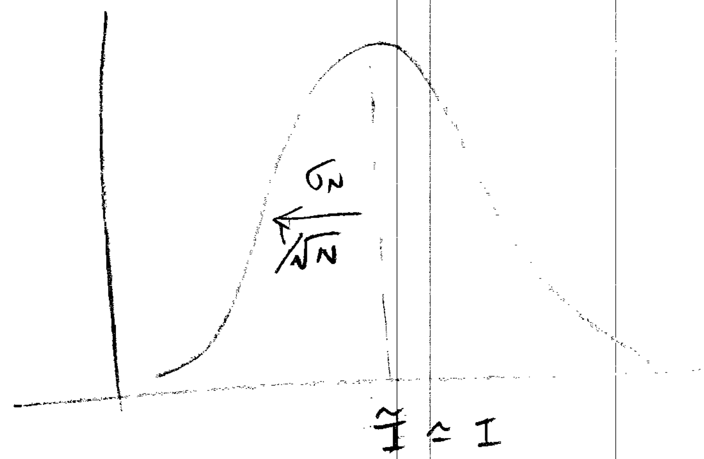
In general, histogram of Integral(N) for many diff. runs.



Note: The dist of an avg tends to be normal even if the dist from which the avg is computed is non-normal.

$I \sim \langle f \rangle$.

By Central Limit Theorem, for Large N,

dist ~ gaussian with width $1/\sqrt{N}$

so, as N ↑, estimate get better ~ $1/\sqrt{N}$!

☆ On the other hand, from your (ind. exercise),

$\Delta(N)$ (SR) ~ h^4 or $\frac{1}{N^4}$ $\left(h = \frac{(b-a)}{N}\right)$
(in 1D)

$\left(\varepsilon \lesssim 10^{-5} \right.$, need $N \sim 20 \rightarrow \left. \frac{1}{N^4} \lesssim 10^{-5} \right)$

★ the type of errors are different :

MC — <u>probabilistic</u>

— more pts → <u>statistic</u> gets better !

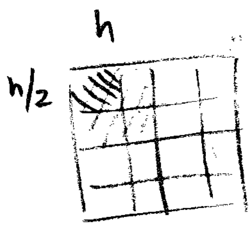
★ convergence depends on the averaging process $\sim \frac{1}{\sqrt{N}}$

<u>AND</u> not on dimensionality of integral !

SR (others) — <u>approx. in fitting integrant</u>

★ — poly. better approx $f(x)$ if grid is finer !

★ convergence depends on step size h



<u>But</u>, $N \sim h^{-d}$ for d-Dim.

$\begin{cases} h \to h/2 \\ 4 \to 16 \end{cases}$

e.g. to $\frac{1}{2}h$, $N(\tfrac{1}{2}h) = 2^d N(h)$!

so, accuracy in SR (others) depends on dimension of integral !

bottom line:

- If $d < 4$, other method will in general requires less function calls to get good approx.

  $\varepsilon \sim h^4$ SR

  $N \sim h^{-d} \rightarrow h \sim N^{-1/d} \rightarrow \varepsilon \sim N^{-4/d}$

- If $d \gtrsim 4$, MC is comparable in efficiency. For d large, MC usually converge faster.

Practical way to test for accuracy

$$I_N - I_{N'} < \varepsilon$$

N & N' different set of N #s.

If yes, $\bar{I}_{2N} = \langle I_N, I_{N'} \rangle$

If NO, $I_{2N'}$ with different set of $2N$ #s

compare $I_{2N'}$, $\bar{I}_{2N}$

<u>example:</u> thermodynamics (integral over phase space)

$$\bar{u} = \frac{\int u\, e^{-E/kT}\, dp^{3N}\, dq^{3N}}{\int e^{-E/kT}\, dp^{3N}\, dq^{3N}}$$

for N particles!

→ this type of <u>HIGH</u> dim integral is basically intractable but with MC.

(Answer might not be accurate but it serves well as rough estimate!)

Other advantages:

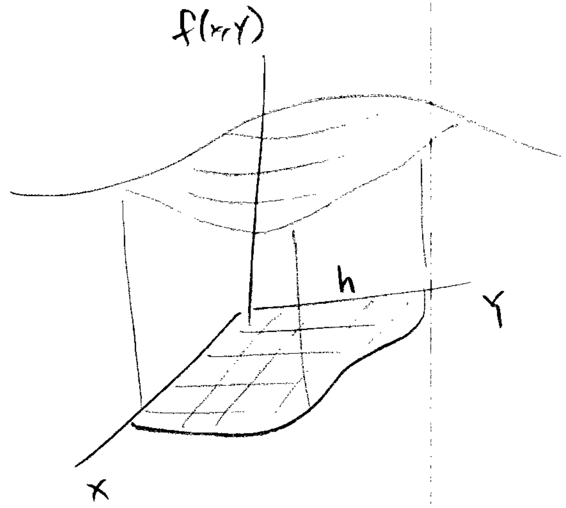
① - it is slow, but it always works! MC might give <u>estimates</u>)
(if all else fails.

