

Monte Carlo methods

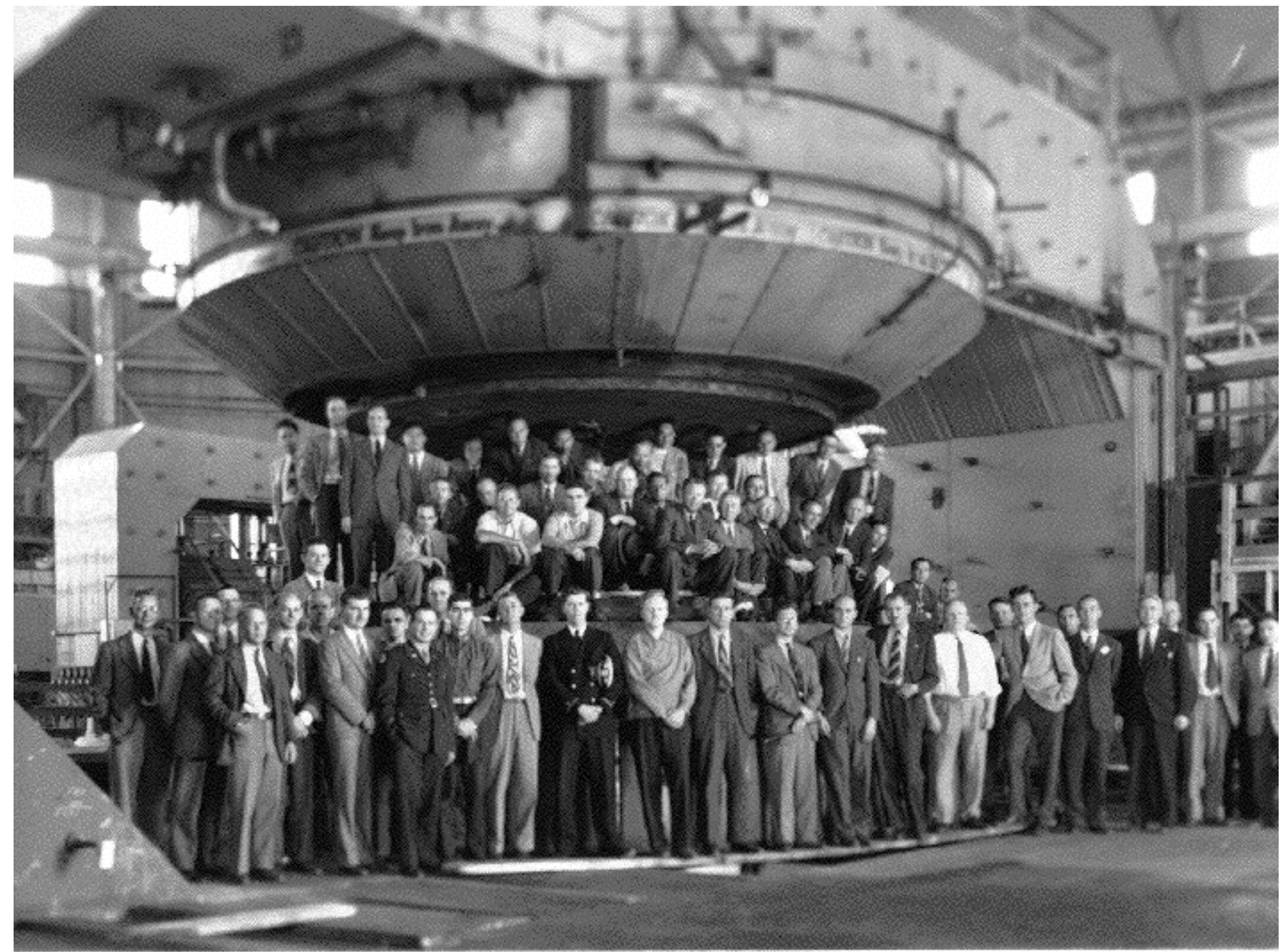
Stochastic Processes in Science Inference

- History of Monte Carlo Methods
- Application of MC to probabilistic inference
- A simple MC simulation
- MC simulations applications in Urban Science - Traffic flow, Resque
- Rejection & Importance Sampling

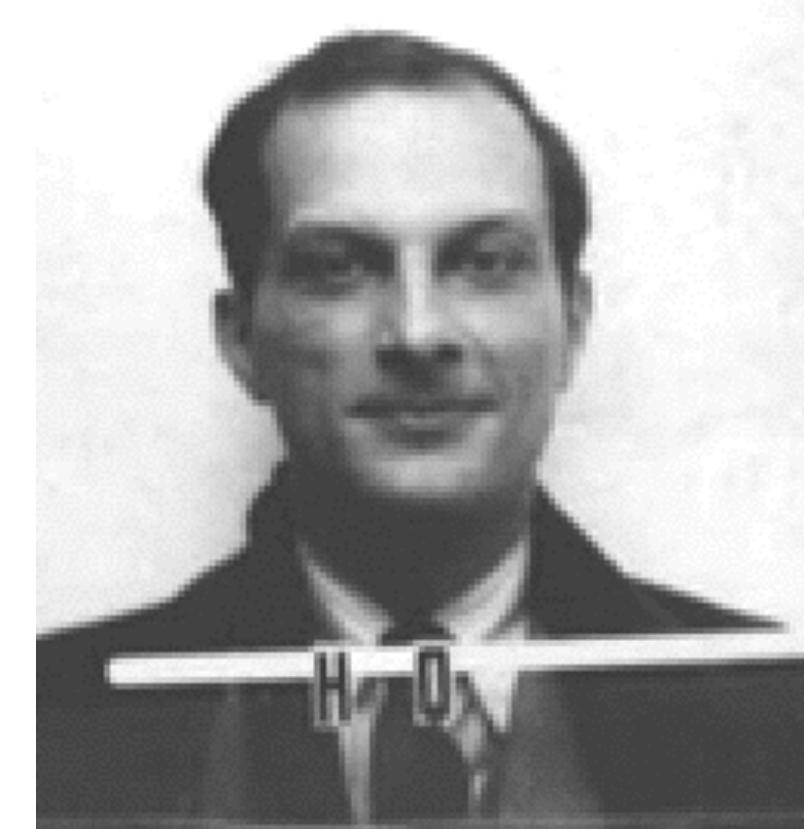
Markov Chain Monte Carlo

- Markovian Processes and Markov chains
- Bayes theorem and the posterior distribution
- Metropolis Hasting (and Gibbs sampling) MCMC
- Affine Invariant MCMC
- convergence criteria

