the brute force method (Simple sampling). For this we consider two topics.

*•* The first topic deals with change of variables, and is linked to the cumulative function *P*(*x*) of a PDF *p*(*x*). Obviously, not all integration limits go from x = 0 to x = 1, rather, in DATA Science we are often confronted with integration domains like *x ∈* [0*,∞*] or *x ∈* [*−∞,∞*] etc. Since all random number generators give numbers in the interval *x ∈* [0*,* 1], we need a mapping from this integration interval to the explicit one under

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the uniform distribution. PA MonteCarl

**Concept of Importance Sampling**

*•* The next topic deals with the shape of the integrand itself. Let us for the sake of simplicity just assume that the integration domain is again from x = 0 to x = 1. If the function to be integrated *f*(*x*) has sharp peaks and is zero or small for many values of *x ∈* [0*,* 1], most samples of *f*(*x*) give contributions to the integral I which are negligible. As a consequence we need many *N* samples to have a sufficient accuracy in the region where *f*(*x*) is peaked. What do we do then? We try to find a new PDF *p*(*x*) chosen so as to match *f*(*x*) in order to render the integrand smooth. The new PDF *p*(*x*) has in turn an x domain which most likely has to be mapped from the domain of

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*p*(*y*)*dy* = *dx* (24) PA MonteCarl

**Importance Sampling -Change of variables**

*•* Consider uniform distribution

*p*(*x*)*dx* =*dx* (for 0 *≤* x *≤* 1)

=0 else(21)

with *p*(*x*) = 1 and satisfying

*∞*

*−inf ty*

*p*(*x*)*dx* = 1 (22)

All random number generators provided in the program library generate numbers in this domain. When we attempt a transformation to a new variable *x → y* we have to conserve the probability

*p*(*y*)*dy* = *p*(*x*)*dx* (23)

which for the uniform distribution implies

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improvements over the brute force Monte Carlo. PA MonteCarl

**Importance Sampling -Change of variables**

Let us assume that *p*(*y*) is a PDF different from the uniform PDF *p*(*x*) = 1 with *x ∈* [0*,* 1]. If we integrate the last expression we arrive

at

*x*(*y*) =

*y* 0

*p*(*y*)*dy*(25)

which is nothing but the cumulative distribution of *p*(*y*), i.e.

*x*(*y*) = *P*(*y*) =

*y* 0

*p*(*y*)*dy*(26)

This is an important result which has consequences for eventual 22

*y* = *a* + (*b − a*)*x* (30) PA MonteCarl

**Change of variables- an example**

Suppose we have the general uniform distribution

*p*(*y*)*dy* =*dy*

*b − a*(for a *≤* y *≤* b)

=0 else

If we wish to relate this distribution to the one in the interval *x ∈* [0*,* 1] we have

*p*(*y*)*dy* =*dy*

(27)

*b − a*(for a *≤* y *≤* b) = *dx* (28)

and integrating we obtain the cumulative function

*dy*

*b − a*(29)

yielding

*x*(*y*) =

*y* 0

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We can rewrite our integral as PA MonteCarl

**Importance Sampling**

*•* With the aid of the above variable transformations we address now one of the most widely used approaches to Monte Carlo integration, namely importance sampling. It will be helpful to sample a function which has peak as we need to consider many more sampling points near the peak.

*•* Let us assume that *p*(*y*) is a PDF whose behavior resembles that of a function F defined in a certain interval [*a, b*]. The normalization condition is

*b*

*p*(*y*)*dy* = 1 (31) *a*

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*p*(*y*(*x*)) *dx* (35) PA MonteCarl **Importance Sampling**

*I* =

*b a*

*F*(*y*)*dy* =

*b a*

*p*(*y*)*F*(*y*)

*p*(*y*)*dy* (32)

Since random numbers are generated for the uniform distribution *p*(*x*) with *x ∈* [0*,* 1], we need to perform a change of variables *x → y*

through

*x*(*y*) =

where we used

*y a*

*p*(*y*)*dy*(33)

*p*(*x*)*dx* = *dx* = *p*(*y*)*dy* (34)

If we can invert *x*(*y*), we find *y*(*x*) as well. With this change of variables we can express the integral of Eq. 32 as

*I* =

*b a*

*p*(*y*)*F*(*y*)

*p*(*y*)*dy* =

25

*b a*

*F*(*y*(*x*))

variable in terms of the old one. PA MonteCarl

**Importance Sampling**

meaning that a Monte Carlo evalutaion of the above integral gives

*b*

*F*(*y*(*x*))

*N*

*F*(*y*(*xi*))

*p*(*y*(*x*)) *dx* =

*a*

*i*=1

*p*(*y*(*xi*)) (36)

The advantage of such a change of variables in case *p*(*y*) follows closely *F* is that the integrand becomes smooth and we can sample over relevant values for the integrand. It is however not trivial to find such a function *p*.

The conditions on p which allow us to perform these transformations are

1. p is normalizable and positive definite,

2. it is analytically integrable and

3. the integral is invertible, allowing us thereby to express a new 26

distribution *p*(*y*). See Example below. PA Mont~~e~~Carl

**Important Note**

*•* The average is over y(x) distribution.

Therefore above equation 35 can be rewritten as

*I* =

*b a*

*p*(*y*)*F*(*y*)

*p*(*y*)*dy* =

*b a*

*p*(*y*)

*F*(*y*) *p*(*y*)

*dy* = *Ep*(*y*)

*F*(*y*) *p*(*y*)

(37)

is actually expectation value of

with distribution *p*(*y*).

