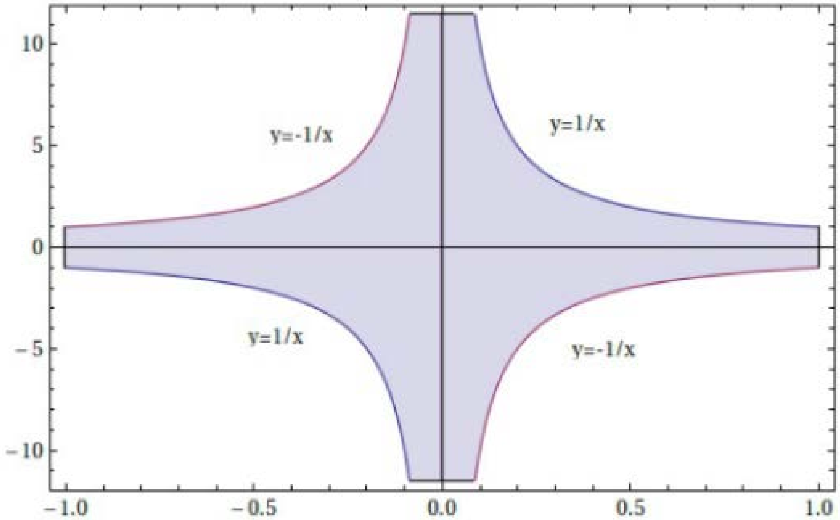
Monte Carlo integration

Exercises

1. Calculation of an area
2. Integration of an analytical function.
   - 2.a With random sampling.
   - 2.b With importance sampling.

1. Calculation of an area.

Evaluate the area enclosed between the curves $y = \pm 1/x$ within the values x ∈ [-1,+1] , y ∈ [-11,+11] represented in the figure.
Note that the exact value is A_{exact}= 13.5916.

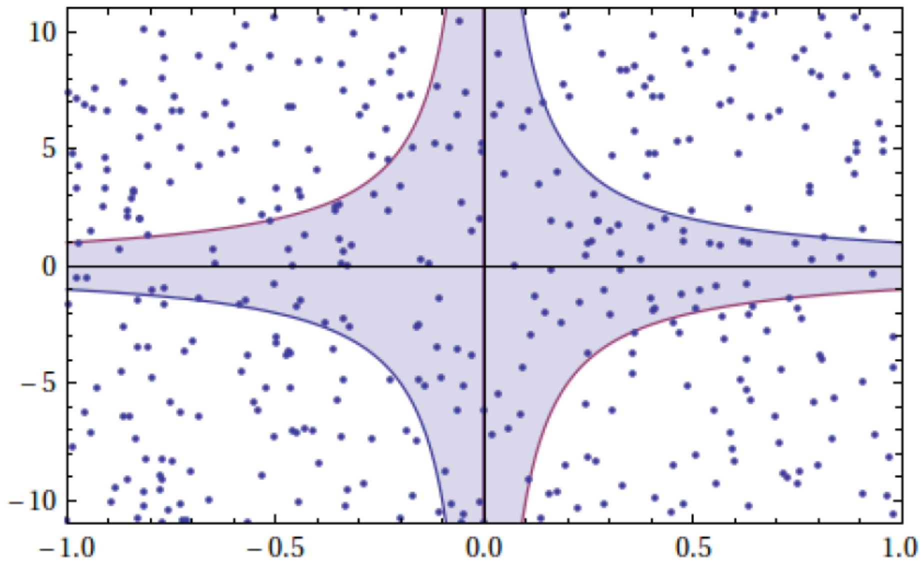


Procedure:

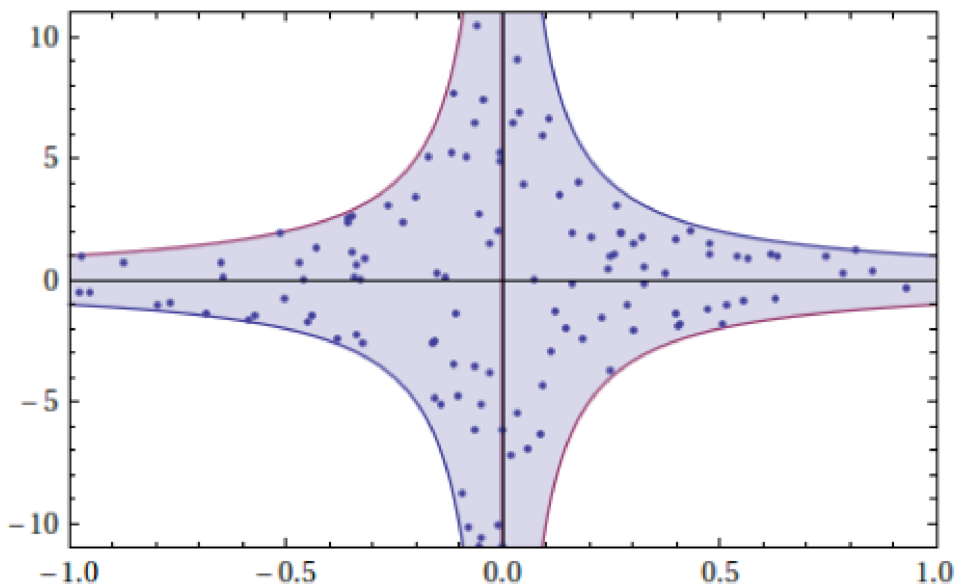
Generate at random a number N of points (x_i, y_i)

x_i: from a uniform distribution between [-1,+1]

y_i: from a uniform distribution between [-11,+11]



Calculate the number of points N_{hit} inside the region of interest:



Estimate the area as:

$$A(N) = 2 \times 22 \times \left[\frac{N_{hit}}{N}\right]$$

- Run several MC series with N= {100 ~ 10 000 000}

→ For each N:

- Calculate the mean value of the area:

$$\boxed{< A(N) >= \frac{1}{M} \sum_{i=1}^{M} A_i(N)}$$

M: number of calculations with N cycles

- Calculate its standard deviation σ (variance is defined as σ^2):

$$\boxed{\sigma(N) = \sqrt{< (A(N) - A_{exact})^2 >}}$$

- Plot $\sigma\ (N)$ versus $N^{-1/2}$

2. Integration of an analytical function.

Exercise statement : numerical calculation of

$$I = \int_0^\infty \int_0^\infty \int_0^\infty \text{Sin}[x1 + x2 + x3]^2 \, (x1\, x2\, x3\, \text{Exp}[-x1^2 - x2^2 - x3^2]) \, dx3 \, dx2 \, dx1$$

within 1 % accuracy

Hint : the result is

$$\frac{\pi\,(3 - 6\,\text{DawsonF}[1]) + 2\,e^2\,\text{DawsonF}[1]\,\left(3 - 6\,\text{DawsonF}[1] + 4\,\text{DawsonF}[1]^2\right)}{16\,e^2}$$

```
N[%]
0.0564563
```

Admisible error : $\frac{\%}{100}$

0.000564563

So the aim is to get 3 correct digits after the decimal point, the fourth digit may fluctuate.

2.a With random sampling.

a) MC calculation without Importance Sampling :

Generate a large sample of points (x1, x2, x3) in the domain

$$\{x1 \in [0, a],\ x2 \in [0, a],\ x3 \in [0, a]\} \qquad \text{with } a \to \infty$$

distributed uniformily, and evaluate

$$I = \int_0^a \int_0^a \int_0^a \mathrm{Sin}[x1 + x2 + x3]^2 \left(x1\ x2\ x3\ \mathrm{Exp}\left[-x1^2 - x2^2 - x3^2\right] \right) dx3\, dx2\, dx1 =$$

$$a^3 \left(\left\langle \mathrm{Sin}[x1 + x2 + x3]^2 \left(x1\ x2\ x3\ \mathrm{Exp}\left[-x1^2 - x2^2 - x3^2\right] \right) \right\rangle \right.$$

In practice, we can limit ourselves to using a = 7.5, since for example

$$\mathrm{Exp}\left[-x1^2 - x2^2 - x3^2\right] /. \{x1 \to 7.5\} \sim 3.7 \times 10^{-25}\ \mathrm{Exp}\left[-x2^2 - x3^2\right] \leqslant 3.7 \times 10^{-25}$$

Some results:

