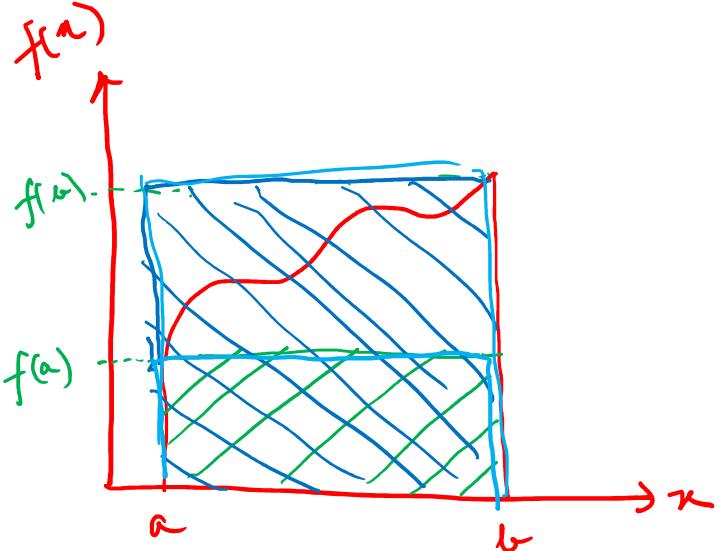
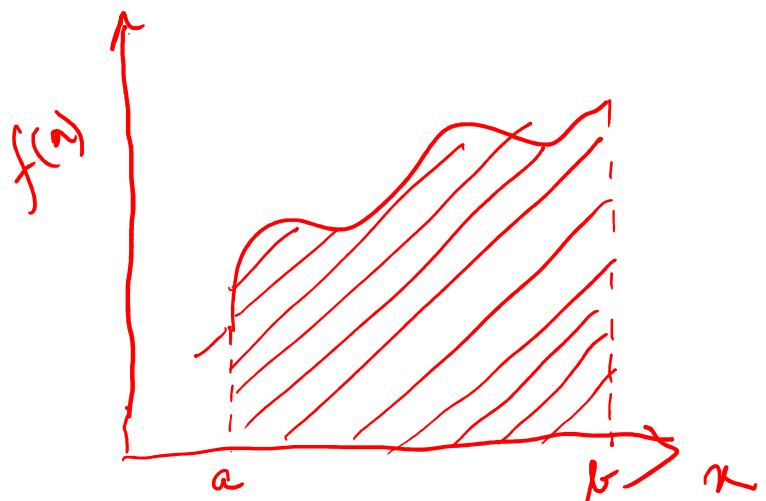


Topics to be covered

- Why we need to do numerical integration?
- Deterministic vs. stochastic methods of integration
- Examples of deterministic methods: Rectangular, trapezoidal, etc. and their limitations
- Random nos., random no generators, testing of random numbers
- Monte Carlo (MC) integration:
 - A. Introduction to MC integration ←
 - B. Errors in MC integration ←
 - C. Improvement of MC integration
 - 1. Hit & miss/ Acceptance & rejection method ←
 - 2. Change of variables ←
 - 3. Importance sampling ←
 - D. Multi dimensional integration using MC.←

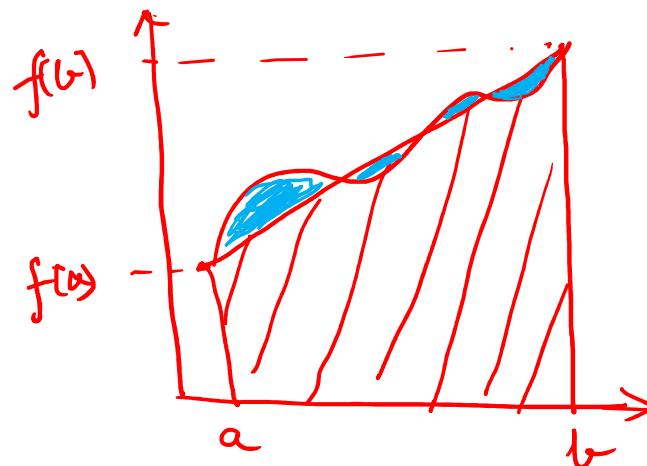


$I = \int_a^b f(x) dx$

= Area ~~under~~ ^{of} curve.

$I \approx (b-a) f(a)$
underestimating

$I \approx (b-a) f(b)$
overestimating



$\int_a^b f(x) dx$

$f(x) = x$ or $ax+by$

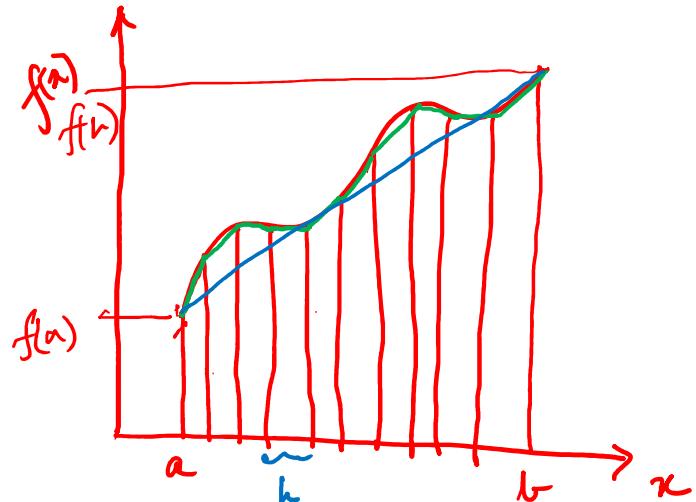
$x|f(a)$ Don't
...| know
-| $f(a)$ relate
-| to x

