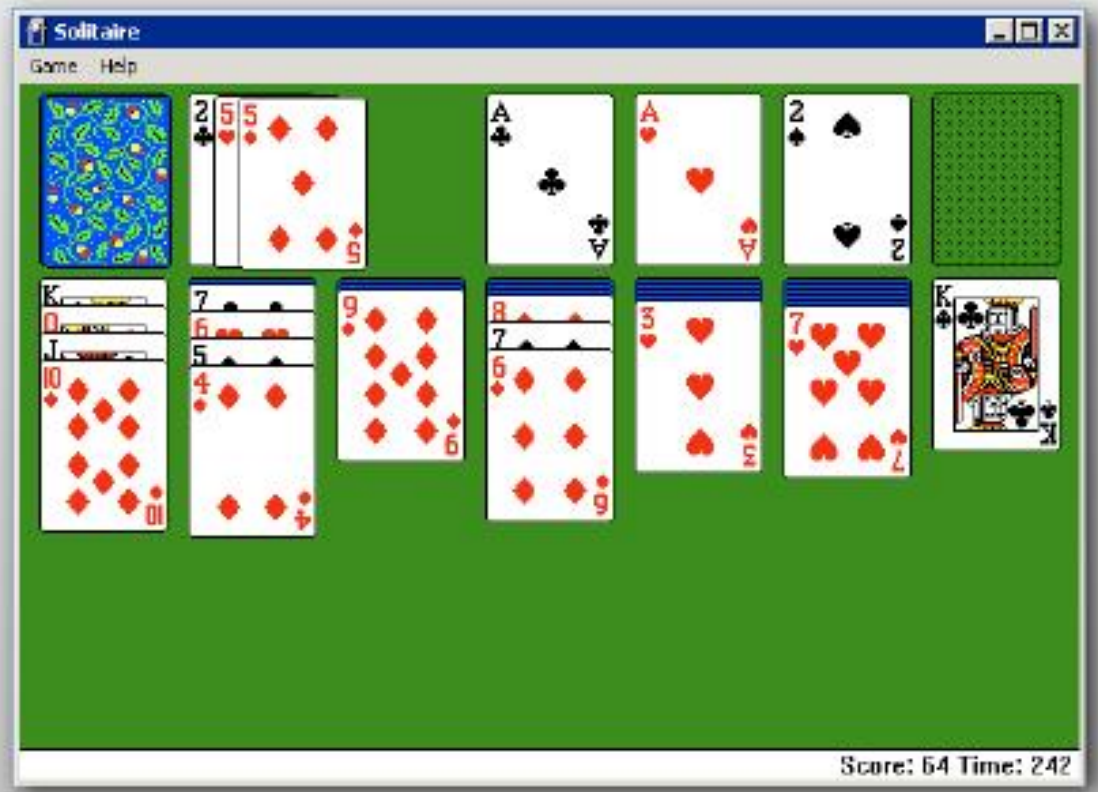
Ulam: the Monte Carlo Method

- What is the probability to win in Solitaire?
  - Ulam's answer: play it 100 times, count the number of wins and you have a pretty good estimate



Integração Númérica por Monte Carlo

Nas regras de integração numérica obtemos para o integral de função formulas do tipo :

$$\int_a^b f(x)dx = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)dx = \frac{(b-a)}{n} \sum_{i=1}^{n} f_{i-1} + \mathcal{O}(h)$$

Esta regra também pode ser vista do ponto de vista estatístico:

$$\int_a^b f(x)dx = (b-a) < f >$$

Integração Númérica por Monte Carlo. Monte Carlo primitivo.

