i.e. $\int_a^b f(x)\,dx =$

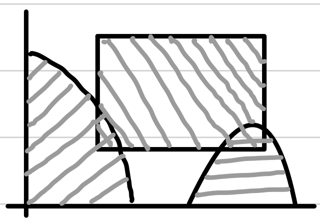
n:

Count hits n_{hit} as number of points

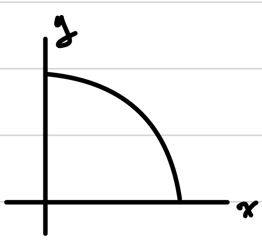
"Hit-or-miss MC" -

- call $\rho =$, uncertainty in I is

Useful for

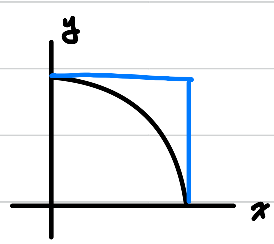
e.g. want area of  -

-

E.g. 

unit quarter circle

$A = \frac{\pi}{4}$ $\rightarrow$



Note: Ratio of areas is

$\frac{\pi}{4} = I \approx$ Area $=$ where $g(x,y) =$

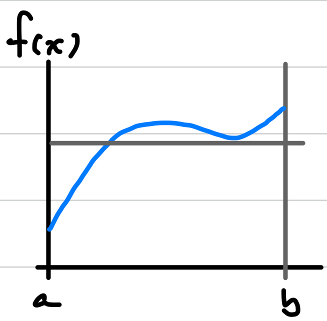
```
sum = 0
do i = 1, N
    x_i =
    y_i =
    if (              ) then

    endif
enddo
area =
```

MC Approach #2 "Sample Mean Method"

Recall definition for

$\langle f \rangle =$ - ave. value of



$\langle f \rangle$

estimate $\langle f \rangle$ by

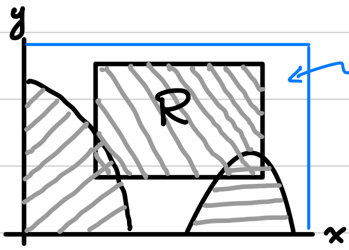
Generate RNs

Calculate $\langle f \rangle \approx$

$\Rightarrow \int_a^b f(x)\,dx =$

- works well for

For domains with complicated geometries



want I

$I \approx$

where $H(x,y) = \begin{cases} \\ \end{cases}$

Metropolis Algorithm and Thermodynamics

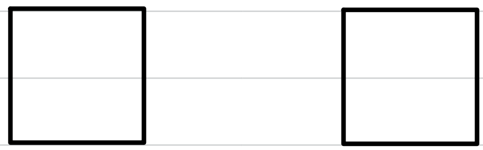
Consider a container filled with a fluid -

- at temperature T. Particle and

, as well as system properties like

, are different at .

System samples different configurations



Thermodynamic average of some property is

$\langle f \rangle =$

- p_i
- f_i

Could randomly, uniformly

- MANY,
- vast majority of states

Better to sample states

$\langle f \rangle =$

But how do we

In thermal equilibrium

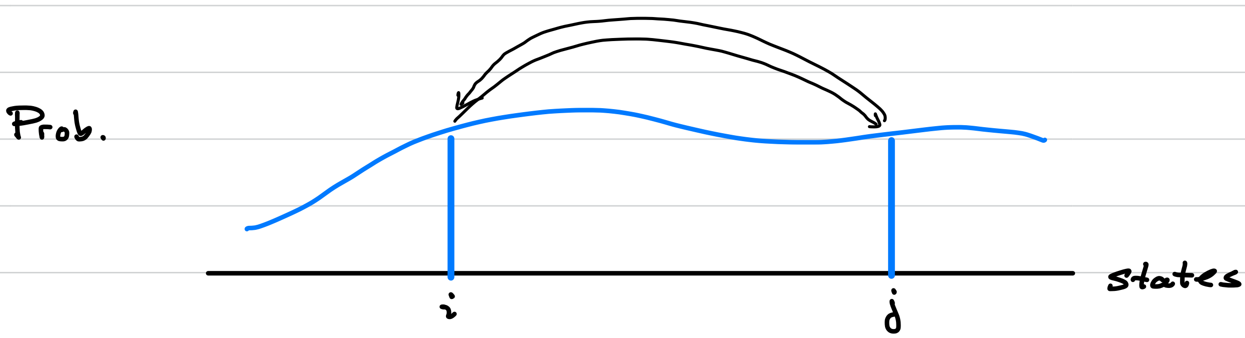
- E_i is , $\beta =$, $k_B \doteq$

$Z =$ is the

- normalization factor such that

We will invoke

$T_{i \to j}$ is transition probability



- ensures that distribution of states remains ,
i.e.
by balancing " " between every pair of states.

- allows construction of

$T_{i\to j} =$

Two parts to $T_{i\to j}$:

$\alpha_{i\to j}$

$acc_{i\to j}$

Detailed balance $\quad p_i T_{i\to j} = p_j T_{j\to i}$

$\to$ construct algorithm such that

e.g. trial particle coordinate
works, since, say, generating $x_j =$ from $x_i =$
is just a likely as generating

but for
since you can generate
but you can't generate

Detailed balance $\Rightarrow$

ΔE is

a couple of possibilities for the acceptance probability

→ $acc_{i \to j}$ = drawback: requires expensive

→ $acc_{i \to j}$ =

i.e. If energy decreases,
If energy increases,

As T increases,
→ all proposed states
→ uphill energy moves

Algorithm
1) choose 1 of N particles

2) consider a new state j

3) if
4) if

5) if state did not change,

6) Carry out steps

7) Do many