$$I \approx (b-a) \left[\frac{f(b)+f(a)}{2} \right]$$

Trapezoidal rule

Can we improve the estimate? Composite Trapezoidal Rule

$I = \text{Sum over area of all trapezoids}$



$$h = \frac{b-a}{n} \quad x_0 = a, x_n = b$$

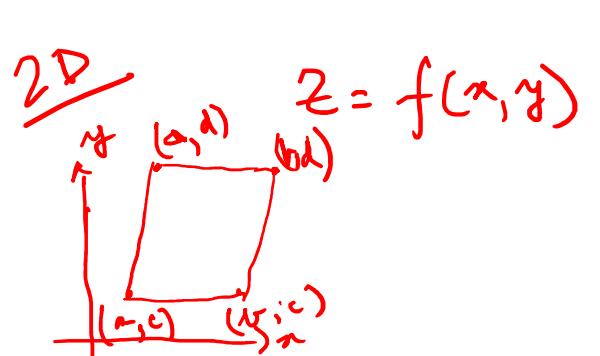
$$I = \sum_{i=1}^n I_i \quad \text{①} \quad I_i = h \left(\frac{f(x_{i-1}) + f(x_i)}{2} \right) \quad \text{②}$$

Plug in ② in ①

$$I = \frac{h}{2} \left[\left\{ f(x_0) + f(x_1) \right\} + \left\{ f(x_1) + f(x_2) \right\} + \dots + \left\{ f(x_{n-1}) + f(x_n) \right\} \right]$$

$$I = \frac{h}{2} \left[f(a) + f(b) + 2 \sum_{k=1}^{n-1} f(x_k) \right]$$

$$\text{Error} \sim O(h^2) \sim O(n^{-2})$$



$$I = \int_a^b \int_c^d z \, dx \, dy$$

$$\left. \begin{array}{l} [a, b] \\ [c, d] \end{array} \right\} \begin{array}{l} n \text{ sub-intervals each width} \\ h = \frac{b-a}{n}, x_i = x_0 + ih \\ i=0, 1, \dots, n \end{array}$$

$$k = \frac{d-c}{n} \quad y_j = y_0 + jk, j=0, 1, \dots, n$$

$$\begin{aligned} I_{2D} &= \frac{hk}{4} \left[f(a, c) + f(b, c) + f(a, d) + f(b, d) \right] \\ &\quad + 2 \sum_{i=1}^{m-1} f(x_i, c) + 2 \sum_{i=1}^{m-1} f(x_i, d) + 2 \sum_{j=1}^{n-1} f(a, y_j) + 2 \sum_{j=1}^{n-1} f(b, y_j) \\ &\quad + 4 \sum_{j=1}^{n-1} \left(\sum_{i=1}^{m-1} f(x_i, y_j) \right) \end{aligned}$$

$$\text{Error} \sim \frac{O(h^2)}{O(nk^{-2})} + \frac{O(k^2)}{O(n^{-2})}$$

$$\left. \begin{array}{l} O(n^2) \\ k=n \\ N=n^2 \\ m=N^{-2} \\ O(n^2) \sim O(N^{-2}) \\ \sim O(N^{-1}) \end{array} \right\}$$

General k dimension, what will error?

$$N = n^k \Rightarrow n = N^{1/k}$$
$$\text{Error} \sim O(n^{-2}) \sim O\left(\left(N^{1/k}\right)^{-2}\right)$$
$$\sim O(N^{-2/k})$$

$k \uparrow$ Error grid based methods ↑
Quality of my integral ↓

Computational cost ??

$$1D \sim O(n)$$

$$2D \sim O(n^2)$$

$$3D \sim O(n^3)$$

-

-

$$k-D \sim O(n^k)$$

As we increase dimension
computational cost
increases.

Feel of computational cost

10 particles.

$$\text{Dimension} = 3 \times 10 = 30$$

10 grid ~~pts~~ points along each dir.

Total # grid pts. 10^{30}

100 Tflop computer $\Rightarrow 10^{14}$ floating pt operations / s.

Time taken to compute at 10^{30} grid points

$$\sim 10^{16} \text{ s}$$

Age of our universe \sim

$$4.7 \times 10^{17} \text{ s}$$

$$E = \frac{\int dR_1 \dots dR_N \Psi^*(R_1, \dots, R_N) H(R_1, \dots, R_N) \Psi(R_1, \dots, R_N) dR_1 \dots dR_N}{\text{Normalization.}}$$

What is the way out?

$$I = \int_{a_1}^{b_1} \int_{a_2}^{b_2} \cdots \int_{a_M}^{b_M} f(x_1, x_2, \dots, x_M) dx^M$$



Integral of 1D fn. \rightarrow Area under the curve

" 2D " \rightarrow Volume enclosed

" M dimensional fn \rightarrow M+1 dimensional volume

$$I = V^{M+1} = \frac{(b_1 - a_1)(b_2 - a_2) \cdots (b_M - a_M)}{N_1 \cdot N_2 \cdots N_M} \sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2} \cdots \sum_{i_M=1}^{N_M} f(\underline{x}_i)$$

$$N_1 \cdot N_2 \cdots N_M = N$$

$$= (b_1 - a_1)(b_2 - a_2) \cdots (b_M - a_M) \cdot \sum_{i_1=1}^N \cdots \sum_{i_M=1}^N f(\underline{x}_i)$$

$$= \sqrt{N} \langle f \rangle \quad \text{where } \langle f \rangle = \frac{1}{N} \sum_{i=1}^N f(\underline{x}_i) \quad \text{where } \underline{x}_i = [x_{i_1}, x_{i_2}, \dots, x_{i_M}]$$

$$I \sim V^{M+1} = V^M \langle f \rangle$$

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^N f(x_i)$$

Choose x_i 's randomly such that they lie within the volume V^M

— then compute $\langle f \rangle$ using these random x_i 's

$$V^{M+1} \approx V^M \langle f \rangle$$

NEED RANDOM NOS.