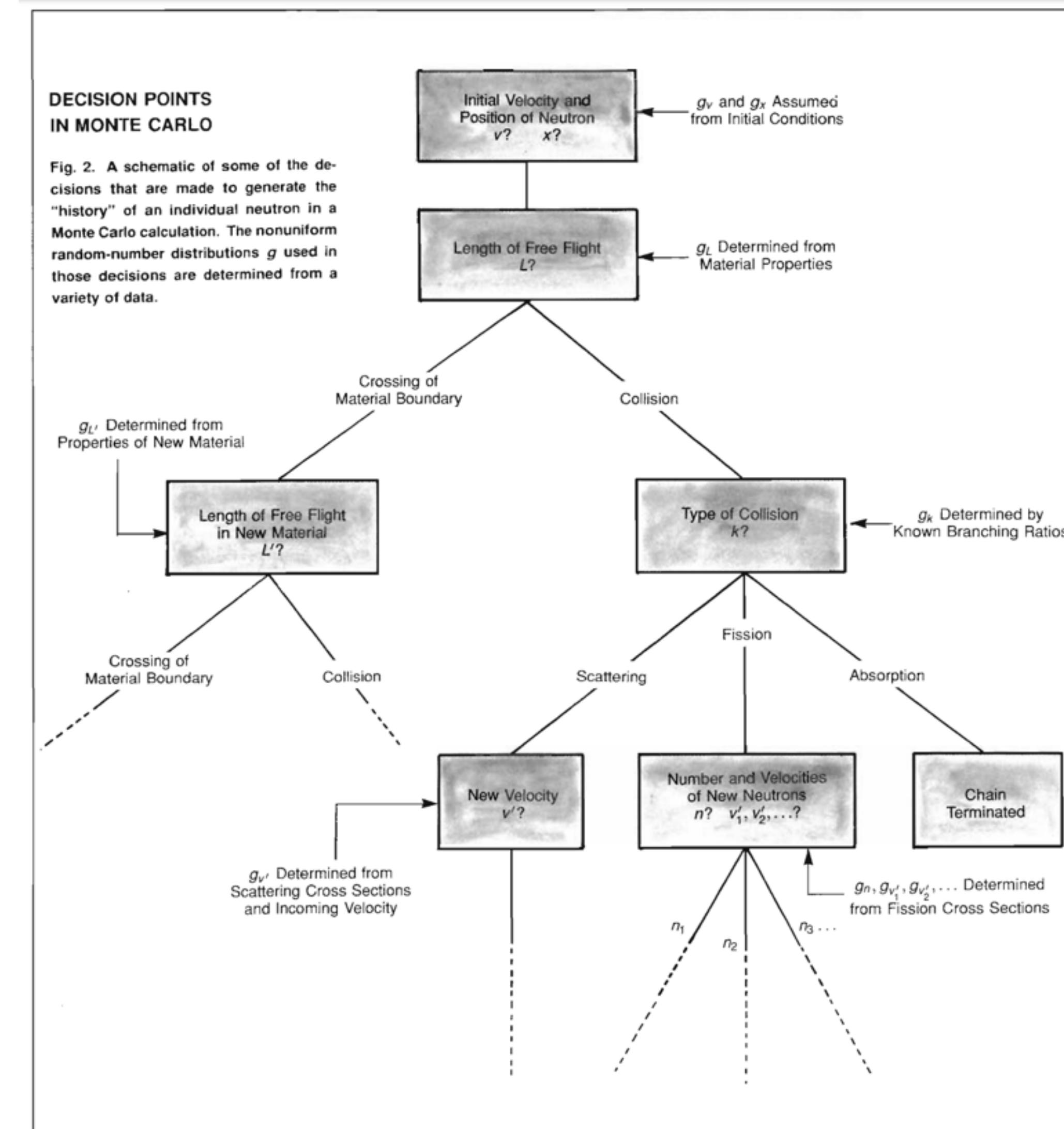
The Manhattan Project



MC - history



Stanislav Ulam





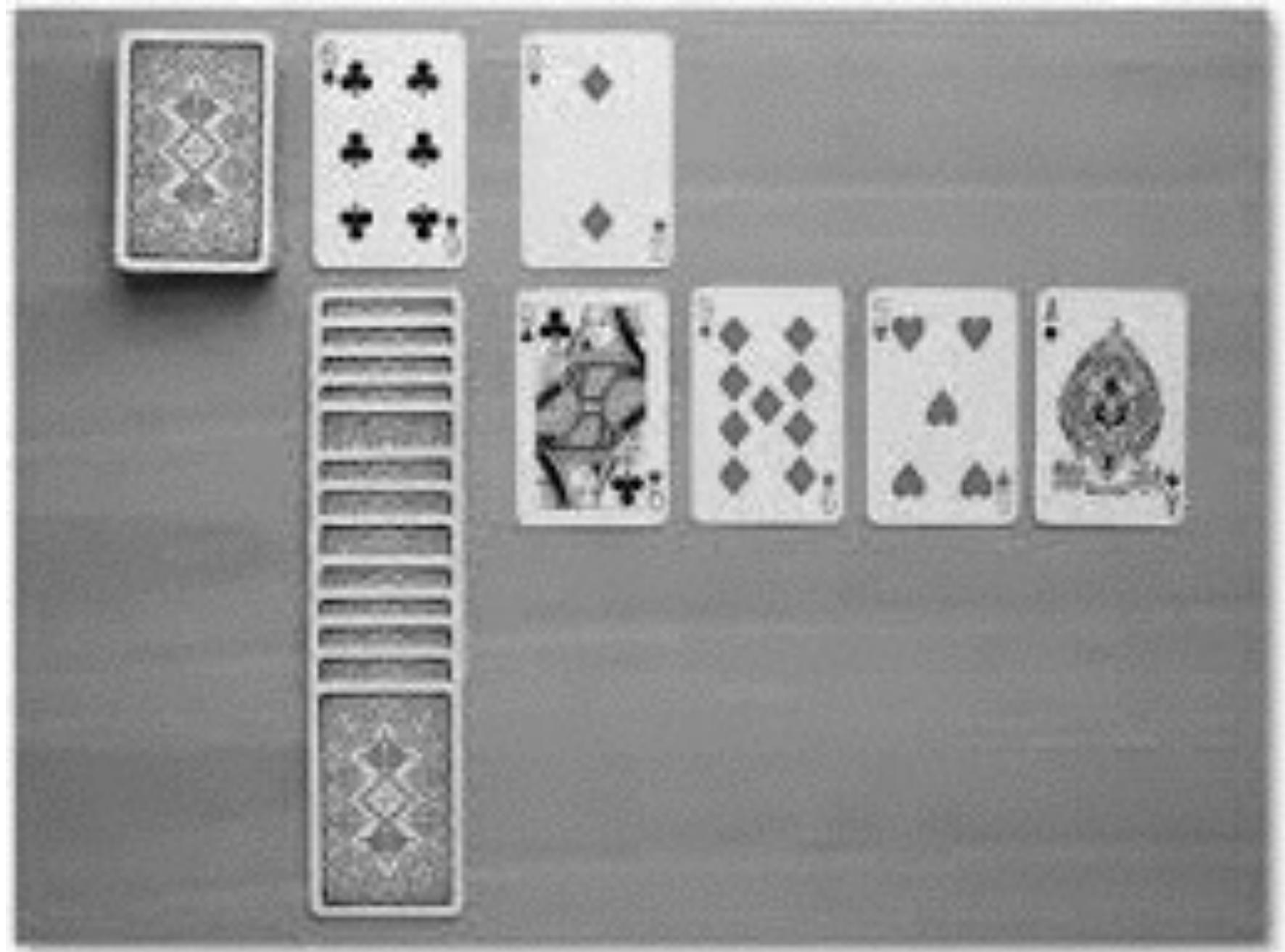
Stanislav Ulam

What are the chances that a Canfield solitaire laid out with 52 cards will come out successfully?

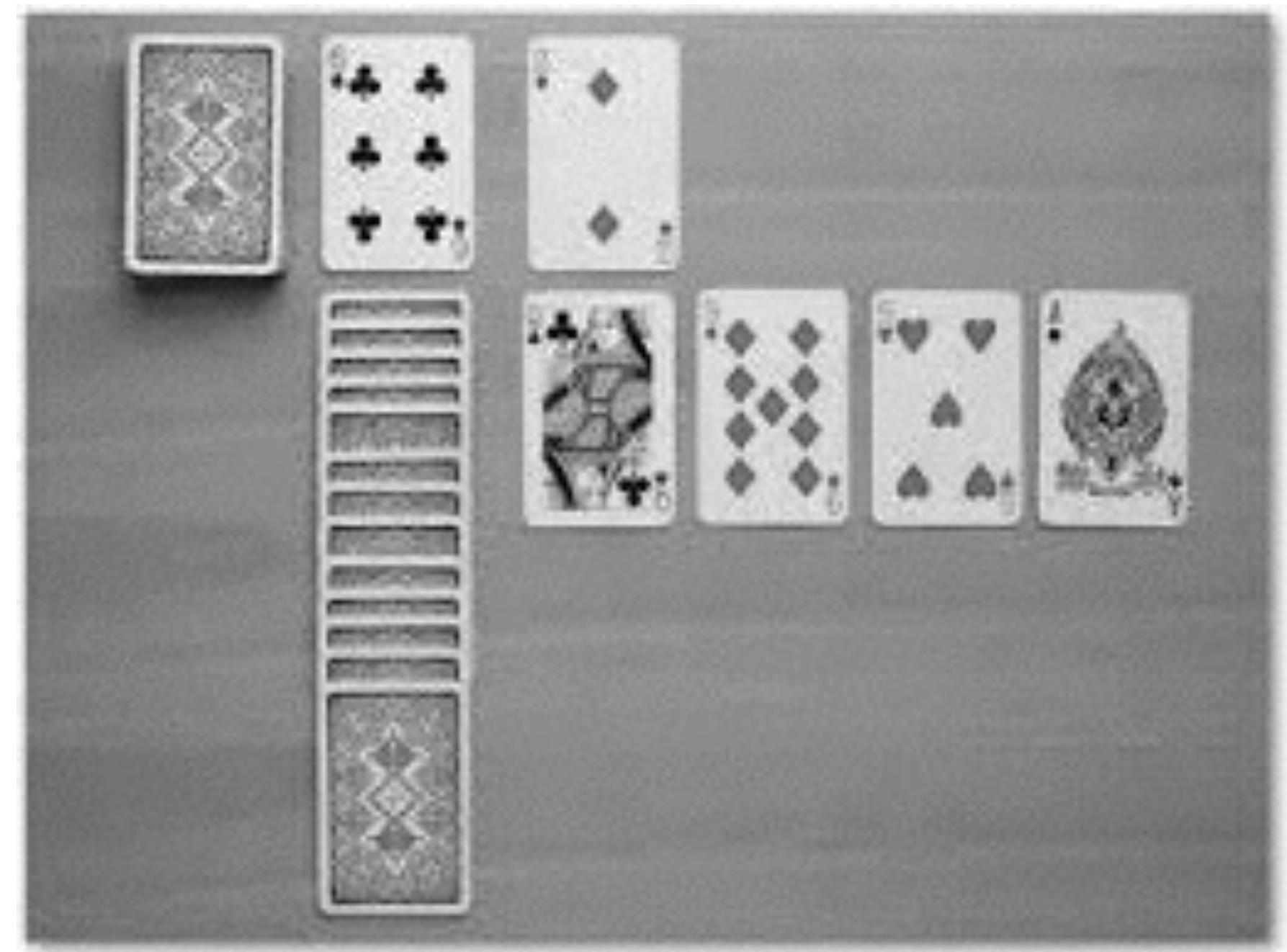
The number of different games is

$$52! = 52 \times 51 \times 50 \dots \times 3 \times 2 \times 1 \sim 8 \times 10^{67}$$

Canfield Solitaire

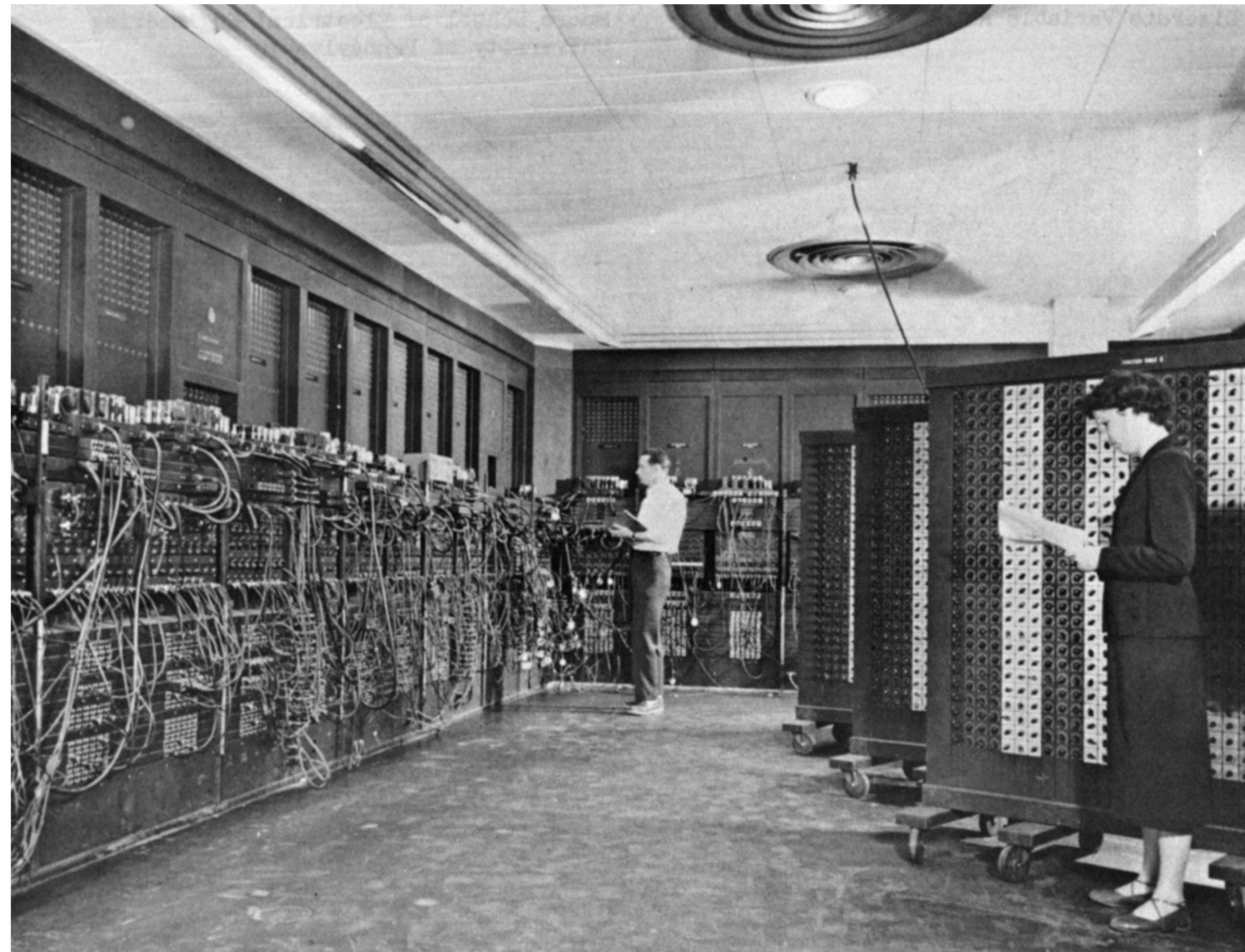


“What are the chances that a Canfield solitaire laid out with 52 cards will come out successfully? After spending a lot of time trying to estimate them by pure combinatorial calculations, I wondered whether **a more practical method than *abstract thinking* might not be to lay it out say one hundred times and simply observe and count the number of successful play”**



