# Random processes and Monte Carlo Simulation

- Monte Carlo integration.
- Non-uniform distributions.
- Random walk.

# Mean value method

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- A simple way to estimate $\langle f \rangle$ is to just measure $f(x)$ at $N$ points, $x_1, x_2, \ldots, x_N$ chosen uniformly between $a$ and $b$:

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

$$I \simeq \frac{b-a}{N} \sum_{i=1}^{N} f(x_i)$$

# Error Analysis

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- Variance on the sum is $N$ times the variance on a single term or $N \mathrm{var} f$.
- Error/standard deviation on the integral:

$$\sigma = \frac{b-a}{N} \sqrt{N \mathrm{var} f} = (b-a) \frac{\sqrt{\mathrm{var} f}}{\sqrt{N}}$$

which goes as $1/\sqrt{N}$ but the variance is smaller!

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- Experiments with different types of distributions

How does one generate non-uniform random number distributions with a uniform random number generators?

# von Neumann Rejection

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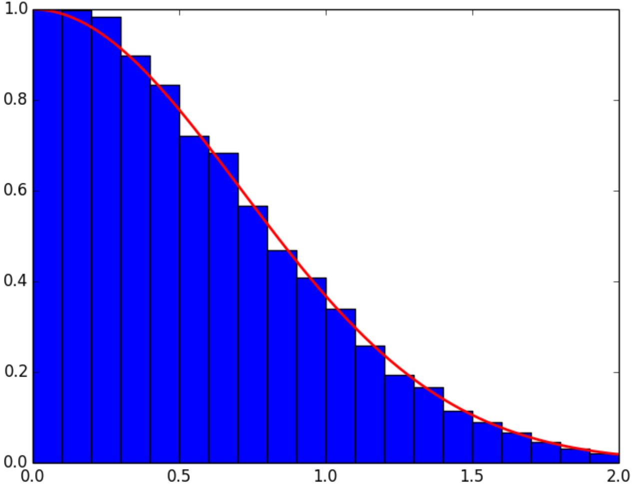
- If $y_i > w(x_i)$ reject $x_i$.
- The $x_i$ so accepted will have the weighting $w(x_i)$.

# von Neumann Rejection

$$w(x) = e^{-x^2} \quad x \in [0, 2]$$



# Inversion method

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- If $z$ is random, $x(z)$ will also be random, with a different distribution $p(x)$.
- Our goal is to choose the function $x(z)$ such that $x$ has the distribution we want.

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- If we can do the integral on the left and solve the equation, we will have the required $x(z)$!

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Thus if we feed the above equation uniformly distributed $z$ in interval $[0, 1]$, it will generate the exponential distribution $x$ for us.

# Gaussian random numbers

- A common problem in physics calculations is the generation of random numbers drawn from a Gaussian (or normal) distribution:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left( - \frac{x^2}{2\sigma^2} \right)$$

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- However, consider two independent random numbers $x$ and $y$ drawn from a Gaussian distribution with the same $\sigma$. The probability that a point $(x, y)$ falls in an element $dxdy$ of the $xy$ plane:

$$p(x)dx \times p(y)dy = \frac{1}{2\pi\sigma^2} \exp\left( - \frac{x^2+y^2}{2\sigma^2} \right) dxdy$$

# Gaussian random numbers

- In polar coordinates:

$$p(r,\theta)drd\theta = \frac{r}{\sigma^2}\exp\left(-\frac{r^2}{2\sigma^2}\right)dr \times \frac{d\theta}{2\pi} \equiv p(r)dr \times p(\theta)d\theta$$

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- Then one can construct $x$ and $y$ as:

$$x = r\cos(\theta) \quad y = r\sin(\theta)$$

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  - In three dimensions there are six possible neighbors.

## Random walk

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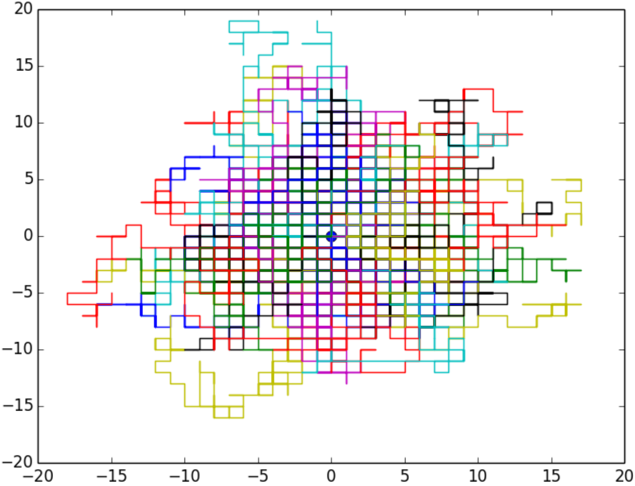
$$\text{In 100 steps, } \langle r \rangle \sim 8.9$$



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Examples of applications:
Spread of inflectional diseases and effects of immunization
Spreading of fire