Numa abordagem de Monte Carlo à integração numérica é feita uma estimativa do valor médio da função no intervalo [a,b] fazendo a média de conjunto de avaliações da função em pontos gerados aleatoriamente em [a,b] , podendo-se ainda estimar a incerteza associada ao valor do integral usando o desvio padrão da amostra:

$$\int_a^b f(x)dx = (b-a)(<f> \pm \sigma_f) \qquad <f> = \frac{\sum_{i=1}^{n} f_i}{n}$$

No Matlab para gerar nº aleatórios usa-se a função:

$$\sigma_{\langle f \rangle} \approx \sqrt{\frac{\langle f^2 \rangle - \langle f \rangle^2}{N}}$$

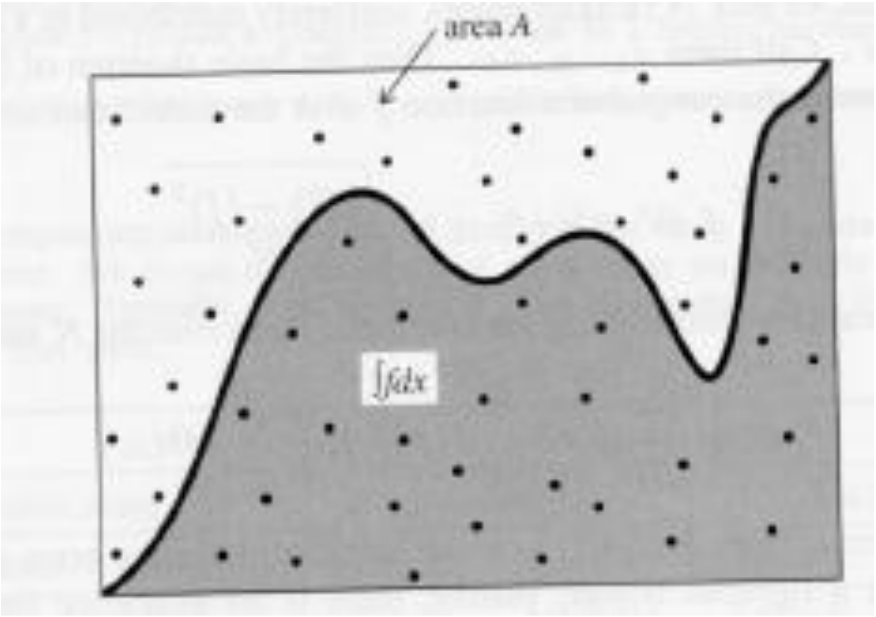
>> rand() para gerar um nº aleatório no intervalo [0,1].

>> rand(N,1) gera um vetor de N nº aleatórios no intervalo [0,1].

Integração Númérica por Monte Carlo. Método da Rejeição.

Outra abordagem para calcular um integral consiste no **método da rejeição**.

1. Gerar ponto $\{x_i, y_i\}$ na caixa usando 2 nº aleatorios
2. Se yi <f(xi) incrementar nº acertos $N_{acertos}$
3. Voltar a 1 e Repetir N vezes
4. Calcular area:



$$A = Area_{caixa} * \left(\frac{N_{acertos}}{N} \pm \sigma_A \right)$$

$$\sigma_A = \frac{1}{\sqrt{N}} \sqrt{\frac{N_{acertos}}{N} - \left(\frac{N_{acertos}}{N} \right)^2}$$

O método da Rejeição é equivalente a usar o Monte Carlo primitivo com: $f(x) = \begin{cases} 1 \; se \; x \; abaixo \; da \; curva \\ 0 \quad se \; acima \; da \; curva \end{cases}$

Método de Monte Carlo.

Geração nº aleatórios com uma distribuição geral f(x).

1. **Para gerar nº aleatórios no intervalo [a,b]**
   x =(b-a)*r +a onde r é nº aleatório em [0,1] com distribuição uniforme.

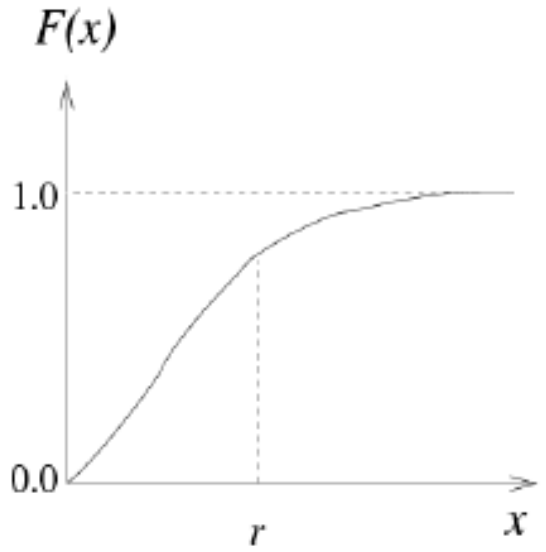
2. **Para gerar nº aleatórios com uma distribuição genérica f(x):**