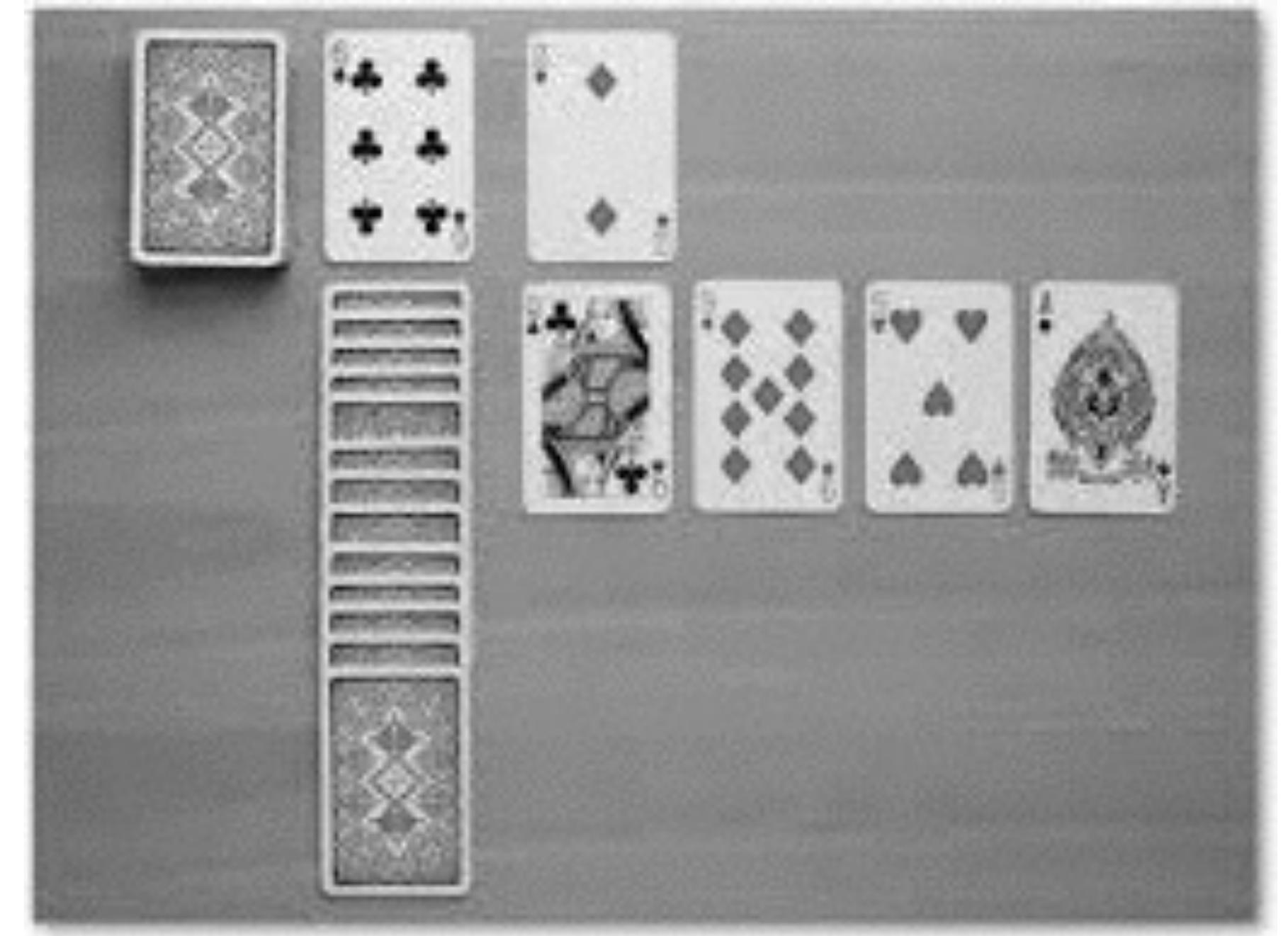
<http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-88-9068>

MC - history



ENIAC It weighed more than 30 short tons (27 t), was roughly 2.4 m × 0.9 m × 30 m (8 × 3 × 100 feet) in size, occupied 167 m² (1,800 ft²), consumed 150 kW of electricity.

500FLOPS vs today's Macbook pro ~1TeraFLOP

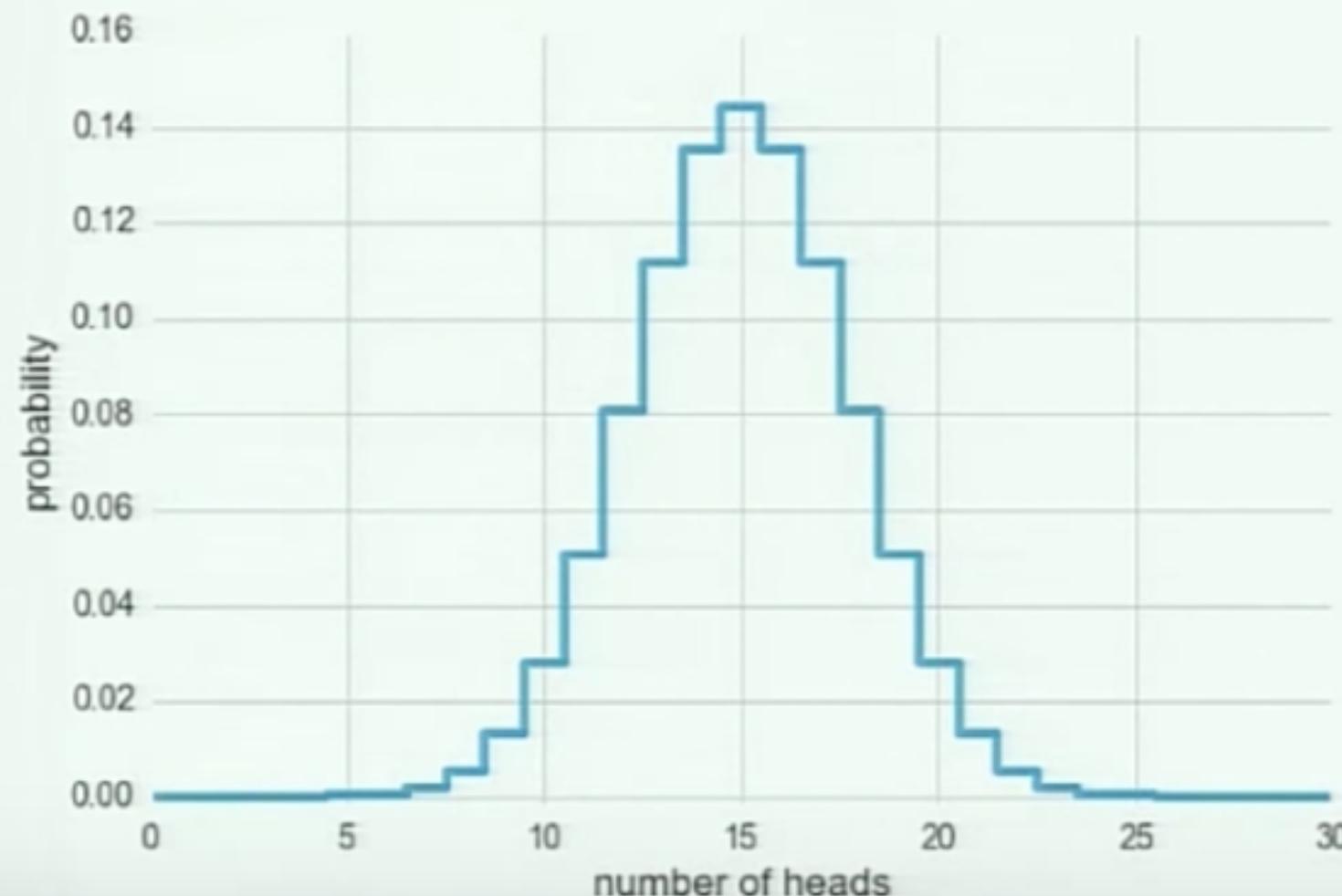


MC - history

Classic Method:

$$N_H = 22, N_T = 8$$

$$P(N_H, N_T) = \binom{N}{N_H} \left(\frac{1}{2}\right)^{N_H} \left(1 - \frac{1}{2}\right)^{N_T}$$



Easier Method:

Just simulate it!

```
M = 0
for i in range(10000):
    trials = randint(2, size=30)
    if (trials.sum() >= 22):
        M += 1
p = M / 10000 # 0.008149
```

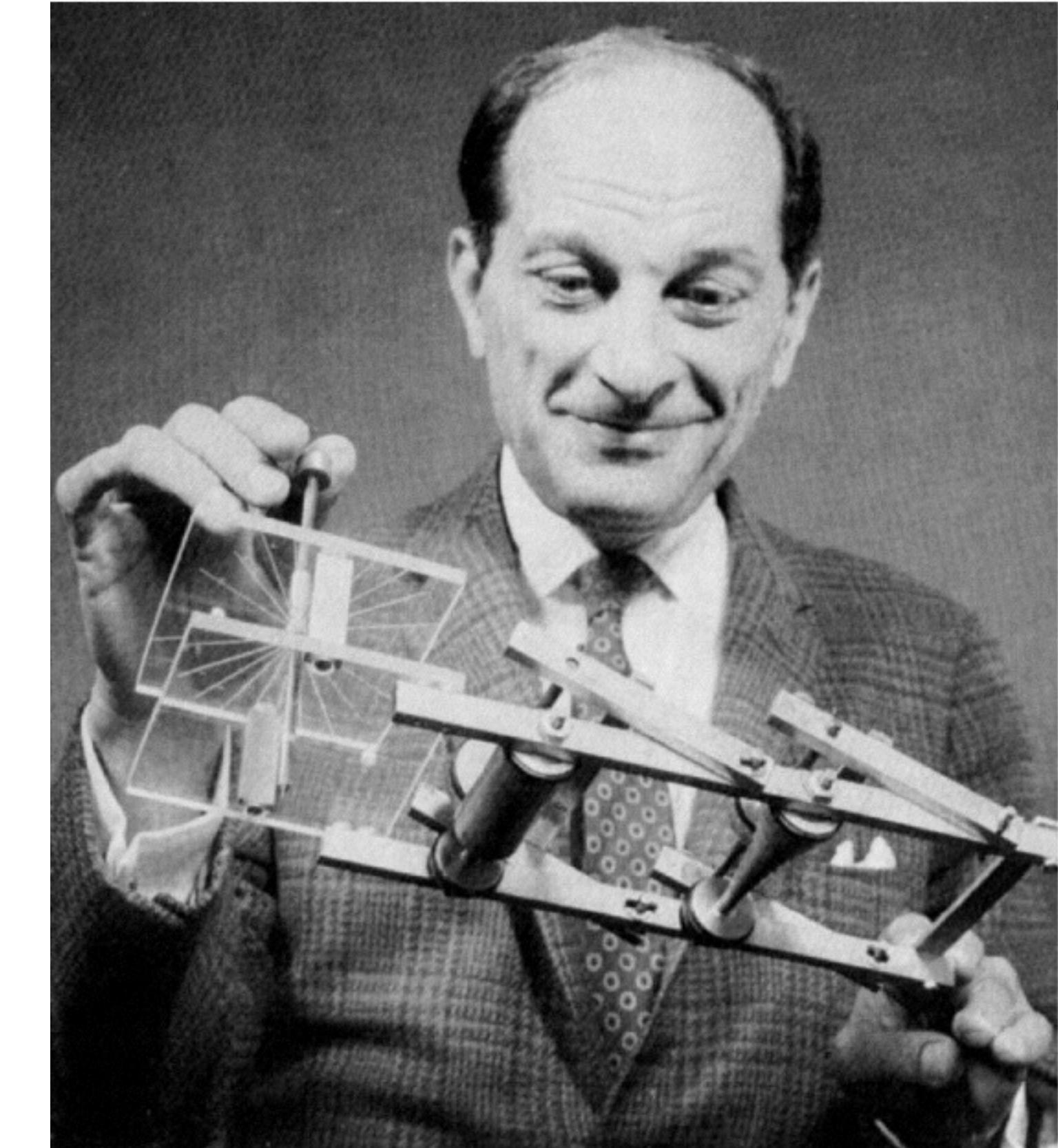
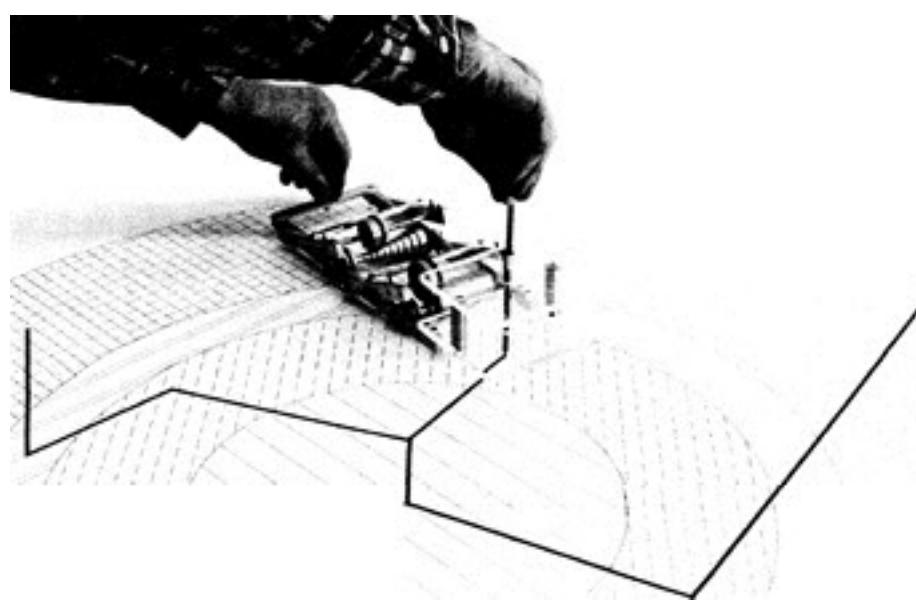
→ reject fair coin at $p = 0.008$