Stochastic Method

Monte Carlo Integration.

Errors in MC integration.

— MC is a statistical average \approx of the fun.

$$\underbrace{V}_{M+1} = \underbrace{V^M}_{\langle f \rangle}$$

What is the error in statistical estimate of $\langle f \rangle$??

Error \rightarrow standard deviation of the probability distribution
fn. of $\langle f \rangle$

For j^{th} measurement $\langle f \rangle_j = \text{Do this } N \Rightarrow \langle f \rangle_j = \frac{1}{N} \sum_{i=1}^N [f(x_i)]_j$.

$$\langle f \rangle = \frac{1}{N} \sum_{j=1}^n \langle f \rangle_j$$

what is the PDF of $\langle f \rangle_j$

Central Limit Theorem.

Central Limit theorem

PDF of $\langle f \rangle_i$ is a normal distribution

& $\sigma_N = \frac{\sigma_c}{\sqrt{N}}$ is the standard deviation of the PDF that has been used to compute one measurement of $\langle f \rangle_j$

$N \rightarrow \infty$ this is accurate.

Reality N is finite

$$\sigma_N = \frac{\sigma}{\sqrt{N-1}}$$

For $N=1$ $\sigma_N \rightarrow \infty$

Compare error of grid based method & MC int.

Grid $\rightarrow O(N^{-2/k})$

MC Int $\rightarrow O(N^{-1/2})$

(i) Error in MC is independent of the dimension of integral

(ii) Grid based methods are more accurate for low dimension.

RANDOM Nos:

Natural random # generator (RNG)

www.random.org ← atmos. noises created by lighting discharge in thunder storms

www.randomnumbers.info ← quantum sources

www.conscious.com ← hardware based random nos.

Random #'s

- (i) Can't be predicted ✓
- (ii) no correlation. -

Pseudo-RNG

- linear congruent / ~~meta~~ modulo generator

$$x_i = (a \cdot \underline{x_{i-1}} + c) \bmod m, i > 0$$

$x_i, a, c, m \rightarrow$ all integers $i=0 \Rightarrow x_0$ is called the seed
 $m \rightarrow$ determines the period.

a & c are crucial to determine the period

$$\rightarrow x_i = (6x_{i-1} + 7) \bmod 5$$

$$x_0 = 2$$

$$\underbrace{2, 4, 1, 3, 0}, \underbrace{2, 4, 1, 3, 0}, \dots$$

$$x_i = (\underline{2} \cdot \underline{x_{i-1}} + \underline{1}) \bmod \underline{5}$$

$$x_0 = 0$$

$$\underbrace{11, 38}, \underbrace{11, 38}, \underbrace{11, 38}, \dots$$

Shift register

Properties of random nos. and their tests.

Generate RN uniform distribution, $x_i = [0, 1]$

$$p(x) = 1$$

(1) Average (μ) and Standard deviation (σ)

Suppose we generate N random #s.
What is the n^{th} moment of the set of N random #s.

$$\langle x^k \rangle = \frac{1}{N} \sum_{i=1}^N x_i^k p(x_i)$$

For uniform dist. $p(x_i) = 1 \Rightarrow \langle x^k \rangle = \frac{1}{N} \sum_{i=1}^N x_i^k$

at $N \rightarrow \infty$ replace \sum by \int

$$\langle x^k \rangle = \int dx x^k = \frac{1}{k+1}$$

$$\mu = \langle x^1 \rangle = 1/2$$

$\boxed{\mu = 0.5}$

$$\sigma = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{1}{\sqrt{12}} \approx 0.2886$$

$\boxed{\sigma = 0.2886}$

(b) Degree of correlation (auto-correlation function)

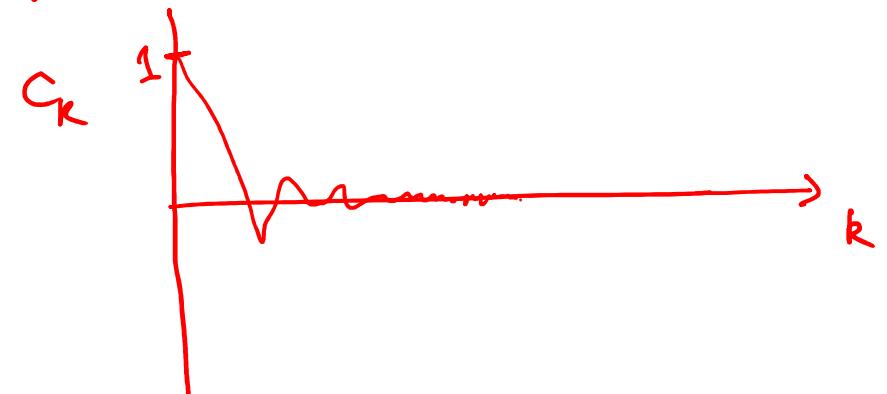
$$c_k = \frac{\langle x_{i+k} x_i \rangle - \langle x_i \rangle^2}{\langle x_i^2 \rangle - \langle x_i \rangle^2}, \quad \langle x_{i+k} x_i \rangle = \frac{1}{N-k} \sum_{i=1}^{N-k} x_i x_{i+k}$$