   Seja f(x) tal que: $\int_{-\infty}^{\infty} f(x)dx = 1$

   Então podemos calcular a função cumulativa associada a f(x) : $F(x) = \int_{-\infty}^{x} f(t)dt$

   2.1 Gerar nº aleatório u no intervalo [0,1] com dist. uniforme

   2.2 Então $x = F^{-1}(u)$ é um nº aleatório com distribuição f(x).



Método de Monte Carlo

Geração nº aleatórios com uma distribuição geral f(x).

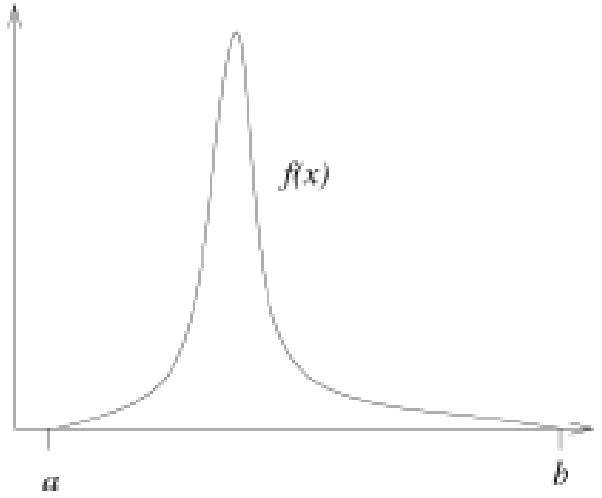
Se f(x) não é invertível temos de usar o **método da rejeição de Von Neumann.**

Seja f(x) tal que: $\int_{-\infty}^{\infty} f(x)dx = 1$

1. Gerar par de nº aleatórios $\{x,y\}$ no intervalo [0,1] com distribuição uniforme.
2. Se y < f(x) aceitar na sequência de nº aleatórios $\{x_i\}$.
3. Repetir a partir de 1.

Método de Monte Carlo. Amostragem por importância.

Por vezes o processo de integração é mais eficiente concentrando os pontos da amostra apenas em certas regiões do domínio, em vez de gerar os nº aleatórios com distribuição uniforme em todo o domínio.



Vamos gerar a amostra com uma distribuição g(x) normalizada em [a,b] então:

$$I = \int_a^b f(x)dx = \int_a^b \frac{f(x)}{g(x)} g(x)dx = \int_a^b \frac{f(x)}{g(x)} dG(x) \qquad \text{onde} \qquad G(x) = \int_a^x g(x)dx$$

Fazendo a mudança de variável r=G(x) com r [0,1] , temos:

$$I = \int_{G(a)}^{G(b)} \frac{f(G^{-1}(r))}{g(G^{-1}(r))} dr$$

ou $$I = \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i^{(g)}))}{g(x_i^{(g)})}$$

onde $x_i^{(g)}$ são nº aleatórios gerados com distribuição g(x).

Exemplo: Comparar o integral usando amostragem por importância ($g(x)=e^{-x}$) e método geral.

$$I = \int_0^1 e^{-x^2} dx$$

Método de Monte Carlo. Cadeias de Markov.

If a configuration in phase space is denoted by X, the probability for configuration according to Boltzman is

$$\rho(X) = \frac{1}{Z} e^{-E(X)/k_B T}$$

where Z is the partition function. This probability is usually not known because the partition function is practically impossible to calculate for most systems.

How to sample over the whole phase space for a general problem? How to generate configurations?

- **Brute force**: generate a truly random configuration X and accept it with probability $e^{-\beta E(X)}$ where all $E > 0$. Successive X are **statistically independent**.

  VERY INEFFICIENT

- **Markov chain**: Successive configurations X_i, X_{i+1} are **NOT** statistically independent but are distributed according to the choosen disribution (such as Boltzman distribution).