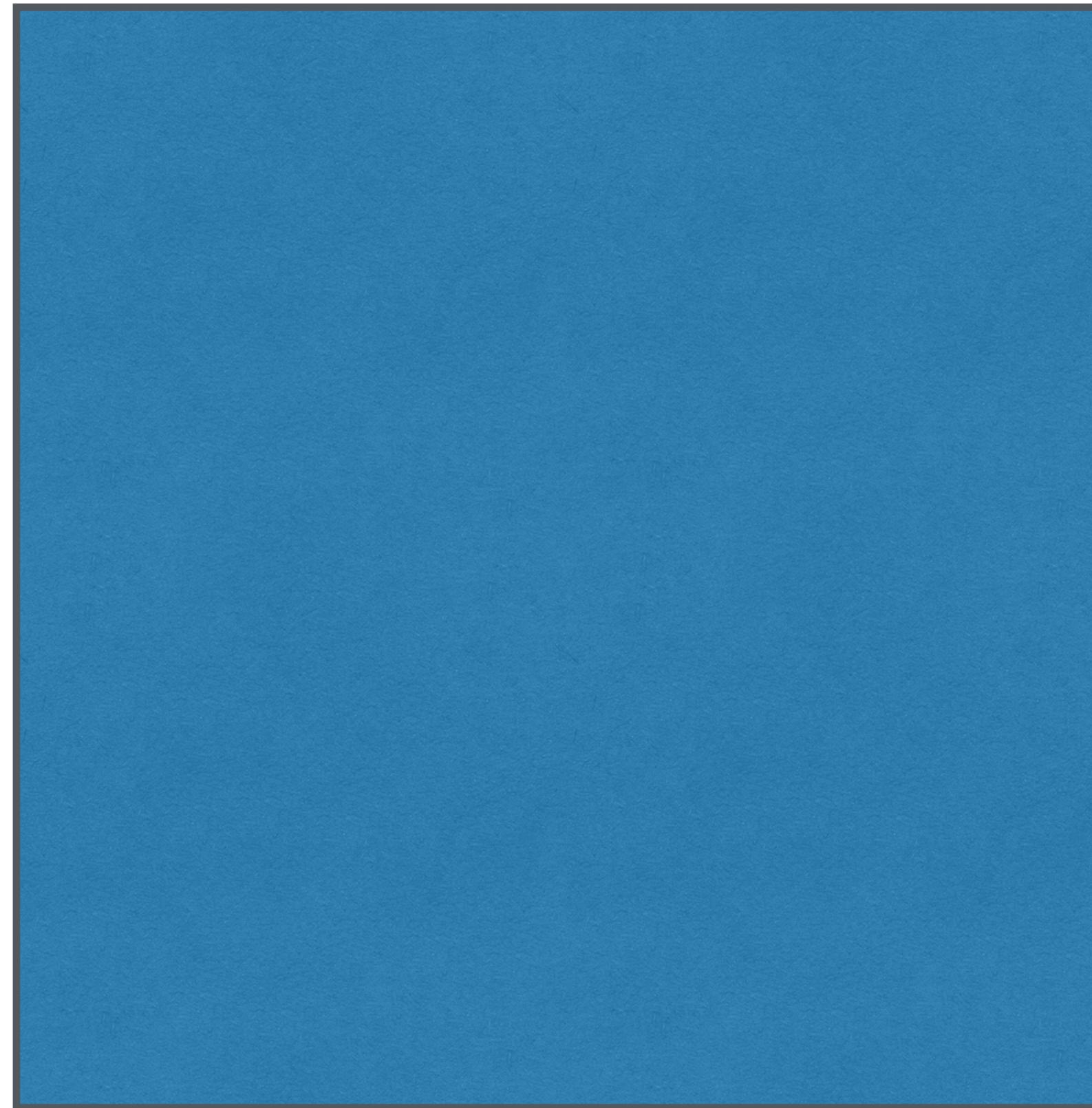
Statistics for Hackers, Jake Vanderplas PyCon16
<https://www.youtube.com/watch?v=lq9DzN6mvYA>

The Fermiac

Enrico Fermi looked really smart with his predictions...