$k=0$

$$\boxed{c_k = 1}$$

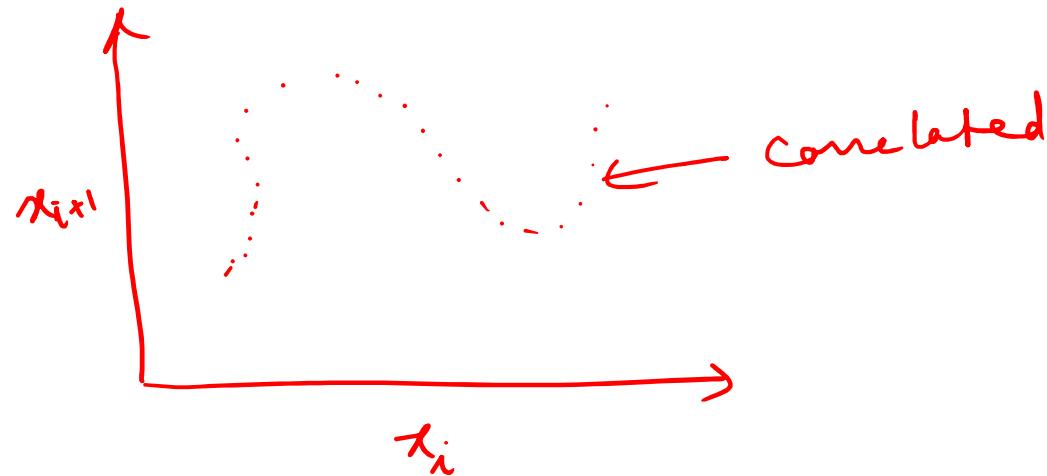
For 0 correlation / uncorrelated #s

Reality $c_k = 0$ / $c_k \rightarrow \infty$ / very small

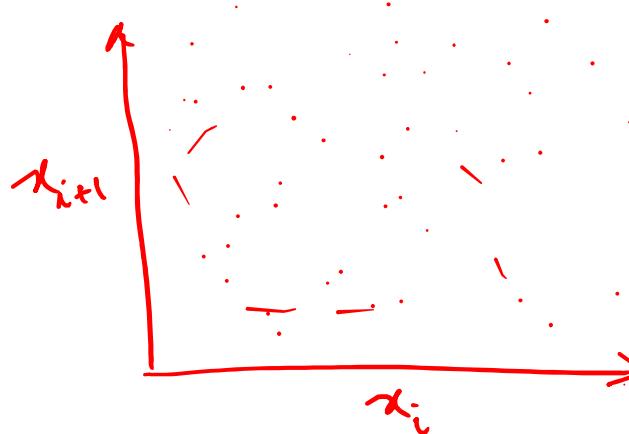


(c) Scatter plot

$x_i \quad x_{i+1}$



← correlated



← uncorrelated/
random

Random # generators in Fortran

RANDOM_NUMBER(β)

$\beta \rightarrow$ array / scalar
REAL

Fortran gives real RN
between $[0, 1]$
with uniform distribution

RANDOM_SEED([SIZE, PUT, GET])

SIZE \rightarrow Scalar, integer, INTENT(OUT)
No. of integers used to hold the seed

PUT \rightarrow Arrays, integer, INTENT(IN)
Size array \geq # returned by SIZE
value to be used as initial seed

GET \rightarrow Arrays, integers, INTENT(OUT)
current value of the seed

Usage of RANDOM NUMBER generator in Fortran

```
ubuntu [Running] - Oracle VM VirtualBox
random_number_var_seed.f90 + (~mc_int/computational_physics_2014/programs) - VIM
random_number_var_seed.f90 + (~mc_int/computational_physics_2014/program... x pghosh@pghosh-VirtualBox: ~/rahul/Modeling%20of%20Pt-H_20%20
PROGRAM ranseed
! how to change the seed for generating random nos.
IMPLICIT NONE

! ----- variables for portable seed setting -----
INTEGER :: i_seed, i, n=6
INTEGER, DIMENSION(:), ALLOCATABLE :: a_seed
INTEGER, DIMENSION(1:8) :: dt_seed
! ----- end of variables for seed setting -----
REAL :: r<--> RN

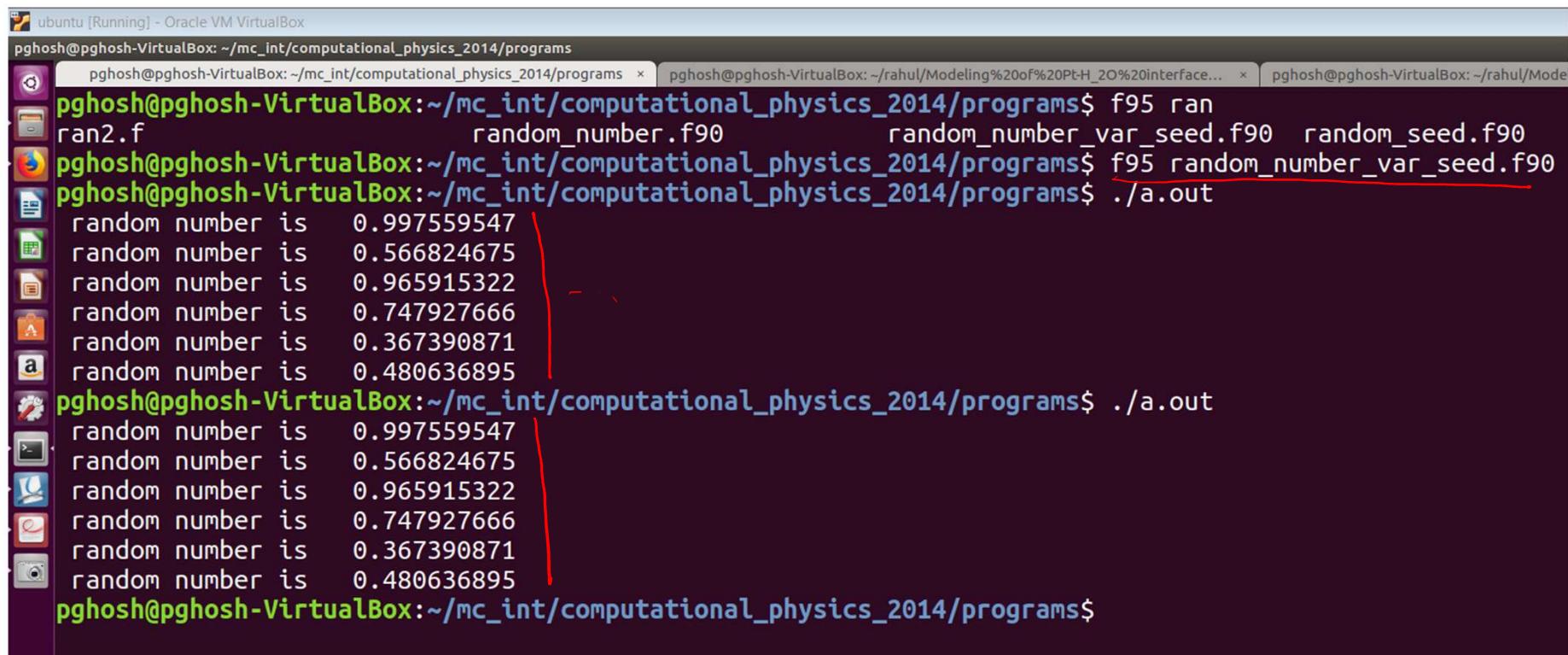
! ----- Set up random seed portably -----
CALL RANDOM_SEED(size=i_seed)
write(*,*) i_seed
ALLOCATE(a_seed(1:i_seed))
CALL RANDOM_SEED(get=a_seed)
CALL DATE_AND_TIME(values=dt_seed)
DO i=1,8
    a_seed(i)=dt_seed(i)
END DO
a_seed(i_seed)=dt_seed(8); a_seed(1)=dt_seed(8)*dt_seed(7)*dt_seed(6)
CALL RANDOM_SEED(put=a_seed)
DEALLOCATE(a_seed)
! ----- Done setting up random seed -----
DO i=1,n
    CALL RANDOM_NUMBER(r)
    WRITE(6,*) 'random number is ',r
END DO
END PROGRAM ranseed
```