Método de Monte Carlo. Cadeias de Markov.

- *Truly random* or *uncorrelated* sequence of configurations satisfies the identity

$$P(X_1, X_2, \cdots, X_N) = P_1(X_1) P_1(X_2) \cdots P_1(X_N)$$

- *Markov chain* satisfies the equation

$$P(X_1, X_2, \cdots, X_N) = P_1(X_{N-1})\, T(X_{N-1} \to X_N)$$

This means that a Markov chain has no memory of the earlier states **N-2, …., 1**

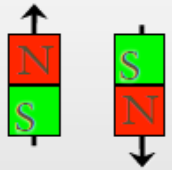
The dificulty in generating ρ(X) can be avoided using **Markov chains**, since each new state is generated directly from the previous state. This can be done because in this case we only need to consider the relative probabilities of the two successive states N-1 and N.

Método de Monte Carlo. Algoritmo de Metropolis.

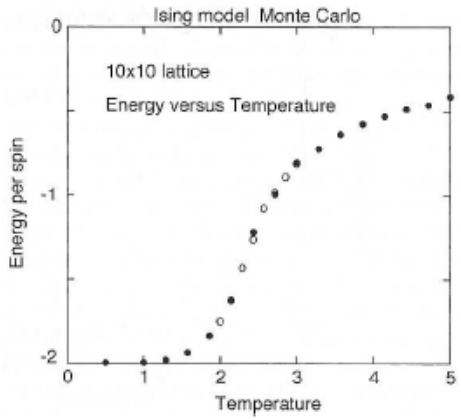
1. Generate an initial state i.
2. Attempt to change the configuration from i to j.
3. Compute $\Delta E = E_j - E_i$.
4. If $\Delta E \leq 0$, accept the change and replace state i by state j. Goto 2.
5. If $\Delta E > 0$, generate a uniform random number $r \in [0, 1]$.
   Calculate $w = \exp(-\Delta E / k_B T)$.
6. If $r < w$, accept the change and replace state i by state j. Goto 2.
7. If $r > w$, then reject the change and keep state i. Goto 2.

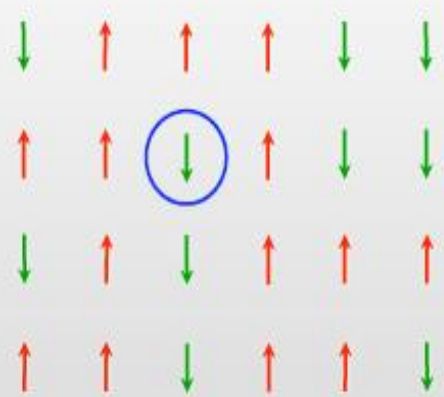
Método de Monte Carlo. Algoritmo de Metropolis.

- Ising model
  - molecular magnets with two states
  - north pole up or down



$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$





- Phase transition:
  - low temperatures: magnetically ordered

↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑

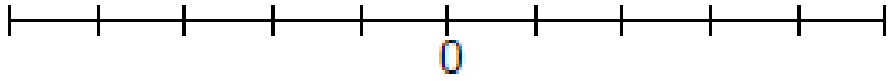
  - high temperatures : disordered

↑↓↓↑↓↑↑↓↓↓↑↑↓↑↓↓↑↑↓↑↓↓

1. Pick a random spin and propose to flip it
2. Accept the flip with probability $P = \min\left[1, e^{-(E_{new} - E_{old})/T}\right]$
3. Perform a measurement independent of whether the proposed flip was accepted or rejected!

Método de Monte Carlo. Passeios aleatórios.

Let us first consider the simplest possible case, a random walker in a one-dimensional lattice:



Say that a walker begins at $x = 0$, and that all steps are of equal length l. After each time interval τ the walker has an equal probability of moving left or right. The direction of each step is independent of the previous one. Let us denote the displacement at each step by s_i, for which

$$s_i = \begin{cases} +l \text{ with 50\% probability} \\ -l \text{ with 50\% probability} \end{cases}$$

Then after N steps (time $N\tau$) in the random walk, the position (and displacement) x of the walker is

$$x(N) = \sum_{i=1}^{N} s_i$$

Método de Monte Carlo. Passeios aleatórios.