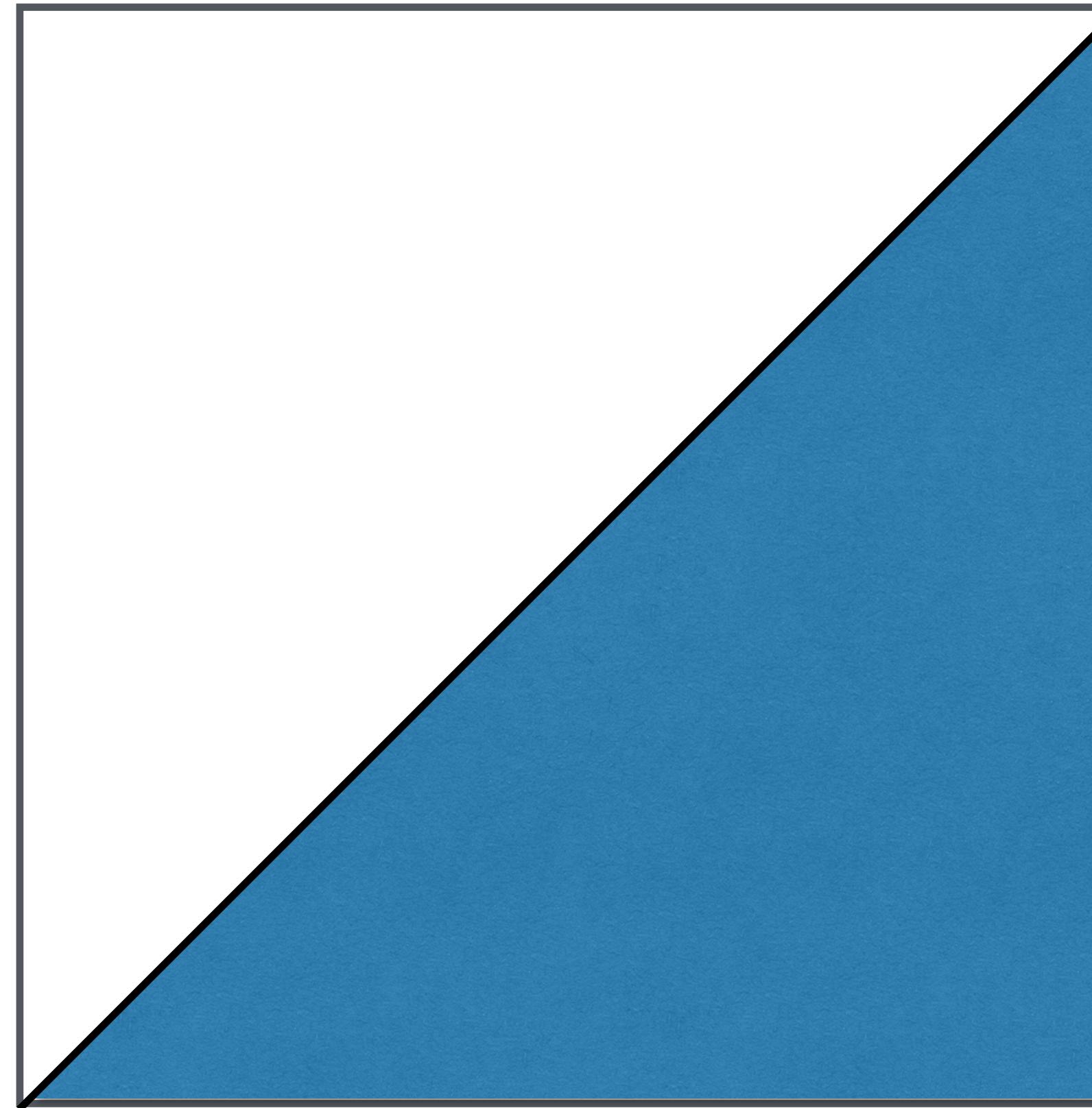
MC - motivation: expectations



Area: base x height

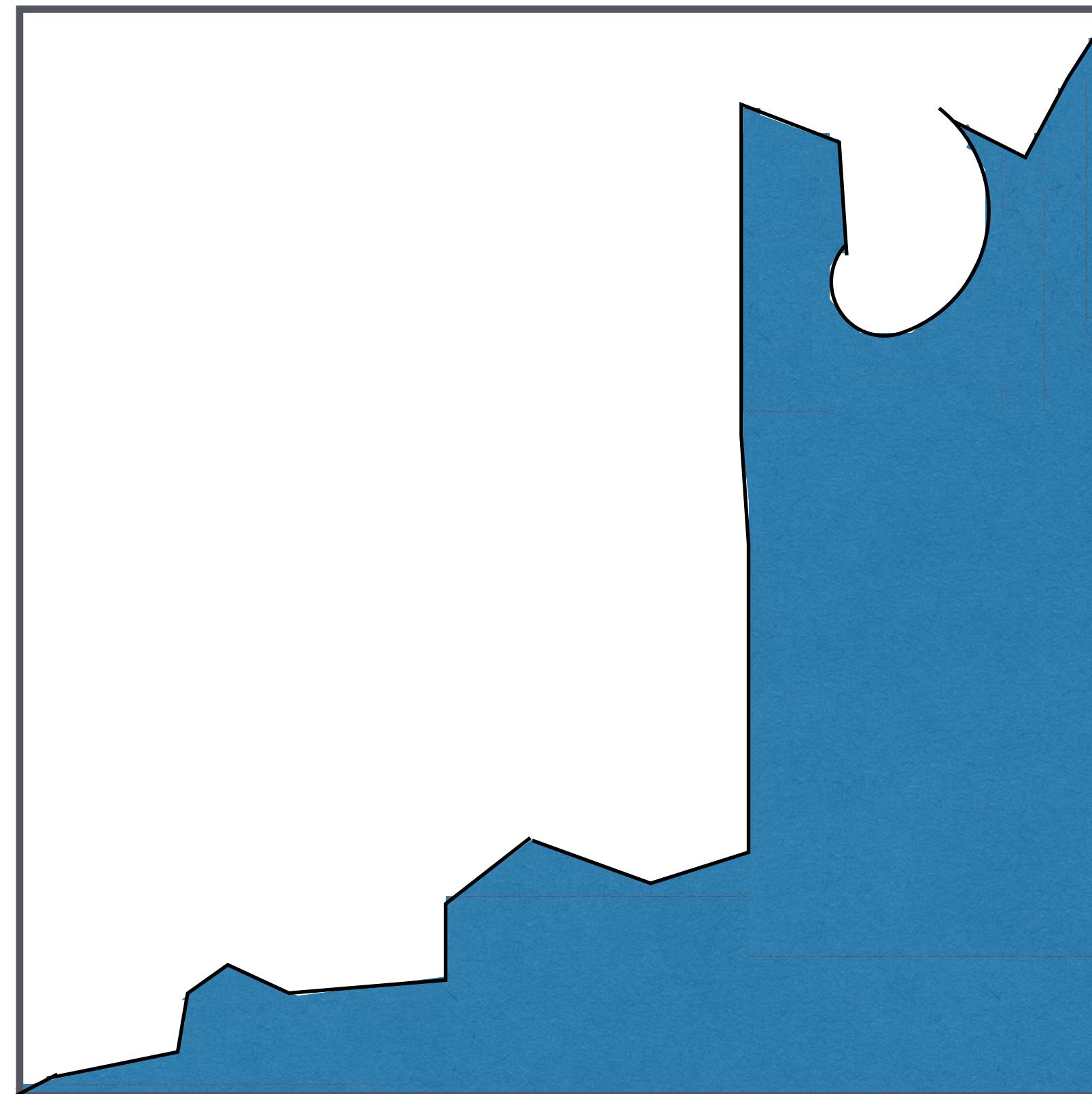


MC - motivation: expectations



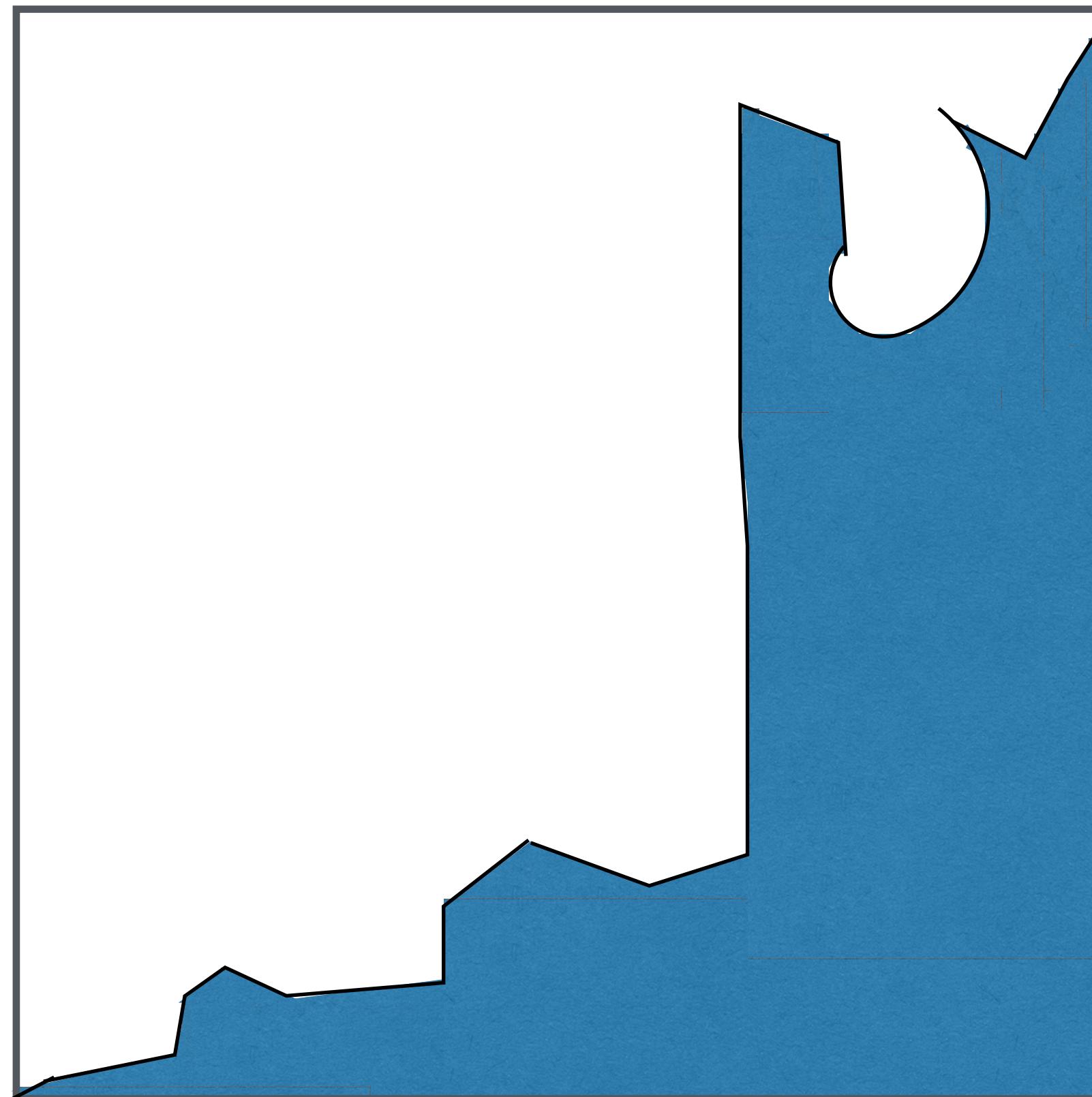
Area: $\frac{\text{base} \times \text{height}}{2}$

MC - motivation: expectations



Area: ??????

MC - motivation: expectations



Area: ??????



MCArea.ipynb

federica bianco - Monte Carlo methods

MC - motivation: expectations

Why am I bothering with areas? - Expectation values are related to areas

Mean

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

$$\begin{aligned}\vec{x} &= [0, 2, 6, 15, 2] \\ \langle x \rangle &= 25 / 5 = 5\end{aligned}$$

MC - motivation: expectations

Why am I bothering with areas? - Expectation values are related to areas

Mean of a sample

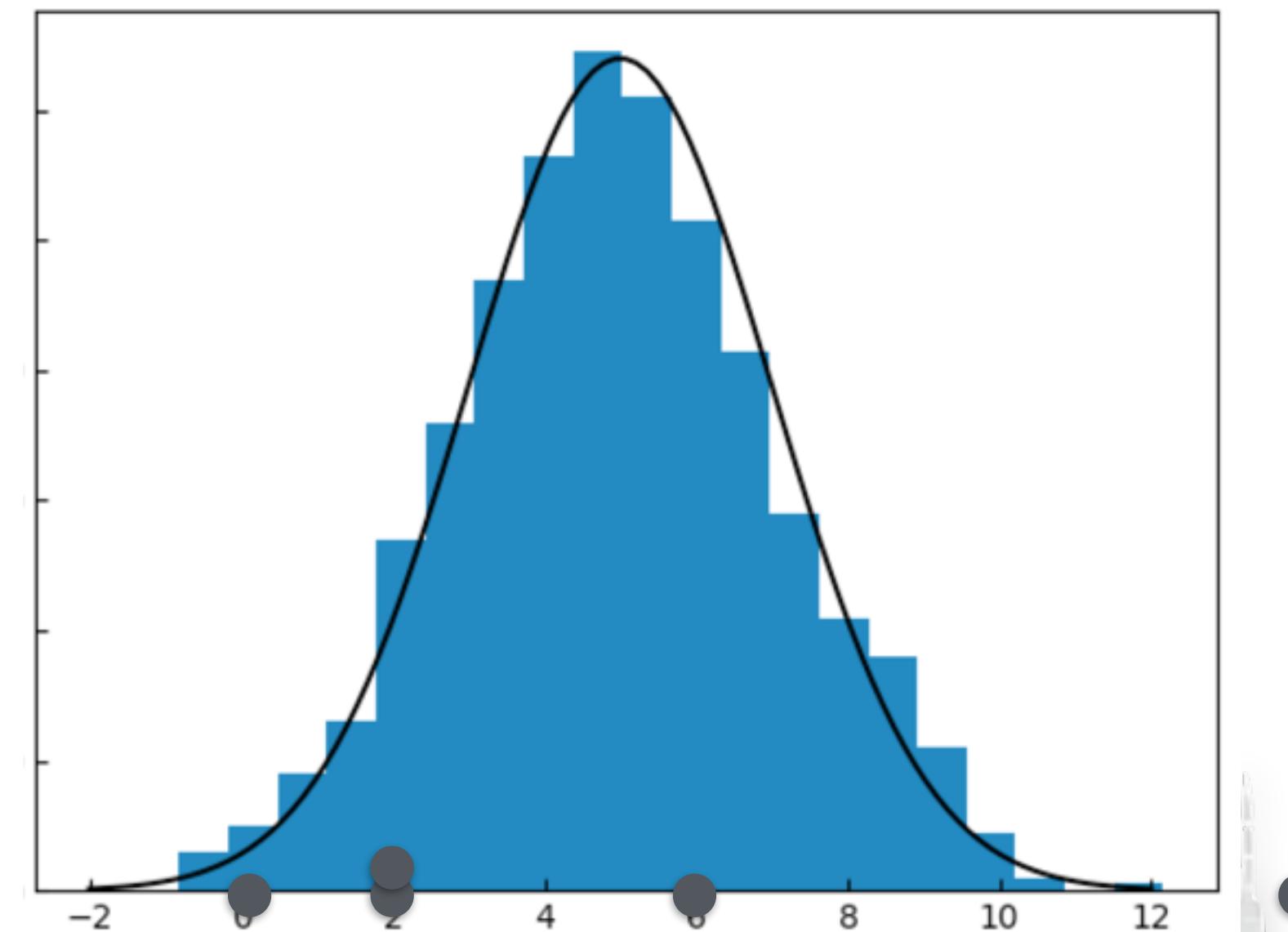
$$\langle \vec{x} \rangle = \frac{1}{N} \sum_{i=1}^N N(x_i)$$