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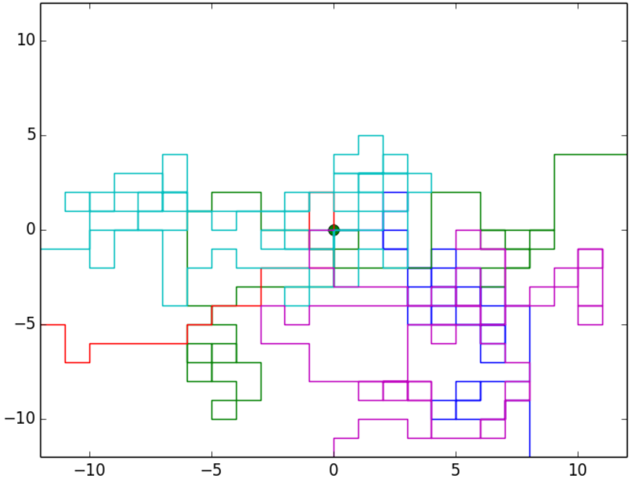
- Condition: the walker can not step back
- Goal: find average number of steps to get out the city

$$\text{To escape } 24 \times 24, \langle n \rangle \sim 92$$



# Random processes and Monte Carlo Simulation

- Importance Sampling and Statistical mechanics.
- Markov Chain Monte Carlo.
- Simulated Annealing

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- We can take the approach that we will calculate the sum via Monte Carlo (random sampling). In that case, we will chose $N$ random states, $k = 1 \dots N$ and calculate:

$$\langle X \rangle \simeq \frac{\sum_{k=1}^{N} X_k P(E_k)}{\sum_{k=1}^{N} P(E_k)}$$

The denominator is needed to normalize the weighted average correctly..

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- But this is ideally suited for importance sampling!

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- Making the particular choice $g_i = X_i P(E_i)/w_i$:

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- Then:

$$\langle X \rangle = \left\langle \frac{X_i P(E_i)}{w_i} \right\rangle_w \sum_i w_i$$

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- In this case, we get:

$$\langle X \rangle \simeq \frac{1}{N} \sum_{k=1}^{N} \frac{X_k P(E_k)}{w_k} \sum_i w_i$$

Note that the first sum is only over the states that we sample, but the second sum is over all states $i$ and has to be calculated analytically!

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- In other words, we just choose $N$ states in proportion to their Boltzmann probabilities and take the average of $X$ over them..
- Unfortunately, we are not done yet – The catch is that it is not easy to pick states with probability $P(E_i)$. This is because to calculate $P(E_i)$, we need to know the partition function, $Z$.

# Markov Chain

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- Consider a single step in the process – Suppose that the previous state for the step before this one, was state $i$.
- For the new state, instead of choosing randomly, we will make some change (usually small) to the state $i$ so as to create a new state.
- The choice of the new state is determined probabilistically by a set of transition probablilities $T_{ij}$ that give the probability of changing from state $i$ to $j$.

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- When we take many steps and generate the entire chain, the complete set of states that we move through is a correct sample of the Boltzmann distribution and we can average any quantity we like over these states.

- The trick lies in choosing $T_{ij}$:

$$\sum_j T_{ij} = 1$$

and also

$$\frac{T_{ij}}{T_{ji}} = \frac{P(E_j)}{P(E_i)} = \frac{e^{-\beta E_j}/Z}{e^{-\beta E_i}/Z} = e^{-\beta(E_j - E_i)}$$

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- The Boltzmann distribution is a fixed point of the Markov chain.

# Metropolis algorithm

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- This scheme will satisfy all the criterion of the transition probability: $\frac{T_{ij}}{T_{ji}} = e^{-\beta(E_i - E_j)}$

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6. Go to step 2.

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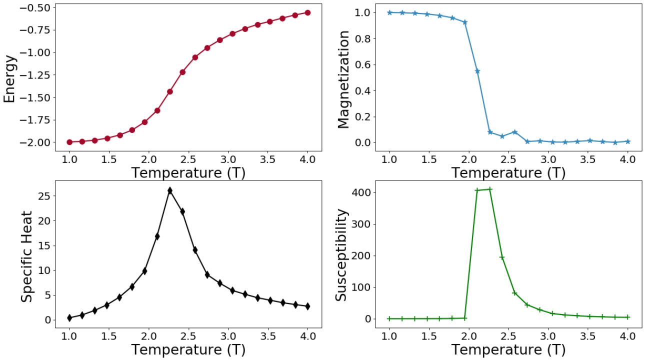
- The number of moves that you chose to take you from $i$ to $j$ should be the same as from $j$ to $i$.
- One has to choose a move set such that every possible state is reachable.
- That the Markov chain will go to Boltzmann distribution is proved but, how long will it to take to reach equillibrium is not known.

# Ising Model

$$E = -\sum_{\langle ij \rangle} s_i s_j$$



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- As one lowers the temperature, the system should land in the ground-state!