Let us now think about what the average distance the walker has moved is. It is immediately obvious that with the equal probabilities to go left and right,

$$\langle x(N) \rangle = 0$$

and the displacement squared is

$$x^2(N) = \left(\sum_{i=1}^{N} s_i \right)^2 = \sum_{i=1}^{N} s_i \sum_{j=1}^{N} s_j = \sum_{i=1}^{N} s_i^2 + \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} s_i s_j \qquad s_i s_j = \begin{cases} +l^2 \text{ with 50\% probability} \\ -l^2 \text{ with 50\% probability} \end{cases}$$

Hence the average after N steps will be

$$\langle x^2(N) \rangle = l^2 N$$

This equation is called the **Einstein relation** after a certain physicist who first derived it back in 1905 [A. Einstein, Ann. Phys. 17 (1905) 549].

$$\langle x^2(t) \rangle = 2Dt \qquad D \equiv l^2/2\tau \text{ and } t = N\tau$$

Método de Monte Carlo. Passeios aleatórios.

Relação com processo de difusão.

Let us begin by writing the random walk behaviour in terms of a so called **master equation.** Let $P(i, N)$ denote the probability that a walker is at site i after N steps. Since walkers have an equal probability to walk left and right, it is clear that

$$P(i, N) = \tfrac{1}{2}P(i + 1, N - 1) + \tfrac{1}{2}P(i - 1, N - 1)$$

To get a continuum limit with familiar names for the variables, we can identify

$$t = N\tau \qquad \text{and} \qquad x = il$$

$$P(x/l, t/\tau) = \tfrac{1}{2}P(x/l + 1, t/\tau - 1) + \tfrac{1}{2}P(x/l - 1, t/\tau - 1)$$

since the probability is independent of the length or time scales, $aP(x, t) = P(ax, t) \quad bP(x, t) = P(x, bt)$

$$P(x, t) = \tfrac{1}{2}P(x + l, t - \tau) + \tfrac{1}{2}P(x - l, t - \tau)$$

Método de Monte Carlo. Passeios aleatórios.

Relação com processo de difusão.

We rewrite this by subtracting $P(x, t-\tau)$ and dividing by τ

$$\frac{P(x,t) - P(x,t-\tau)}{\tau} = \frac{P(x+l,t-\tau) + P(x-l,t-\tau) - 2P(x,t-\tau)}{2\tau}$$

$$\frac{\partial P(x,t)}{\partial t} \approx \frac{l^2}{2\tau}\frac{\partial^2 P(x,t)}{\partial x^2}$$

In the limit $\tau \to 0, l \to 0$ but where the ratio l^2/τ is finite, this becomes an exact relation. If we further *define* $D \equiv l^2/2\tau$ we get the equation

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}$$

one possible solution of this is a Gaussian of the form $P(x,t) = \frac{N}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}$

Método de Monte Carlo

Transporte de particulas. Passeio aleatório 1D assimétrico.

The input parameters are the thickness of the plate t, the capture probability p_c, and the mean free path λ. The scattering probability is $p_s = 1 - p_c$. We begin with $z = 0$ and implement the following steps:

1. Determine if the neutron is captured or scattered. If it is captured, then add one to the number of captured neutrons and go to step 5.
2. If the neutron is scattered, compute $\cos\theta$ from (11.62) and ℓ from (11.63). Change the z-coordinate of the neutron by $\ell \cos\theta$.

$$z_{i+1} = z_i + l.\cos(\theta)$$

3. If $z < 0$, add one to the number of reflected neutrons. If $z > t$, add one to the number of transmitted neutrons. In either case skip to step 5 below.
4. Repeat steps 1–3 until the fate of the neutron has been determined.
5. Repeat steps 1–4 with additional incident neutrons until sufficient data has been obtained.

$$\ell = -\lambda \ln r, \qquad (11.63)$$

$$\cos\theta = 1 - 2r. \qquad (11.62)$$