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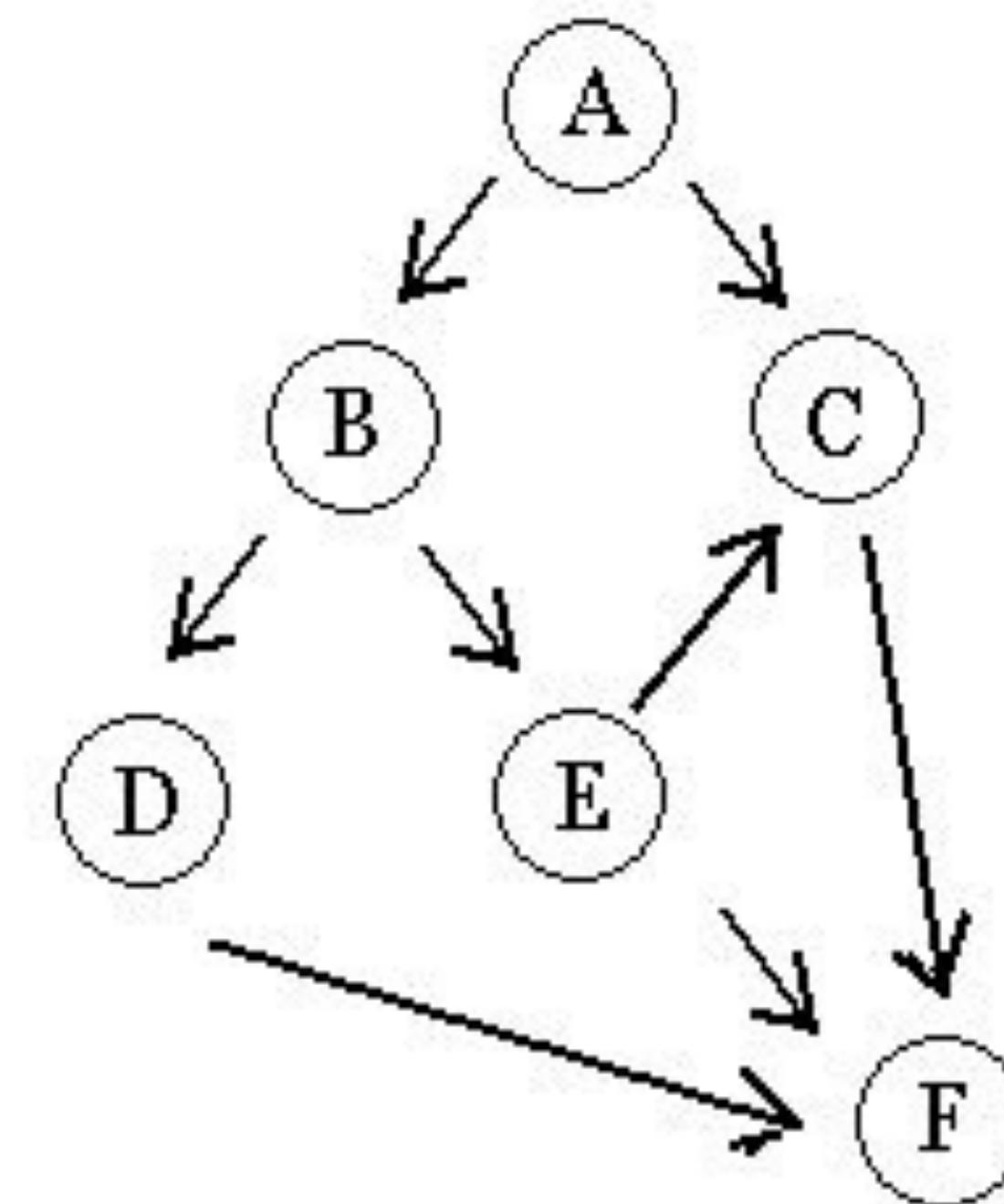
Mean of a
continuous
distribution

$$mean(X) = E[X] = \int X f(X) dX$$

$$Var(X) = E[X^2] - (E[X])^2.$$



MC - motivation: simulations



Sample

$$A \sim P(A)$$

$$B \sim P(B|A)$$

$$C \sim P(C|A,E)$$

$$D \sim P(D|B)$$

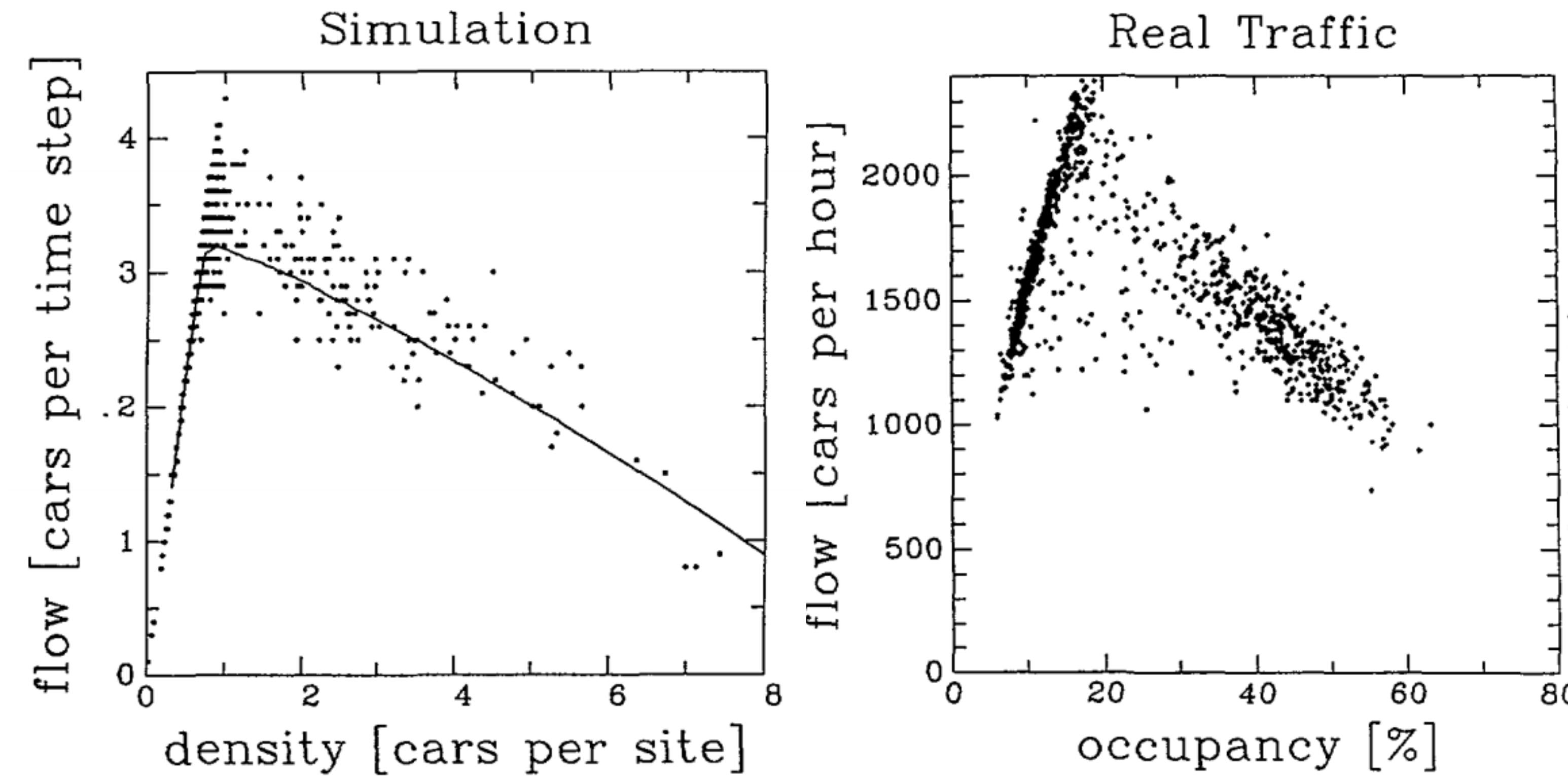
$$E \sim P(E|B)$$

$$F \sim P(F|C,D,E)$$

A long history of MC simulation in traffic flow analysis

A cellular automaton model for freeway traffic

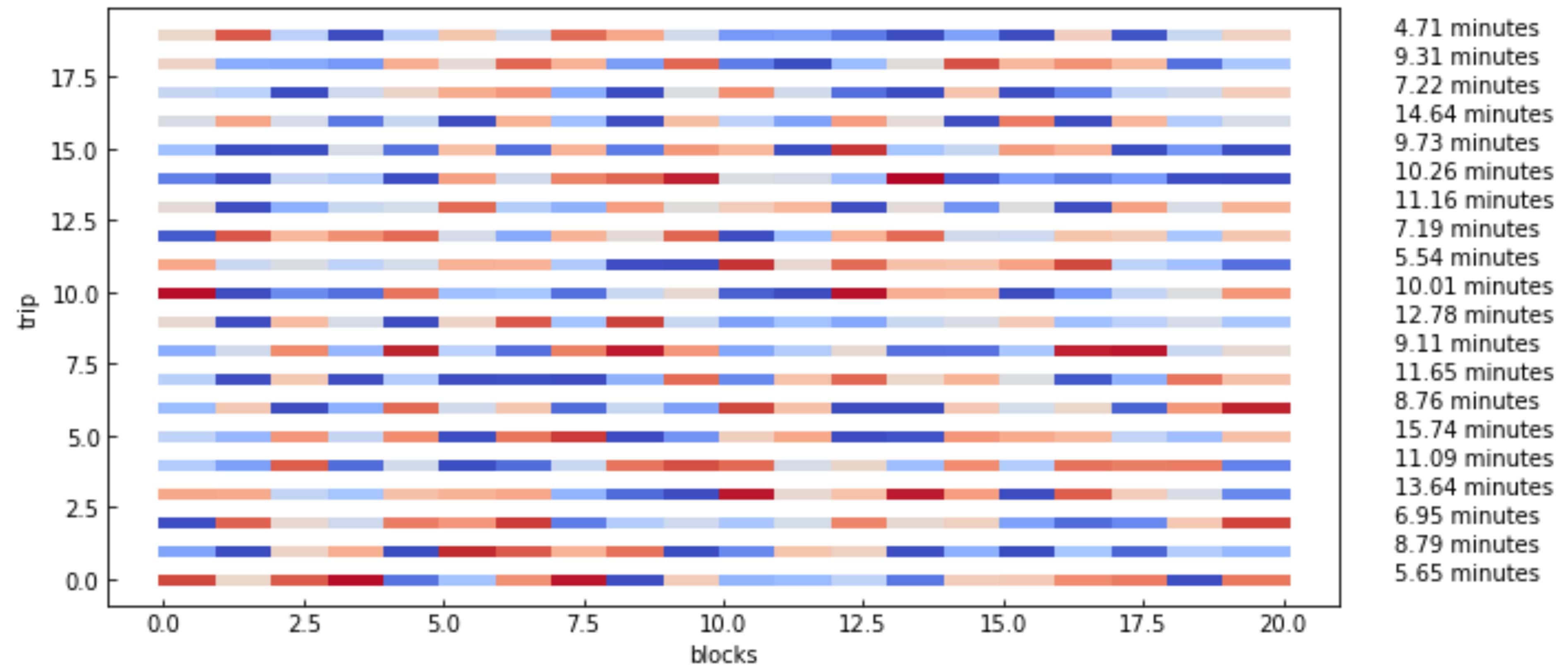
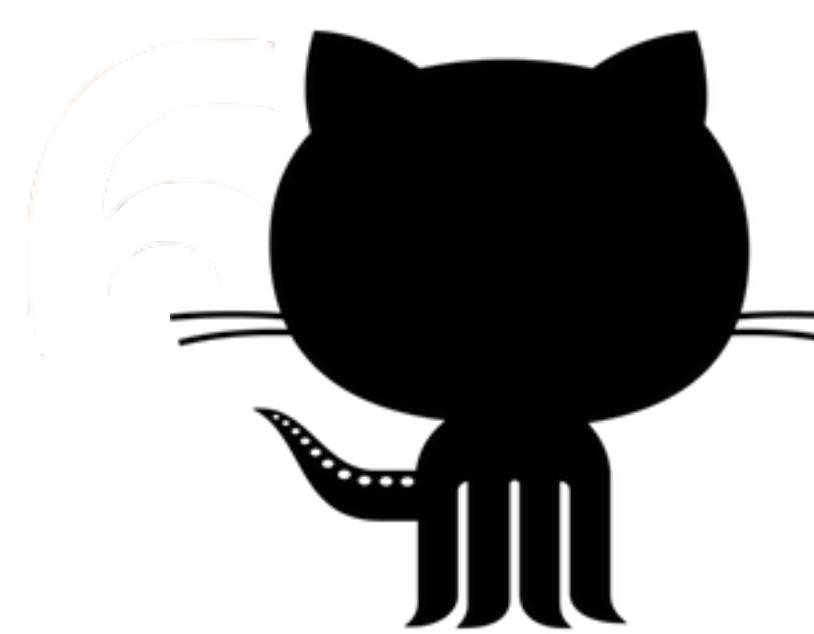
Nagel & Schreckenber 1992