SIZE → # , INTENT(OUT)
PUT → array , * (IN)
GET → array , * (OUT)

DATE_AND_TIME

→ YEAR
→ MONTH
→ DAY
→ DIF~~T~~
→ HR
→ MIN
→ SEC.
→ mill.sec.

Usage of RANDOM NUMBER generator in Fortran



The screenshot shows a terminal window on an Ubuntu system within a VirtualBox environment. The user is in the directory `~/mc_int/computational_physics_2014/programs`. They compile three source files: `ran2.f`, `random_number.f90`, and `random_number_var_seed.f90` using the command `f95 ran`. Then, they compile the `random_number_var_seed.f90` file alone using the command `f95 random_number_var_seed.f90`. Finally, they run both versions of the program, `./a.out`, which outputs six random numbers each time. A red bracket is drawn around the first three output lines from the second run, indicating a comparison between the two compilation approaches.

```
pghosh@pghosh-VirtualBox:~/mc_int/computational_physics_2014/programs$ f95 ran  
ran2.f          random_number.f90      random_number_var_seed.f90  random_seed.f90  
pghosh@pghosh-VirtualBox:~/mc_int/computational_physics_2014/programs$ f95 random_number_var_seed.f90  
pghosh@pghosh-VirtualBox:~/mc_int/computational_physics_2014/programs$ ./a.out  
random number is  0.997559547  
random number is  0.566824675  
random number is  0.965915322  
random number is  0.747927666  
random number is  0.367390871  
random number is  0.480636895  
pghosh@pghosh-VirtualBox:~/mc_int/computational_physics_2014/programs$ ./a.out  
random number is  0.997559547  
random number is  0.566824675  
random number is  0.965915322  
random number is  0.747927666  
random number is  0.367390871  
random number is  0.480636895  
pghosh@pghosh-VirtualBox:~/mc_int/computational_physics_2014/programs$
```

Usage of RANDOM NUMBER generator in Fortran

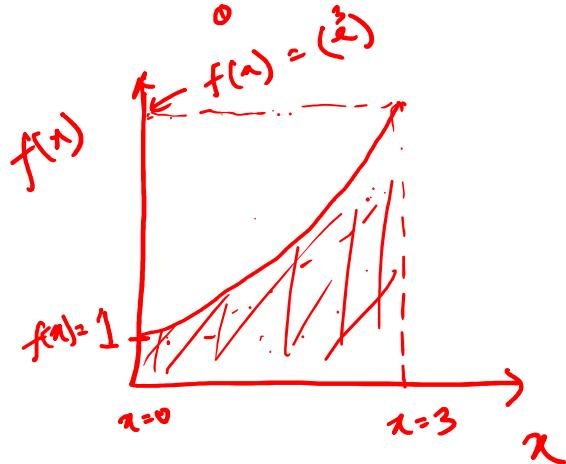
```
ubuntu [Running] - Oracle VM VirtualBox
pghosh@pghosh-VirtualBox: ~/mc_int/computational_physics_2014/programs
pghosh@pghosh-VirtualBox: ~/mc_int/computational_physics_2014/programs x pghosh@pghosh-VirtualBox: ~/rahul/Modeling%20of%20Pt-H_2O%20interface... x pghosh@pghosh-VirtualBox: ~/rahul/Mode
pghosh@pghosh-VirtualBox:~/mc_int/computational_physics_2014/programs$ f95 random_number_var_seed.f90
pghosh@pghosh-VirtualBox:~/mc_int/computational_physics_2014/programs$ ./a.out
random number is  0.505306959
random number is  0.962101996
random number is  0.666360795
random number is  0.141213417
random number is  0.273788571
random number is  0.954724312
}
pghosh@pghosh-VirtualBox:~/mc_int/computational_physics_2014/programs$ ./a.out
random number is  0.441632032
random number is  0.813283026
random number is  0.907419145
random number is  0.150628090
random number is  0.804107785
random number is  0.703152657
}
pghosh@pghosh-VirtualBox:~/mc_int/computational_physics_2014/programs$
```

ran0, ran1, ...