“a” “N”

```
{QuickMC[5.0, 50 000], QuickMC[5.0, 50 000], QuickMC[5.0, 50 000]}
{QuickMC[7.5, 50 000], QuickMC[7.5, 50 000], QuickMC[7.5, 50 000]}
{QuickMC[10., 50 000], QuickMC[10., 50 000], QuickMC[10., 50 000]}

{0.0599594, 0.0579883, 0.0556769}

{0.0572729, 0.0540836, 0.0629879}

{0.0487784, 0.0453447, 0.0632209}
```

Without importance sampling, we can only state that the result lies somewhere in the interval (0.05 ~ 0.06)

```
QuickMC[5.0, 500 000]

0.0568222

ExactValue = 0.056456;
```

2.b With important sampling

b) MC calculation with Importance Sampling :

Generate points a large sample of points (x1, x2, x3)

in the domain $(0 - \infty, 0 - \infty, 0 - \infty)$

according to the distribution probability

$$p[x1, x2, x3] = 8\, x1\, x2\, x3\ \mathrm{Exp}\left[-x1^2 - x2^2 - x3^2\right]$$

$\left(\text{Note that} \quad \int_0^\infty \int_0^\infty \int_0^\infty p[x1, x2, x3]\; dx3\, dx2\, dx1 = 1\right)$

Let's rewrite I as

$$I = \int_0^\infty \int_0^\infty \int_0^\infty f[x1, x2, x3]\, p[x1, x2, x3]\, dx3\, dx2\, dx1 =$$

$$\left(\frac{\int_0^\infty \int_0^\infty \int_0^\infty f[x1, x2, x3]\, p[x1, x2, x3]\, dx3\, dx2\, dx1}{\int_0^\infty \int_0^\infty \int_0^\infty p[x1, x2, x3]\, dx3\, dx2\, dx1} \right) \left(\int_0^\infty \int_0^\infty \int_0^\infty p[x1, x2, x3]\, dx3\, dx2\, dx1 \right)$$

with $f[x1, x2, x3] = \frac{1}{8} \mathrm{Sin}[x1 + x2 + x3]^2$

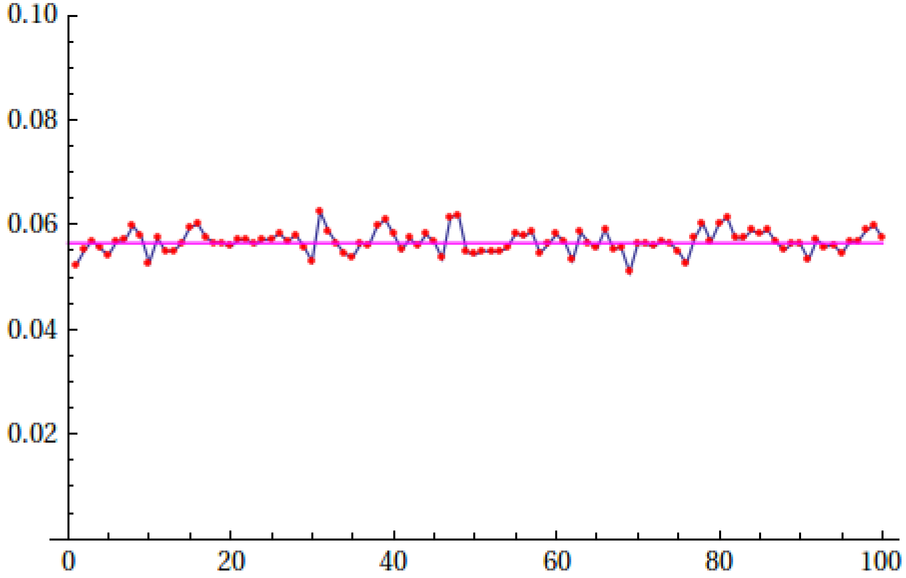
We will evaluate the quotient by means of the replacement:

$$I = \frac{\int_0^\infty \int_0^\infty \int_0^\infty f[x1, x2, x3]\, p[x1, x2, x3]\, dx3\, dx2\, dx1}{\int_0^\infty \int_0^\infty \int_0^\infty p[x1, x2, x3]\, dx3\, dx2\, dx1} \longrightarrow I = \frac{\langle f[x1, x2, x3] \rangle_{MC}}{\langle 1 \rangle_{MC}}$$

Note that $\frac{\langle f[x1, x2, x3] \rangle_{MC}}{\langle 1 \rangle_{MC}}$ can be obtained on a (large) sample of points, independently of the size of the sample.