- 1) **Acceleration:** if the velocity v of a vehicle is lower than v_{\max} and if the distance to the next car ahead is larger than $v + 1$, the speed is advanced by one [$v \rightarrow v + 1$].
- 2) **Slowing down (due to other cars):** if a vehicle at site i sees the next vehicle at site $i + j$ (with $j \leq v$), it reduces its speed to $j - 1$ [$v \rightarrow j - 1$].
- 3) **Randomization:** with probability p , the velocity of each vehicle (if greater than zero) is decreased by one [$v \rightarrow v - 1$].
- 4) **Car motion:** each vehicle is advanced v sites.

Through the steps one to four very general properties of single lane traffic are modelled on the basis of integer valued probabilistic cellular automaton rules [9, 10]. Already this simple model shows nontrivial and realistic behavior. Step 3 is essential in simulating realistic traffic flow since otherwise the dynamics is completely deterministic. It takes into account natural velocity fluctuations due to human behavior or due to varying external conditions. Without this randomness, every initial configuration of vehicles and corresponding velocities reaches very quickly a stationary pattern which is shifted backwards (i.e. opposite the vehicle motion) one site per time step.

MC - Urban Applications



[MCstreetLight.ipynb](#)

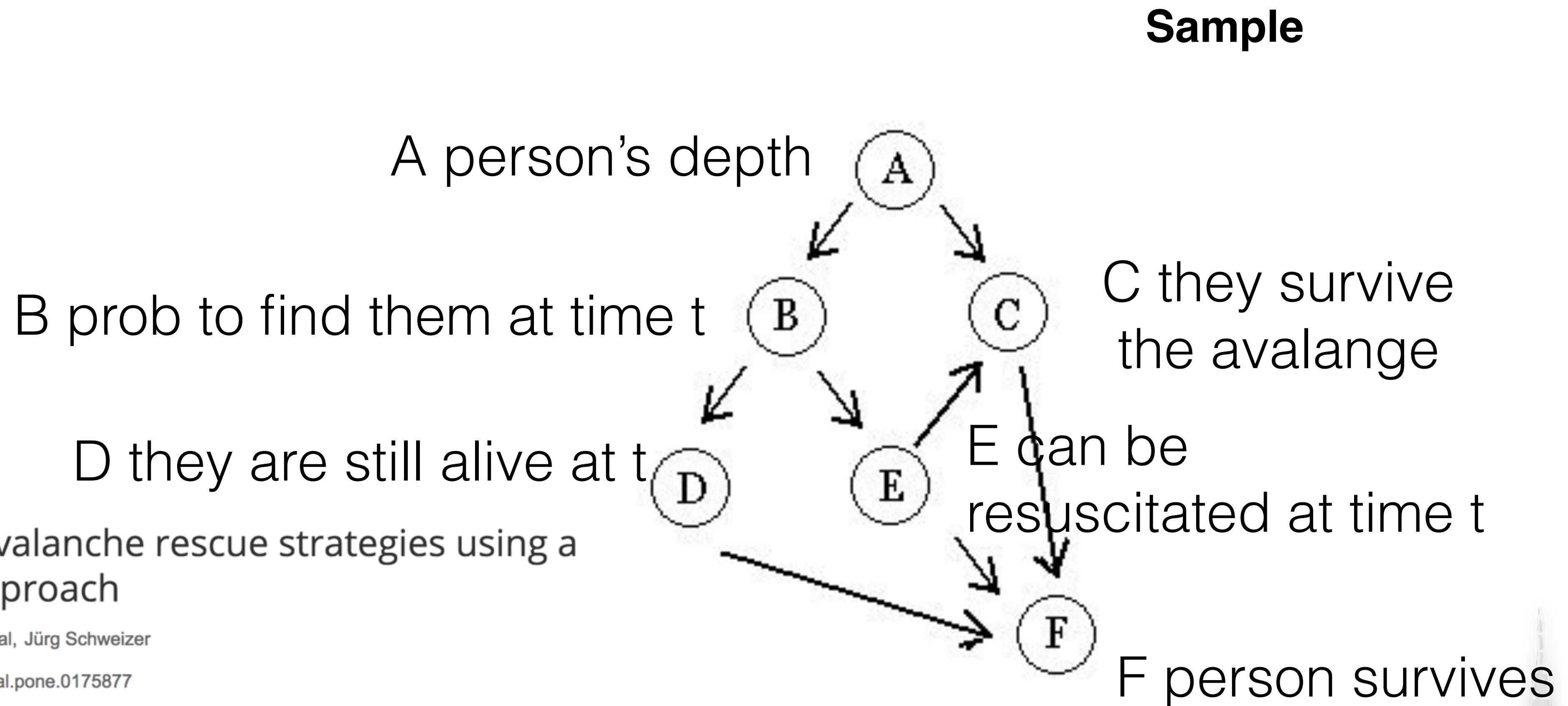
federica bianco - Monte Carlo methods

A concept for optimizing avalanche rescue strategies using a Monte Carlo simulation approach

Ingrid Reiweger  , Manuel Genswein , Peter Paal, Jürg Schweizer

Published: May 3, 2017 • <https://doi.org/10.1371/journal.pone.0175877>

<http://journals.plos.org/plosone/article?id=10.1371/journal.pone.0175877>



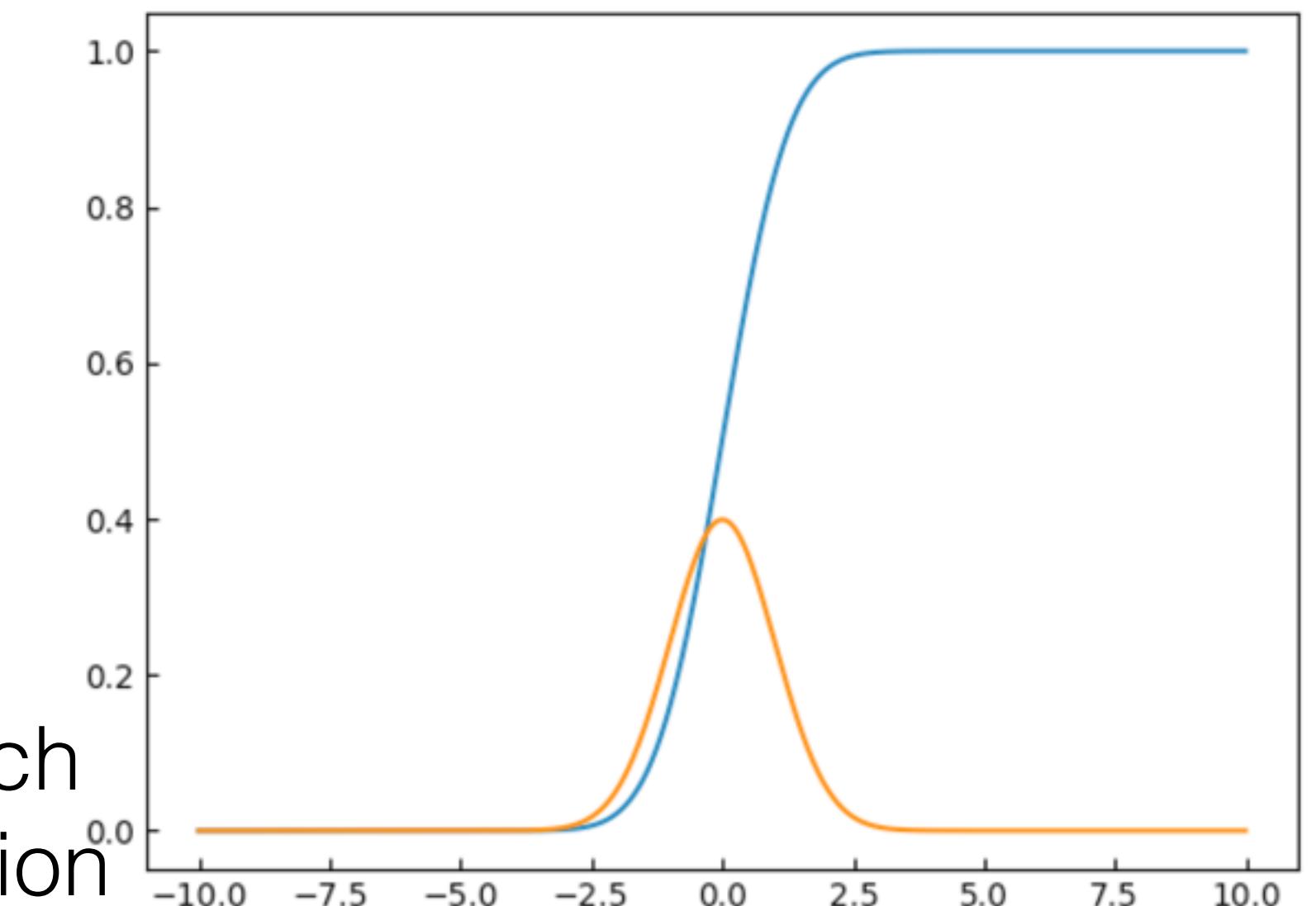
MC - motivation: sampling

SetUp 1:

1. I have a distribution described by some formula $P(x)$ (its PDF)
2. The function can be integrated : e.g. Gaussian

$$P(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \quad \int P(x)dx = \frac{1}{2} \left[1 + \operatorname{erf}\left(\frac{x-\mu}{\sigma\sqrt{2}}\right) \right]$$

3. If I can *take the integral* of the PDF $P(x)$ I can calculate the CDF $F(x)$
4. If I know *and can invert* $F(x)$ (i.e. calculate $F^{-1}(u)$) I know at which percentile a value is and I can directly sample from the distribution



