i.e. $\int_a^b f(x)\,dx = H(b-a)\,\dfrac{n_{hit}}{n} = I$

$n$: # of random points used

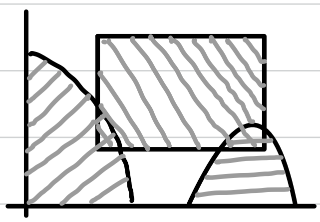
Count hits $n_{hit}$ as number of points $(x_i, y_i)$ that satisfy $y_i \le f(x_i)$

"Hit-or-miss MC" - need uniform RN generator

- call $\rho = \dfrac{n_{hit}}{n}$, uncertainty in $I$ is $H(b-a)\sqrt{\dfrac{\rho-\rho^2}{n}}$

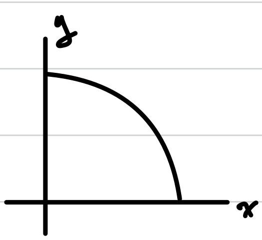
Useful for

e.g. want area of



- difficult classically
- For MC, use "if" statements to determine if $(x_i, y_i)$ is a "hit" or not.

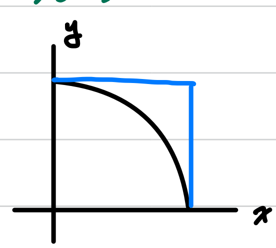
E.g.




unit quarter circle

$A = \dfrac{\pi}{4}$

->




Note: Ratio of areas is $\dfrac{\pi r^2}{4 r^2} = \dfrac{\pi}{4}$

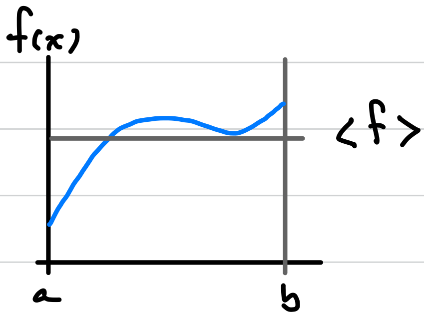
$$\frac{\pi}{4} = I = \text{Area} = \int_0^1 dx \int_0^1 dy\; g(x,y) \qquad \text{where } g(x,y) = \begin{cases} 1, & x^2+y^2 \le 1 \\ 0 & \text{otherwise} \end{cases}$$

```
sum = 0
do i = 1, N
    x_i = rand on 0,1
    y_i = rand on 0,1
    if ( x_i^2 + y_i^2 <= 1 ) then
        sum = sum + 1
    endif
enddo
area = sum/N
```

## MC Approach #2 "Sample Mean Method"

Recall definition for

$$\langle f \rangle = \frac{1}{b-a}\int_a^b f(x)\,dx$$ – ave. value of $f$ on $[a,b]$




estimate $\langle f \rangle$ by sampling $f(x)$

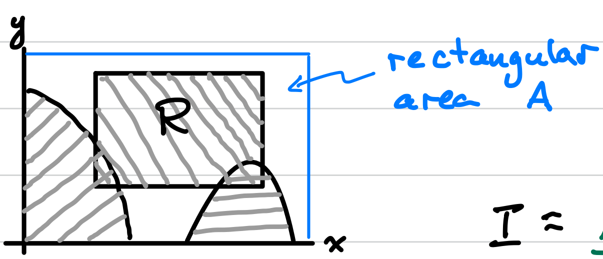
Generate RNs uniformly on $[a,b]$

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

$$\Rightarrow \int_a^b f(x)\,dx = \frac{b-a}{N}\sum_{i=1}^{N} f(x_i)$$

- works well for high $d$

For domains with complicated geometries




want $I = \int_R dx\,dy\, f(x,y)$

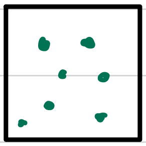
$$I \approx \frac{A}{N}\sum_{i=1}^{N} f(x_i, y_i)\, H(x_i, y_i)$$

where $H(x,y) = \begin{cases} 1 & \text{if } (x,y) \text{ inside } R \\ 0 & \text{if } (x,y) \text{ outside } R \end{cases}$

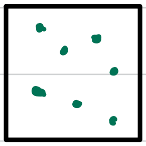
# Metropolis Algorithm and Thermodynamics

Consider a container filled with a fluid - a collection of molecules - at temperature $T$. Particle positions and velocities, as well as system properties like potential energy, are different at different times.

System samples different configurations



$t_1$



$t_2$

Thermodynamic average of some property $f$ is

$$\langle f \rangle = \sum_{\text{all possible configuration}} f_i \, p_i$$

- $p_i$ probability of config $i$
- $f_i$ property of config $i$

Could randomly, uniformly sample all possible particle configurations, but

- MANY, too many configurations
- vast majority of states have negligible $p_i$

Better to sample states according to $p_i$ and use

$$\langle f \rangle = \frac{1}{N} \sum_i f_i$$

But how do we generate a sequence of states sampled from (the equilibrium distribution) $p$ ?

