Lesson 11

http://www.chem.unl.edu/zeng/joy/mclab/mcintro.html
http://www.phys.ufl.edu/courses/phy7097-cmt/fall08/lectures/dufty111008.pdf

Monte Carlo methods

*) How to approximate the value of Pi.

We know that the area of a circle is Pi*R^2.
Pick a circle of radius R=1 and surround it with a square of side 1.
Select just quadrant where the possible values of x and y in the square can vary from 0 to 1.
Get various random numbers in this range for both x and y.
Use Pythagoras to find the hypotenuse of the respective triangles.
If this value is <= 1, it belongs to the 1/4 of the circle.
We sum all the points in this condition. The result is proportional to area of the 1/4 of the circle.
We have:
(Number of points in 1/4 of circle)/(Total number of points) = (area of 1/4 of circle)/(area of square)=(Pi*R^2/4)/R^2

```
Clear[shade, tot, sideX, sideY, hypo];
shade = 0;
tot = 10 000;
Do[
  sideX = RandomReal[];
  sideY = RandomReal[];
  hypo = Sqrt[sideX^2 + sideY^2];
  If[hypo ≤ 1., shade = shade + 1];
  , {k, 1, tot}];


Print["From Monte Carlo we get Pi=", 4. shade / tot];
Print["The actual value is ", 1. Pi]
```

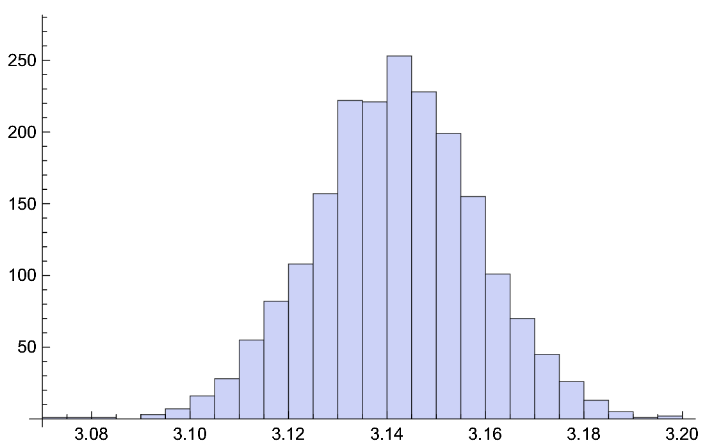
```
From Monte Carlo we get Pi=3.1572

The actual value is 3.14159
```

*) Find 2000 values of Pi using the method above.
What is the average and the variance?
Show a histogram with the distribution of those values.

```
Clear[tot, Nrea];
Nrea = 2000;
tot = 10 000;
Do[
  Clear[shade, sideX, sideY, hypo];
  shade = 0;
  Do[
   sideX = RandomReal[];
   sideY = RandomReal[];
   hypo = Sqrt[sideX^2 + sideY^2];
   If[hypo ≤ 1., shade = shade + 1];
   , {k, 1, tot}];
  pip[kk] = 4. shade / tot;
  , {kk, 1, Nrea}];
```

```
Clear[la];
la = Table[pip[kk], {kk, 1, Nrea}];
Print["Average:"];
Sum[la〚kk〛, {kk, 1, Nrea}] / Nrea
Print["Variance:"];
Sum[la〚kk〛^2, {kk, 1, Nrea}] / Nrea - (Sum[la〚kk〛, {kk, 1, Nrea}] / Nrea)^2
Histogram[la]
```

```
Average:
3.14164
Variance:
0.000276191
```



*) <u>Birthday Problem.</u>

We want to find out the probability that out of 30 people two share a birthday.

Person 1
Person 2: prob=364/365 of no overlap with the first;
Person 3: prob=363/365 of no overlap with 1 and 2;
Person 4: prob=362/365 of no overlap with 1, 2 and 3;
...
Person 30: prob=336/365 of no overlap with any person above;

The probability of having no shared birthdays is then (364/365)*(363/365)*(362/365)...(336/365) =

```
Product[1. × (365 - k) / 365, {k, 1, 29}]
```

```
0.293684
```

So the probability of having at least one pair of people having the same birthday is 71%.

Let us find this probability with the Monte Carlo Approach:
1) Pick 30 random numbers in the range [1.365].
2) Check to see if any of the thirty are equal.
3) Go back to step 1 and repeat 10000 times.
4) Report the fraction of trial that have matching birthdays.

```
Clear[trials, Npeople, matches];
trials = 10 000;
Npeople = 30;
matches = 0;

Do[
  Clear[radlis];
  radlis = Table[RandomInteger[{1, 365}], {k, 1, Npeople}];

  Do[
   Do[
     If[radlis[[k]] == radlis[[k + j]], {matches = matches + 1, Goto[end]}];
     , {j, 1, Npeople - k}];
   , {k, 1, Npeople - 1}];
  Label[end];

  , {m, 1, trials}];
1. matches / trials
```

```
0.7032
```

*) <u>Numerical integration.</u>

$$\int_a^b f(x)\,dx \sim \sum_{i=0}^{n-1} f(x_i)\,\Delta x$$

$$\Delta x = (b-a)/n$$

Different methods can be used to solve the integral above [see Lesson05 and Test 2]

MonteCarlo:
-) Select random numbers between a and b to compute f(x)
-) Compute the sum to approximate the integral

Solve the examples below exactly and with Monte Carlo:

(i) $\int_0^1 x\, dx$

(ii) $\int_0^2 x^2\, dx$

(iii) $\int_0^\pi \sin(x)\, dx$

```
Clear[Nt];
Nt = 10 000;

Print["Item (i)"]
Print["Exact:"];
Integrate[1. x, {x, 0, 1}]
Print["Monte Carlo:"];
Sum[RandomReal[], {k, 1, Nt}] (1. / Nt)

Print["Item (ii)"]
Print["Exact:"];
Integrate[1. x^2, {x, 0, 2}]
Print["Monte Carlo:"];
Sum[RandomReal[{0, 2}]^2, {k, 1, Nt}] (2. / Nt)

Print["Item (iii)"]
Print["Exact:"];
Integrate[1. Sin[x], {x, 0, Pi}]
Print["Monte Carlo:"];
Sum[Sin[RandomReal[{0, Pi}]], {k, 1, Nt}] (Pi / Nt)
```

```
Item (i)
Exact:
0.5
Monte Carlo:
0.502353
```

Item (ii)

Exact:

2.66667

Monte Carlo:

2.67117

Item (iii)

Exact:

2.

Monte Carlo:

1.9979