Results for 100 MC runs

```
Show[ListLinePlot[mcdata, PlotRange → {0, 0.1}], ListPlot[mcdata, PlotStyle → {Red}],
 ListLinePlot[{{0, 0.0564563}, {100, 0.0564563}}, PlotStyle → {Magenta}]]
```




```
exactval = 0.056456

Mean[mcdata]

0.0566936
```

Extend the calculation to the 11 - dimensional case :

$$\int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \mathrm{Sin}[x1 + x2 + x3 + x4 + x5 + x6 + x7 + x8 + x9 + x10 + x11]^2$$

$$\left(x1\ x2\ x3\ x4\ x5\ x6\ x7\ x8\ x9\ x10\ x11\ \mathrm{Exp}\left[-x1^2 - x2^2 - x3^2 - x4^2 - x5^2 - x6^2 - x7^2 - x8^2 - x9^2 - x10^2 - x11^2\right] \right)$$

$$dx11\, dx10\, dx9\, dx8\, dx7\, dx6\, dx5\, dx4\, dx3\, dx2\, dx1$$

Exact result :

$$\int_0^\infty\int_0^\infty\int_0^\infty\int_0^\infty\int_0^\infty\int_0^\infty\int_0^\infty\int_0^\infty\int_0^\infty\int_0^\infty\int_0^\infty \mathrm{Sin}[x1+x2+x3+x4+x5+x6+x7+x8+x9+x10+x11]^2 \left(x1\,x2\,x3\,x4\,x5\,x6\,x7\,x8\,x9\,x10\,x11\,\mathrm{Exp}\left[-x1^2-x2^2-x3^2-x4^2-x5^2-x6^2-x7^2-x8^2-x9^2-x10^2-x11^2\right]\right) dx11\,dx10\,dx9\,dx8\,dx7\,dx6\,dx5\,dx4\,dx3\,dx2\,dx1 =$$

$$\frac{1}{4096\,e^{11}}\sqrt{\pi}\Big(11\,e^{10}\,\mathrm{Erfi}[1]+165\,e^{8}\,\pi\,\mathrm{Erfi}[1]\left(-3+\mathrm{Erfi}[1]^2\right)-55\,e^{9}\sqrt{\pi}\left(-1+\mathrm{Erfi}[1]^2\right)+$$
$$462\,e^{6}\,\pi^2\,\mathrm{Erfi}[1]\left(5-10\,\mathrm{Erfi}[1]^2+\mathrm{Erfi}[1]^4\right)-330\,e^{7}\,\pi^{3/2}\left(1-6\,\mathrm{Erfi}[1]^2+\mathrm{Erfi}[1]^4\right)+$$
$$330\,e^{4}\,\pi^3\,\mathrm{Erfi}[1]\left(-7+35\,\mathrm{Erfi}[1]^2-21\,\mathrm{Erfi}[1]^4+\mathrm{Erfi}[1]^6\right)-462\,e^{5}\,\pi^{5/2}\left(-1+15\,\mathrm{Erfi}[1]^2-15\,\mathrm{Erfi}[1]^4+\mathrm{Erfi}[1]^6\right)+$$
$$55\,e^{2}\,\pi^4\,\mathrm{Erfi}[1]\left(9-84\,\mathrm{Erfi}[1]^2+126\,\mathrm{Erfi}[1]^4-36\,\mathrm{Erfi}[1]^6+\mathrm{Erfi}[1]^8\right)-$$
$$165\,e^{3}\,\pi^{7/2}\left(1-28\,\mathrm{Erfi}[1]^2+70\,\mathrm{Erfi}[1]^4-28\,\mathrm{Erfi}[1]^6+\mathrm{Erfi}[1]^8\right)+$$
$$\pi^5\,\mathrm{Erfi}[1]\left(-11+165\,\mathrm{Erfi}[1]^2-462\,\mathrm{Erfi}[1]^4+330\,\mathrm{Erfi}[1]^6-55\,\mathrm{Erfi}[1]^8+\mathrm{Erfi}[1]^{10}\right)-$$
$$11\,e\,\pi^{9/2}\left(-1+45\,\mathrm{Erfi}[1]^2-210\,\mathrm{Erfi}[1]^4+210\,\mathrm{Erfi}[1]^6-45\,\mathrm{Erfi}[1]^8+\mathrm{Erfi}[1]^{10}\right)\Big) =$$

0.0002418585339