Acceptance / Rejection Method

After von Neumann

$$I = \int_0^3 \exp(x) dx$$



Hit or Miss Method

uniform dist. $[0, 1]$

for $x [0, 3]$

for $y [0, e^3]$

$$x \in [0, 3]$$

$$y \in [0, e^3]$$

$$x = 3 * \text{rand}$$

$$\rightarrow y = \exp(3) * \text{rand}$$

$$s=0$$

If $y < \exp(x)$ $s = s + 1$

Repeat N no. of times

Fraction of #s in shaded region = $\frac{s}{N}$

$$I \approx 3 * \exp(3) * \frac{s}{N}$$

Improvement of MC

- (i) Error \Rightarrow smaller variance
- (ii) Fewer MC sampling

(i) Change of variables

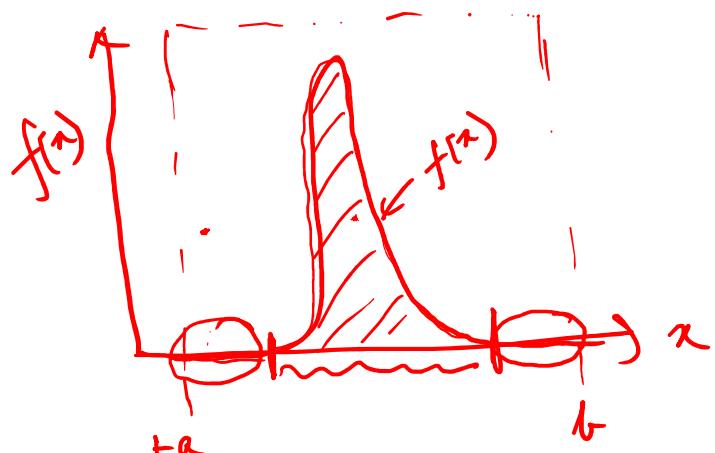
RNG (Fortran)

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

$x \in [0, 1]$

Need map $x \in [0, 1] \rightarrow y \in [a, b]$

(ii) Sampling \Rightarrow Shape of the integrand.



$$\langle H \rangle = \int dx \psi^*(x) H(x) \psi(x)$$

Ensures smooth behaviour in the neighbourhood of the exact solution.

$$I = \int_a^b f(x) dx$$

Quantum mechanics : $\rho(x) = \psi^*(x) \psi(x)$

$\psi \rightarrow \text{normalized}$

$(H(x)) \psi(x) = E \psi(x)$

$$\begin{aligned} &= \int dx \underbrace{\psi^*(x) \psi(x)}_{\rho(x)} \underbrace{\frac{H(x)}{\psi(x)} \psi(x)}_{\tilde{H}(x)} dx \\ &= \int dx \rho(x) \tilde{H}(x) dx \\ &= \int dx \rho(x) E \cancel{\psi(x)} \\ &= \underline{E} \end{aligned}$$

$\tilde{H}(x) = \frac{H(x)}{\psi(x)} \psi(x)$
 $= E$

$\therefore \int dx \rho(x) = 1$

Change variables : Starting : PDF $p(x) = \begin{cases} 1 & \text{for } 0 \leq x \leq 1 \\ 0 & \text{elsewhere} \end{cases}$

$$\int_{-\infty}^{\infty} p(x) dx = 1$$

$x \rightarrow y$ Conservation of probability
 y PDF $\rightarrow p(y)$

$$\underbrace{p(y) dy}_{\text{y'}}$$
 $= \underbrace{p(x) dx}_{\text{x'}}$ $= dx$

$$\int_0^{y'} p(y') dy' = x$$

$$x(y) = \int_0^{y'} p(y') dy'$$

$$y(x)$$

↑
cumulative distribution
of $p(y)$

Ex(1)

$$f(y) dy = \frac{dy}{b-a} \quad a \leq y \leq b$$
$$= 0 \quad \text{Else where.}$$

$$\frac{dy}{b-a} = \frac{f(x)dx}{b-a} = 1 dx$$
$$x(y) = \int_a^y \frac{dx}{b-a} = \frac{y-a}{b-a}$$

$$\boxed{y = a + (b-a)x}$$

$\begin{cases} [0,1] \\ [a,b] \end{cases}$

Ex 2

Exponential distn :

How to apply this to perform the integration??

$$\begin{aligned}
 I &= \int_0^\infty f(y) dy = \int_0^\infty e^{-y} \frac{F(y)}{e^{-y}} dy \\
 &\quad \text{Diagram: A green circle labeled } G(y) = \frac{F(y)}{e^{-y}} \text{ is shown next to the fraction.} \\
 &= \int_0^1 G(y(x)) dx \\
 &\approx \frac{1}{N} \sum_{i=1}^N G(y(x_i))
 \end{aligned}$$

$$f(y) dy = e^{-y} dy$$

$$e^{-y} dy = dx$$

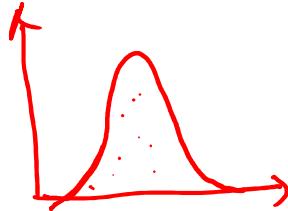
$$x = \int_0^y e^{-y'} dy' = 1 - e^{-y}$$

$$y(x) = -\ln(1-x)$$

$$x \in [0, 1] \quad y \in [0, \infty)$$

where x_i is a random # $[0, 1]$

Importance Sampling:



PDF $p(y) \rightarrow$ matches a fn F defined in
the interval $[a, b]$
Norm. $\int_a^b p(y) dy = 1$

$$I = \int_a^b f(y) dy = \int_a^b (p(y) F(y) / p(y)) dy$$

$$= \int_{y(a)}^{y(b)} \frac{F(y(x))}{p(y(x))} dx$$

$$I \approx \frac{1}{N} \sum_{i=1}^N \frac{F(y(\alpha_i))}{p(y(\alpha_i))} \leftarrow \tilde{F}$$

$$x(y) = \int_a^y p(y') dy' = z \quad \text{Invert}$$

$$y(x) = z \quad \text{Invert}$$

Cond. on $p(y)$

(i) Normalizable, +ve definite

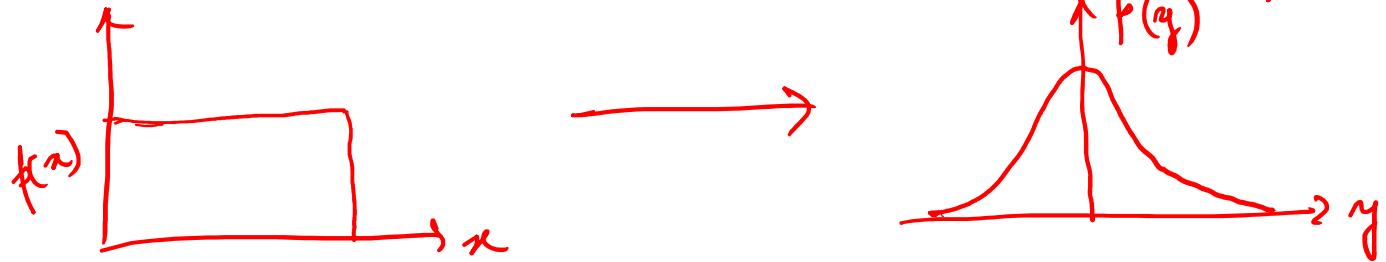
(ii) Integrable analytically

(iii) Invertible.

Error estimate. $\sigma^2 = \frac{1}{N} \sum_{i=1}^N (\tilde{F})^2 - \left(\frac{1}{N} \sum_{i=1}^N \tilde{F} \right)^2$

$$\tilde{F} = \frac{F(y(x_i))}{p(y(x_i))}$$

Uniform disk. \rightarrow normal distribution / Gaussian



$$\underbrace{p(x) dx}_{\text{"1"}} = \underbrace{p(y) dy}_{\text{}}$$

$$x(y) = \int_0^y e^{-y'^2/2} dy' \leftarrow \begin{array}{l} \text{Not possible to integrate} \\ \text{analytically} \\ \text{Error fn.} \end{array}$$

Box - Muller Transform:

$$\underbrace{p(y_1, y_2, \dots) dy_1 dy_2 \dots}_{\text{Joint probability}} = p(x_1, x_2, \dots) \left| \frac{\partial(x_1, x_2, \dots)}{\partial(y_1, y_2, \dots)} \right| dx_1 dx_2 \dots \quad \textcircled{1}$$

$$p(x_1, x_2) = e^{-(x_1^2 + x_2^2)/2} \quad \textcircled{2}$$

Switch to polar coord.

$$x_1 = r_1 \cos \theta_2$$

$$x_2 = r_1 \sin \theta_2$$

$$\frac{\partial(x_1, x_2, \dots)}{\partial(r_1, \theta_2, \dots)} = \frac{\partial(x_1, x_2, \dots)}{\partial(r_1, \theta_2, \dots)} \cdot \frac{\partial(r_1, \theta_2, \dots)}{\partial(y_1, y_2, \dots)} \quad \text{Derivative of all axis w.r.t. } y$$

$$\frac{\partial x_i}{\partial y_j}$$

$$\left. \begin{array}{l} y_1^2 = x_1^2 + x_2^2 \\ y_2 = \tan^{-1}\left(\frac{x_2}{x_1}\right) \end{array} \right\} \quad \textcircled{3}$$

$$p(y_1, y_2) dy_1 dy_2 = e^{-(x_1^2 + x_2^2)/2} \begin{vmatrix} \frac{\partial x_1}{\partial y_1} & \frac{\partial x_1}{\partial y_2} \\ \frac{\partial x_2}{\partial y_1} & \frac{\partial x_2}{\partial y_2} \end{vmatrix} dy_1 dy_2$$

$x_1 = y_1 \cos y_2$
 $x_2 = y_1 \sin y_2$

$$= e^{-y_1^2/2} \begin{vmatrix} \cos y_2 & -y_1 \sin y_2 \\ \sin y_2 & y_1 \cos y_2 \end{vmatrix} dy_1 dy_2$$

$$p(y_1, y_2) dy_1 dy_2 = e^{-y_1^2/2} y_1 dy_1 dy_2$$

$y_2 \in [0, 2\pi]$ Multiply RN from uniform dist.
 $y_1 = (x_1^2 + x_2^2)^{1/2} \Rightarrow y_1 \in [0, \infty)$ $\uparrow [0, 1]$

$$\text{Let } u = \frac{1}{2} y_1^2 \Rightarrow y_1 = \sqrt{2u}$$

$$du = y_1 dy_1$$

$$e^{-y_1^2/2} y_1 dy_1 = e^{-u} du \quad \text{New PDF}$$

$$u = -\ln(1-x') \quad x' \in [0, 1]$$

$$x_1 = y_1 \cos y_2 = \sqrt{-2 \ln(1-x')} \cos y_2$$

$$x_2 = y_1 \sin y_2 = \sqrt{-2 \ln(1-x')} \sin y_2$$

$$y_2 \in [0, 2\pi], \quad x' \in (0, 1)$$

Some more simplification.