*F*(*y*)

*p*(*y*)

**Please note that the average is over the distribution** *p*(*y*) **not over** *p*(*x*)**.**

Therefore in the importance sampling integration you first find the p(y) corresponding to *p*(*x*) *∈* [0*,* 1]. Then find average 36 with

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**Importance Sampling - Examples** (1) Consider the integral

*I* =

1

exp (*−x*2)*dx* (38) 0

Evaluate *I* using (i) brute force (simple sampling) MC with *p*(*x*) = 1 and (ii) importance sampling with *p*(*x*) = *a* exp (*−x*). Improtant Note: You first write Algorithm in each case then write code in python language following the Hints

(a) Obtain average of exp (*−x*2) for *x ∈* [0*,* 1]

(b) Find its variance too.

These are results of Simple sampling.

for importance sampling:

(c) Find *p*(*y*) corresponding to *p*(*x*) = *a* exp (*−x*) from equation 33 where *a* is normalization constant.

(d) Then find the expectation value of exp (*−x*2)

*a* exp (*−x*)

with distribution

*p*(*y*). (e) Find variance also. (f)Compare both errors or variances and

comments on our results.

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1 *−*1*e*(40) PA MonteCarl

**Monte Carlo - More on above examples** *•* **Solution of above example (Importance sampling):**

*I* =

1

exp (*−x*2)*dx* (39) 0

with chosen pdf (probability distribution function) *p*(*x*) = *a* exp(*−x*) such that *x ∈* (0*,* 1) and

1

*a* exp (*−x*)*dx* = 1*.*

0

resulting *a* =*e*

*p*(*x*)*dx* =

1 0

*e−*1.

=*⇒ p*(*x*) = exp (*−x*) 29

*e −* 1(42) PA Mon~~t~~eCarl

**Monte Carlo - More on above examples**

Also check whether p(x) fulfills the criteria for pdf. for this we find *F*(0)

*p*(0) and *F*(1)

*p*(1) . They have to be equal.

Now*F*(0)

*p*(0) =*e*

*e −* 1=*F*(1)

*p*(1) (41)

Since our pdf fulfills the criteria lets find *y*(*x*)*.* For this we perform then the change of variables (via the Cumulative distribution function)

*y*(*x*) =

*x* 0

*p*(*x*)*dx*=

*x* 0

30

*dx*exp (*−x*) *×e*

PA MonteCarl **Monte Carlo - More on above examples**

=*⇒ y*(*x*) = *e*

*e −* 1

after solving for *x* we get;

1 *− e−x*(43)

=*⇒ x* = *−* ln 1 *− y*(1 *− e−*1)(44)

which gives *y* = 0 for *x* = 0 and *y* = 1 for *x* = 1 as required for the property of pdf.

Now we need to find expectation value of

exp (*−x*2)

exp (*−x*)

with distribution *y*(*x*)*.* That is we need to evaluate

1 0

exp (*−x*2)*dx* = 31

exp (*−y*2(*x*)) exp (*−y*(*x*))

both results. PA MonteCarl

**Monte Carlo - More on above examples**

Algorithm:

1. Start

2. import required libraries like random, numpy ..

3. Define n, functions, initialize summ etc

4. start loop over n

5. generate random numbers *x ∈* (0*,* 1)

6. define function *y*(*x*) using above formula from *x* as

*y*(*x*) = *e*

*e−*1

(1 *− e−x*)

7. Get sum of the function exp (*−y*2(*x*))

8. close the loop

exp (*−y*(*x*))

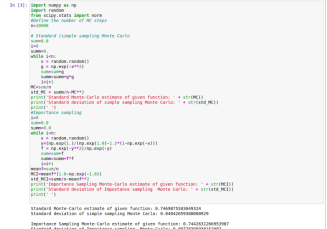
9. Find the integration value i.e. exp (*−y*2(*x*))

exp (*−y*(*x*))

10. You also find variance and hence the error.

The python code is in next page.

Pl note that the code contains the simple sampling also. Compare 32

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**Monte Carlo - More on above examples** 33

minimizes the variance. PA MonteCarl

**Importance Sampling - Examples**

Now compare the variances OR errors due to simple sampling and importance sampling both.

(2) Consider the integral

*I* =

1

*π*

*x*2 + cos2 *xdx* (45) 0

Evaluate *I* using importance sampling with *p*(*x*) = *a* exp (*−x*) where *a* is a constant.

Improtant Note: You first write Algorithm then write code in python language following the Algorithm. Can you find the value of *a* which

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Again you write Algorithm and code. PA MonteCarl

**Monte Carlo Integration - Homework** Consider

*I* =

1 0

*dx*1

1 0

*dx*2*...*

1 0

*dxng*(*x*1*, x*2*, ..., xn*) (46)

with *xi* defined in the interval [*ai, bi*] we would typically need a transformation of variables of the form

*xi* = *ai* + (*bi − ai*) *∗ ti*

if we were to use the uniform distribution on the interval [0*,* 1]. As an example, evaluate

*d***x** *d***y** *g*(**x***,* **y**) (47)

with

*I* =

5 *−*5

*g*(**x***,* **y**) = exp (*−***x**2 *−* **y**2 *−* (**x** *−* **y**)2*/*2) 35

numbers *x* and *s* and perform the test in the latter equation again. PA MonteCarl

**Monte Carlo Acceptance-Rejection method**

It is simple and and appealing method after von Neumann. Assume that we are looking at an interval *x ∈* [*a, b*], this being the domain of the PDF *p*(*x*). Suppose also that the largest value our distribution function takes in this interval is *M* , that is

*p*(*x*) *≤ M x ∈* [*a, b*] (48)

Then we generate a random number *x* from the uniform distribution for *x ∈* [*a, b*] and a corresponding number s for the uniform distribution between [0*, M*]. If

*p*(*x*) *≥ s* (49)

we accept the new value of *x*, else we generate again two new random 36