In thermal equilibrium $p_i = \frac{1}{Z} e^{-\beta E_i}$ (Boltzmann distribution)

- $E_i$ is energy of state $i$, $\beta = \frac{1}{k_B T}$, $k_B \doteq 1.38 \times 10^{-23}$ J/K Boltzmann constant

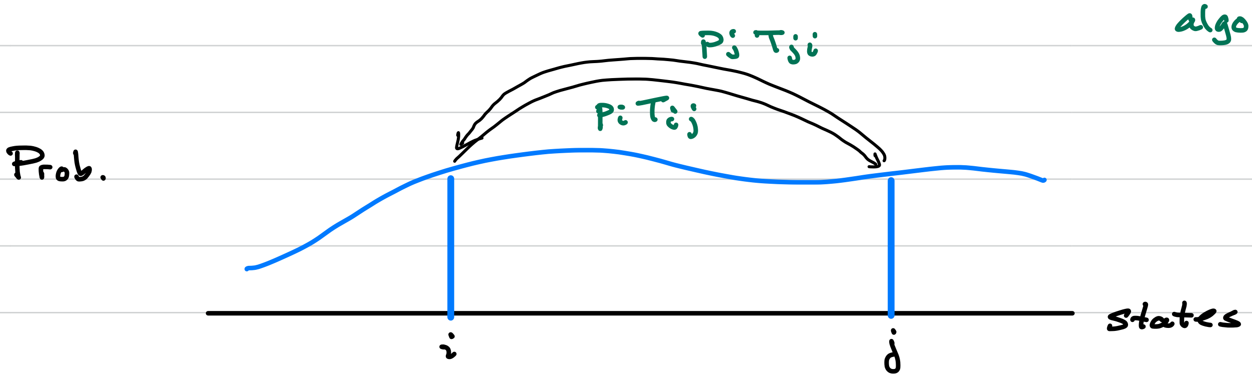
$Z = \sum_{i} e^{-E_i/k_B T}$ (all states) is the "Partition function"

- normalization factor such that $\sum_i p_i = 1$ (system exists in some state)

We will invoke "detailed balance"

$$p_i T_{i \to j} = p_j T_{j \to i}$$

$T_{i \to j}$ is transition probability - prob. that system in state $i$ changes to state $j$ (in a step of the algorithm)




- ensures that distribution of states remains stationary, i.e. unchanging in time (steps of algorithm $\Leftrightarrow$ time) by balancing "probability flux" between every pair of states.

- allows construction of algorithms that generate sets of states sampled according to the Boltzmann distribution.

$$T_{i\to j} = \alpha_{i\to j}\ acc_{i\to j}$$

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

$\alpha_{i\to j}$ prob of selecting a trial state $j$ given the current state $i$

$acc_{i\to j}$ prob. of accepting the proposed change from $i$ to $j$

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

$$p_i\ \alpha_{i\to j}\ acc_{i\to j} = p_j\ \alpha_{j\to i}\ acc_{j\to i}$$

→ construct algorithm such that $\alpha_{i\to j} = \alpha_{j\to i}$

e.g. trial particle coordinate $x_j = x_i + \underset{\text{rand}}{\text{uniform}}(-0.5, 0.5)$

works, since, say, generating $x_j = 6.2$ from $x_i = 6.0$

is just a likely as generating $x_j = 6.0$ from $x_i = 6.2$

but for $x_j = x_i + \text{rand}(0,1)$, $\alpha_{i\to j} \neq \alpha_{j\to i}$

since you can generate $x_j = 6.2$ from $x_i = 6.0$

but you can't generate $x_j = 6.0$ from $x_i = 6.2$

Detailed balance ⇒ $$\frac{acc_{i\to j}}{acc_{j\to i}} = \frac{p_j}{p_i} = \frac{e^{-\beta E_j}}{e^{-\beta E_i}} = e^{-\beta(E_j - E_i)} = e^{-\beta \Delta E}$$

$\Delta E$ is the change in energy that would result from going from state $i$ to state $j$

a couple of possibilities for the acceptance probability

→ $acc_{i\to j} = \dfrac{e^{-\beta \Delta E}}{1 + e^{-\beta \Delta E}}$ drawback: requires expensive calculation of $e^{-\beta \Delta E}$

→ $acc_{i\to j} = \begin{cases} 1 & \text{if } \Delta E \leq 0 \\ e^{-\beta \Delta E} & \text{if } \Delta E > 0 \end{cases}$ i.e. if energy decreases for proposed move

i.e. If energy decreases, accept the move
If energy increases, accept the move with probability $e^{-\beta \Delta E}$

As $T$ increases, $\beta$ decrease and $e^{-\beta \Delta E}$ approaches 1
→ all proposed states accepted at infinite $T$
→ uphill energy moves usually rejected at low $T$

Algorithm

1) choose 1 of $N$ particles at random when system is in state $i$

2) consider a new state $j$ generated by moving/changing the chosen particle, and compute $\Delta E = E_j - E_i$

3) if $\Delta E \leq 0$, change to state $j$

4) if $\Delta E > 0$, generate uniform random number $r \in [0, 1]$, and if $r < e^{-\beta \Delta E}$, then change to state $j$ (accept change)

5) if state did not change, state $i$ is repeated in the sequence of states

6) Carry out steps 1-5 $N$ times. This is 1 MC "sweep" MCS

7) Do many MCS to equilibrate system and to get good statistics.