$$\text{Let } 1-x^2 = s$$

$$x^2 = 0 \quad s=1$$

$$x^2 = 1 \quad s=0$$

$$x_1 = \sqrt{-2 \ln s} \cos \gamma_2$$

$$x_2 = \sqrt{-2 \ln s} \sin \gamma_2$$

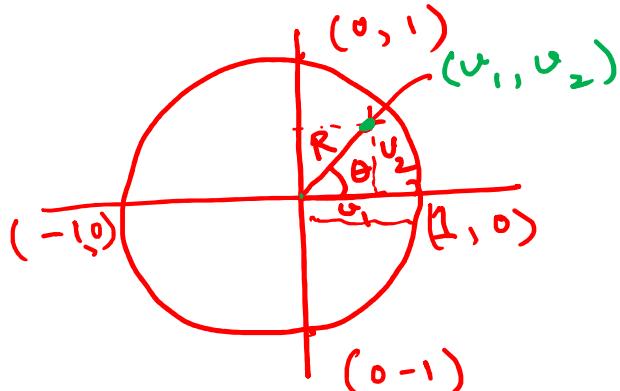
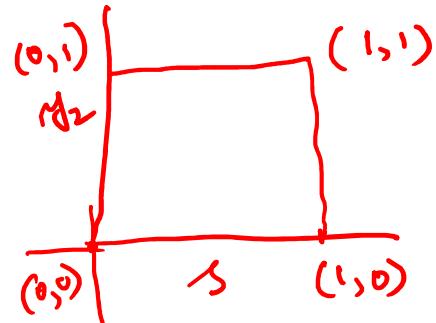
$$x_1 = \sqrt{-2 \ln s} \cos 2\pi \gamma_2$$

$$x_2 = \sqrt{-2 \ln s} \sin 2\pi \gamma_2$$

$$s \in (0, 1]$$

$$\gamma_2 \in [0, 1]$$

Box Muller



Pick up uniform deviates in an unit γ_2 .

Let v_1, v_2
ordinate abscissa

$$R^2 = v_1^2 + v_2^2$$

$$s = R^2 = v_1^2 + v_2^2$$

$$\cos \theta = \frac{v_1}{R} \quad \sin \theta = \frac{v_2}{R}$$

(1) 2 random #s v_1, v_2 from uniform dist $[0, 1]$

) (2) Compute $s \Rightarrow$ IF $s=0$ OR $s>1$

throw away v_1, v_2
else x_1, x_2

Try
the step
again

$v_1, v_2 \rightarrow$ uniform dist. $[0, 1]$

$$x_1 = \sqrt{-2 \ln R^2} \frac{v_1}{R}$$

$$x_2 = \sqrt{-2 \ln R^2} \frac{v_2}{R}$$

Normal / Gaussian dist.

Advantage of Box-Muller Tr.

$$x_1 = \sqrt{-2 \ln s} \cos(2\pi y_2)$$

$$x_2 = \sqrt{-2 \ln s} \sin(2\pi y_2)$$

- 4 Multiplication
- $2\pi \ln s \rightarrow (1)$
 - $2\pi y_2 \rightarrow (1)$
 - $\sqrt{s} \rightarrow \cos/\sin (2)$

1 Sq root

1 ln

2 Trigonometric operation

BM

$$x_1 = \sqrt{-2 \ln R^2} \frac{v_1}{R} \quad R^2 = v_1^2 + v_2^2$$

$$x_2 = \sqrt{-2 \ln R^2} \frac{v_2}{R}$$

(i) No trigonometric fun. evaluation
expensive

5 Multiplication. $R^2 \rightarrow (2) \rightarrow v_1 \cdot v_1; v_2 \cdot v_2$

$2 \cdot \ln \rightarrow (1)$

$\sqrt{\cdot} \frac{v_1}{R}; \sqrt{\cdot} \frac{v_2}{R} \rightarrow (2)$

✓ 1 square root

2 division

✓ 1 ln

Multi-dimensional Integration.

$$\underline{x} = [x_1, x_2, x_3]$$

$$\underline{y} = [x_4, x_5, x_6]$$

$$g(\underline{x}, \underline{y}) = \exp(-\underline{x}^2 - \underline{y}^2 - (\underline{x} - \underline{y})^2/2)$$

* Importance sampling Gaussian PDF: $\frac{1}{\sqrt{\pi}} e^{-x^2}$

$$I = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \left(\prod_{i=1}^6 \frac{1}{\sqrt{\pi}} e^{-x_i^2} \right) \exp(-\underline{x}^2 - \underline{y}^2 - (\underline{x} - \underline{y})^2/2) d\underline{x}_1 d\underline{x}_2 \dots d\underline{x}_6$$

$$I = \pi^3 \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} e^{-\left[(x_1 - x_4)^2 + (x_2 - x_5)^2 + (x_3 - x_6)^2 \right]/2} dy_1 dy_2 \dots dy_6$$

- (1) Brute force MC
- (2) Importance sampling

Avg of this fn.

{Remember to change σ_{BM} to $\sigma = 1/\sqrt{2}$ }

$$I = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} d\underline{x} d\underline{y} g(\underline{x}, \underline{y})$$

6-dimensional Integral

$$\frac{e^{-\underline{x}} f(\underline{x})}{e^{-\underline{x}}}$$

$$\mu = 0$$

$$\sigma = \frac{1}{\sqrt{2}}$$