② - singularities don't bother!

Multidimensional Numerical Integration

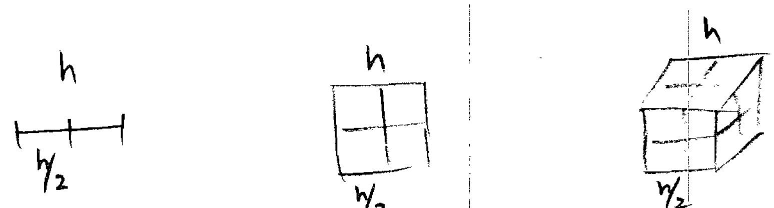
2D:

$$I = \int_a^b \int_c^d f(x,y)\,dx\,dy$$



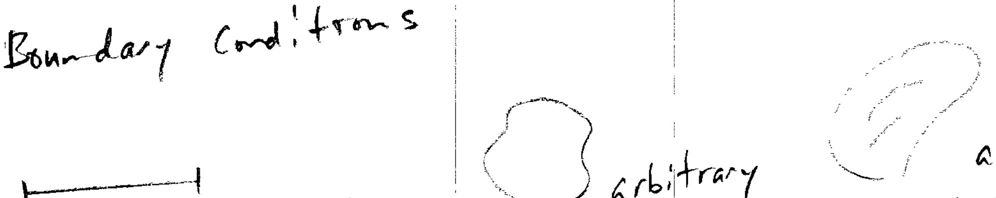
Difficulties with multi-D Integrals:

1. N (# of grid pts / evaluation pts) $\sim h^{-d}$ ← precision needed



$$\frac{N'}{N} = 2^1 \qquad \frac{N'}{N} = 2^2 \qquad \frac{N'}{N} = 2^3$$

2. Boundary Conditions



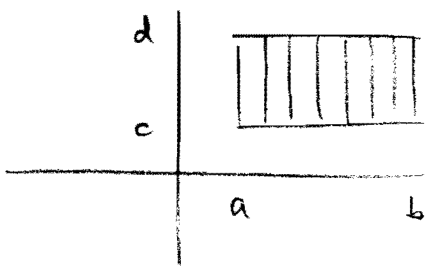
1D → 2pts (simple)

2D - curves, arbitrary

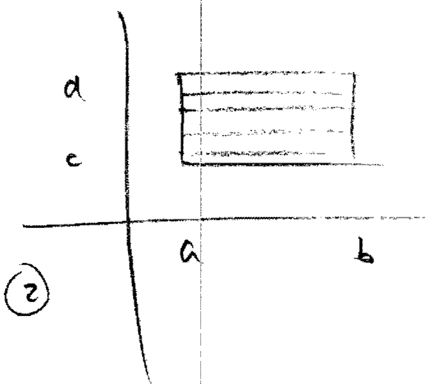
3D - surfaces, arbitrary

Simple Rect Case :

If a, b, c, d in $\int_a^b \int_c^d dx\,dy$ are constant, the integrating domain is a rectangle.



①



②

Solution:

Nested 1D integrators :

① Column first

$$\int_c^b \int_c^d f(x,y)\,dx\,dy = \int_a^b G(x)\,dx$$

where $G(x) = \int_c^d f(x,y)\,dy$

x is a parameter here!

example : Trap rule

Main loop

Do

$I = \frac{1}{2} G(x_0) + G(x_1) + \dots + \frac{1}{2} G(x_N)$, Trap step

$h = h/2$, half interval

while (% error < tol)

function G(x)

Do

$I' = \frac{1}{2} f(x, y_0) + f(x, y_1) + \dots \frac{1}{2} f(x, y_N)$, inner trap step

$h = h/2$

while (% error < tol)

★ function G(x) of outer trap is another integration.

★ Grid in x & y are not necessary identical

★ don't recalculate inner G(x) if you need to half hx in outer loop.

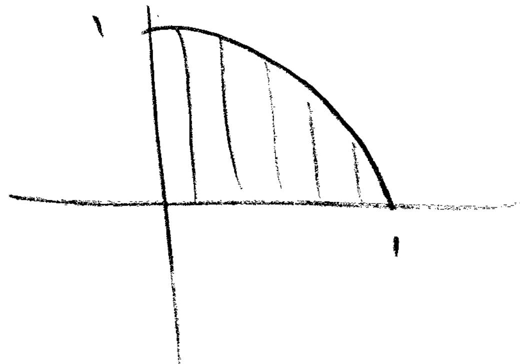
(2) Row first :

$$\int_a^b \int_c^d f(x,y)\, dx\, dy = \int_c^d F(y)\, dy$$

where $F(y) = \int_a^b f(x,y)\, dx$

Other domains :

- know boundary $y = f(x)$

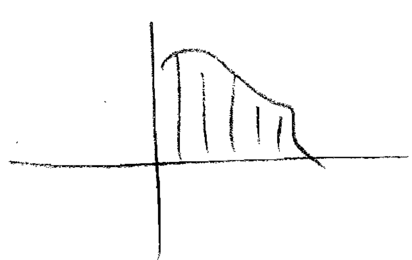


circle

$$I = \int_0^1 \int_0^{\sqrt{1-x^2}} f(x,y)\,dy\,dx$$

☆ need functn $\sqrt{1-x^2}$ to decribe boundary.

- boundary without analytic functon



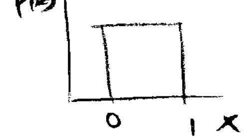
- conditional check for end pt at each column.

- Monte Carlo

Another way to do this average!

– by <u>uniformly</u> but <u>randomly</u> sample pts in $[a,b]$

Then $\underbrace{\langle f \rangle_N = \frac{1}{N} \sum_i f(x_i)}$ $\leftarrow$ $x_i \in P_{\text{uniform}}(x)$.

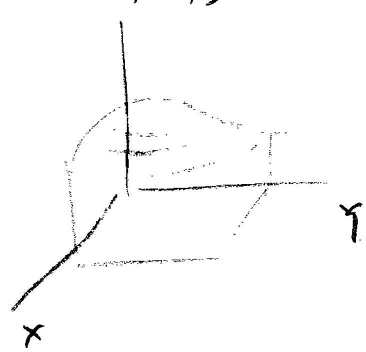


$$\Rightarrow \quad \underline{\int_a^b f(x)\,dx \simeq I_N = (b-a)\langle f \rangle_N}$$

Monte Carlo estimate of integral.

☆ (see 8' for important sampling)

2D MC integration



$$I = \int_a^b \int_c^d f(x,y)\,dx\,dy$$

↑ volume under surface.

$$I \simeq I_N = \underset{\substack{\uparrow \\ \text{area in} \\ \text{domain}}}{(b-a)(d-c)} \underbrace{\frac{1}{N}\sum_i f(x_i,y_i)}_{\langle f \rangle_N}$$

– simple extension to higher D!

(c) Imporper Integrals

Types: (1) $\int_a^b f(x)\,dx$, either a or b = ∞.

(2) $\int_a^b f(x)\,dx$, f(x) is singular at $x \in [a,b]$.

(3) $\int_a^b f(x)\,dx$, $f(x) \to \infty$ at either a, b but $\int_a^b f(x)\,dx < \infty$.

Soln:

(3) – Newton-Cotes Open Formulas
see, press or Natamura

(2),(3) – Monte Carlo method

(2) – Find singularity, partition [a,b]
→ $[a, x_0]$ $[x_0, b]$ then use
Newton - Cotes Open

(2) – choice of grid so that x_i won't land on x_c!

1 - Remap range :

$$\int_a^b f(x)\,dx = \int_{1/b}^{1/a} \frac{1}{t^2} f\left(\frac{1}{t}\right) dt \qquad ab>0.$$

($x = \frac{1}{t}$ substitution)

Can be used with either $a \to \infty$ <u>or</u> $b \to \infty$.

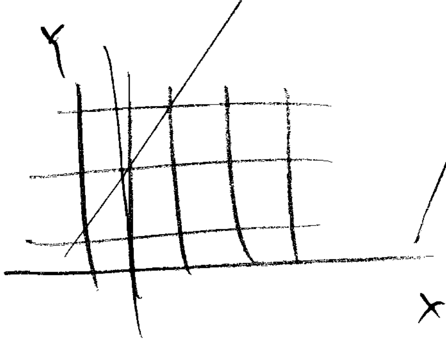
or other change of variables

→ see Press

Monte Carlo Method

(effective for $D \geq 2$ integrals)

(or $f(x)$ singular in $[a,b]$)



grid pts $\sim N^D$

For D large, numerical costly!