MC - motivation: sampling

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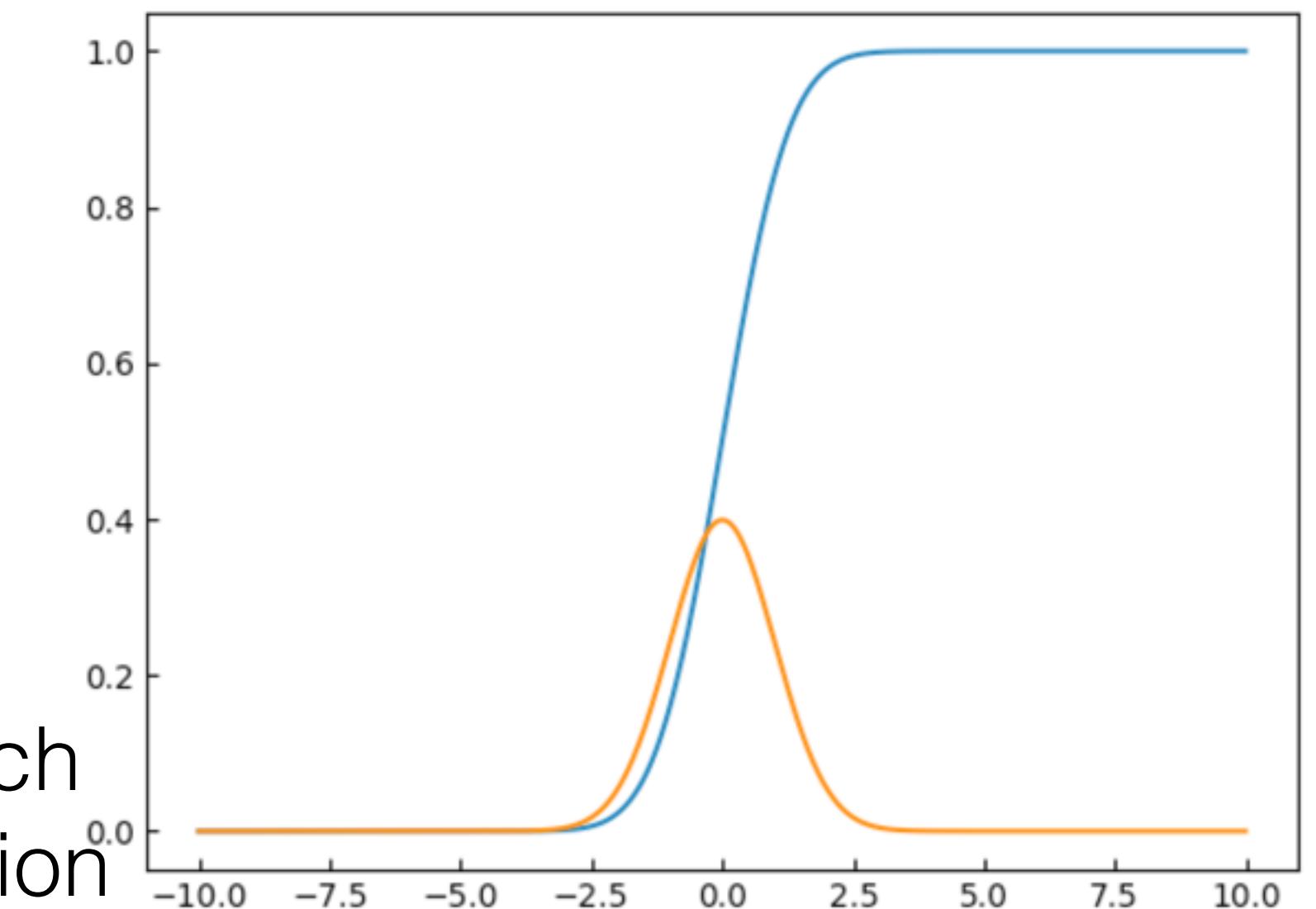
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4. If I know *and can invert* $F(x)$ (i.e. calculate $F^{-1}(u)$) I know at which percentile a value is and I can directly sample from the distribution

WHILE convergence: // $P(x)$ is filled in

draw a uniform random number $u \sim \text{Uniform}[0,1]$

calculate $x = F^{-1}(u)$ // x is a sample from P



Slides on sampling from distributions

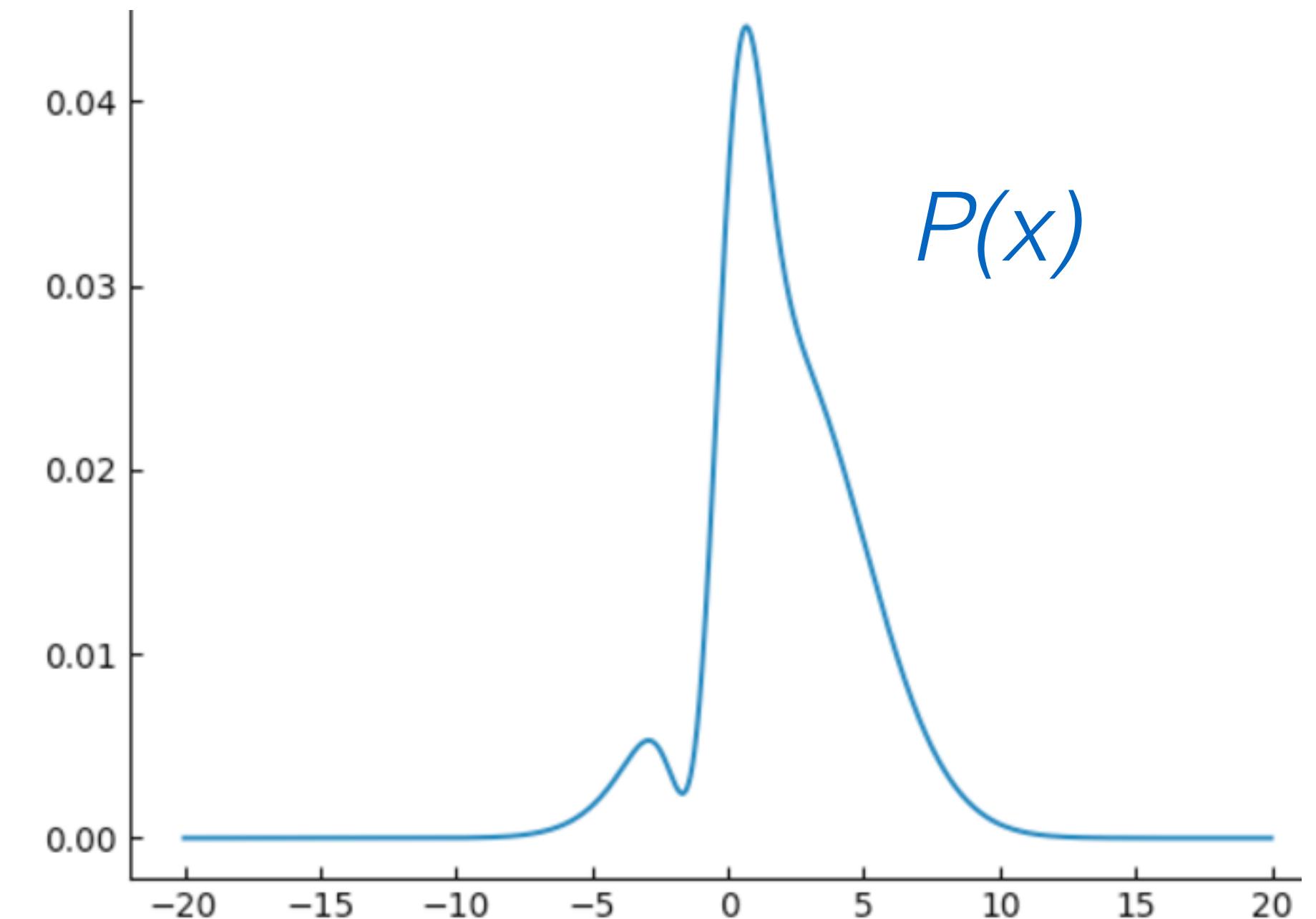
Paul E. Johnson 2015

MC - Rejection Sampling

SetUp 2:

1. I have a distribution described by some formula $P(x)$
2. The function *cannot* be (easily) integrated :

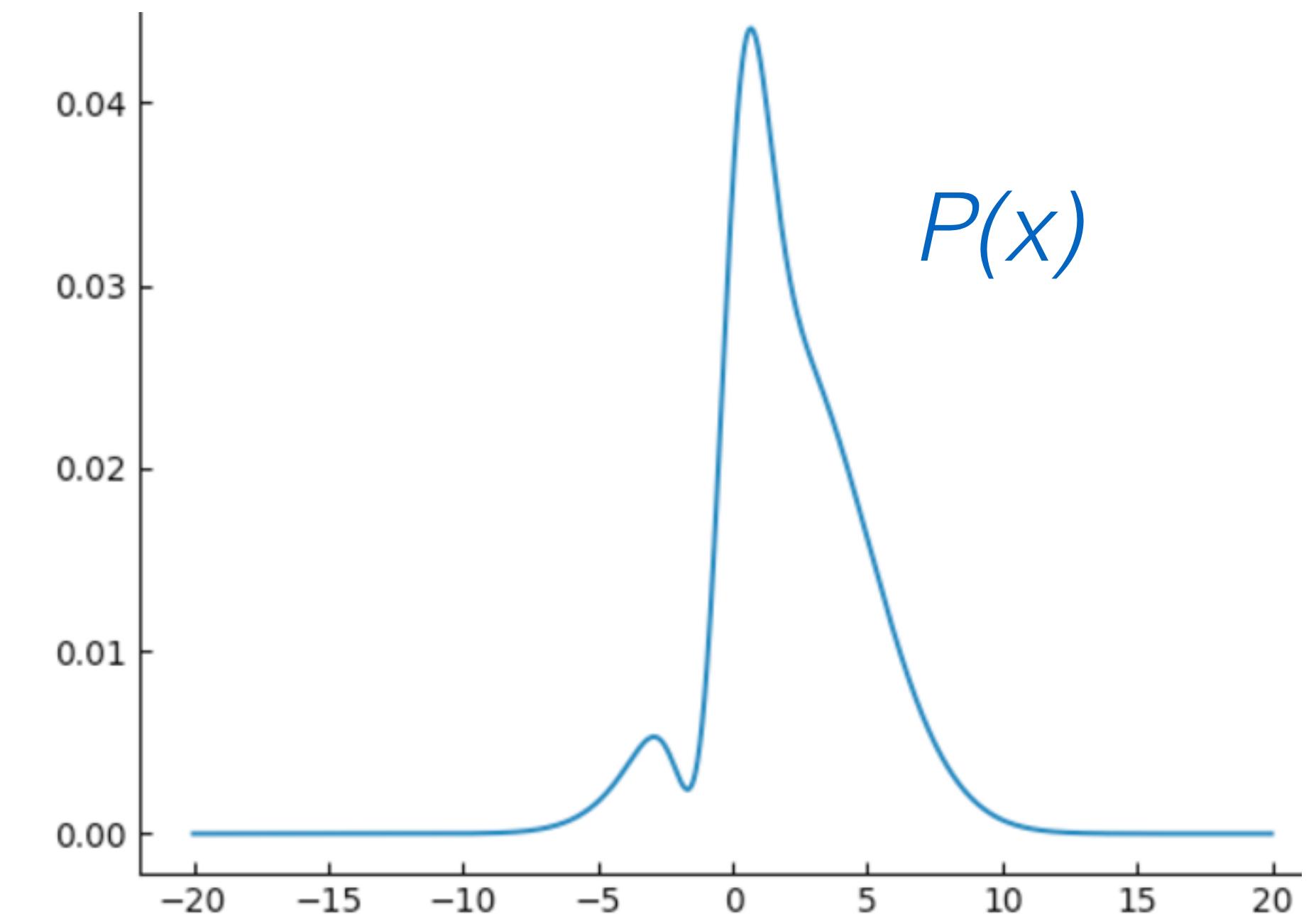
***I dont know how to draw samples
but I can calculate its value at every x***



MC - Rejection Sampling

SetUp 2:

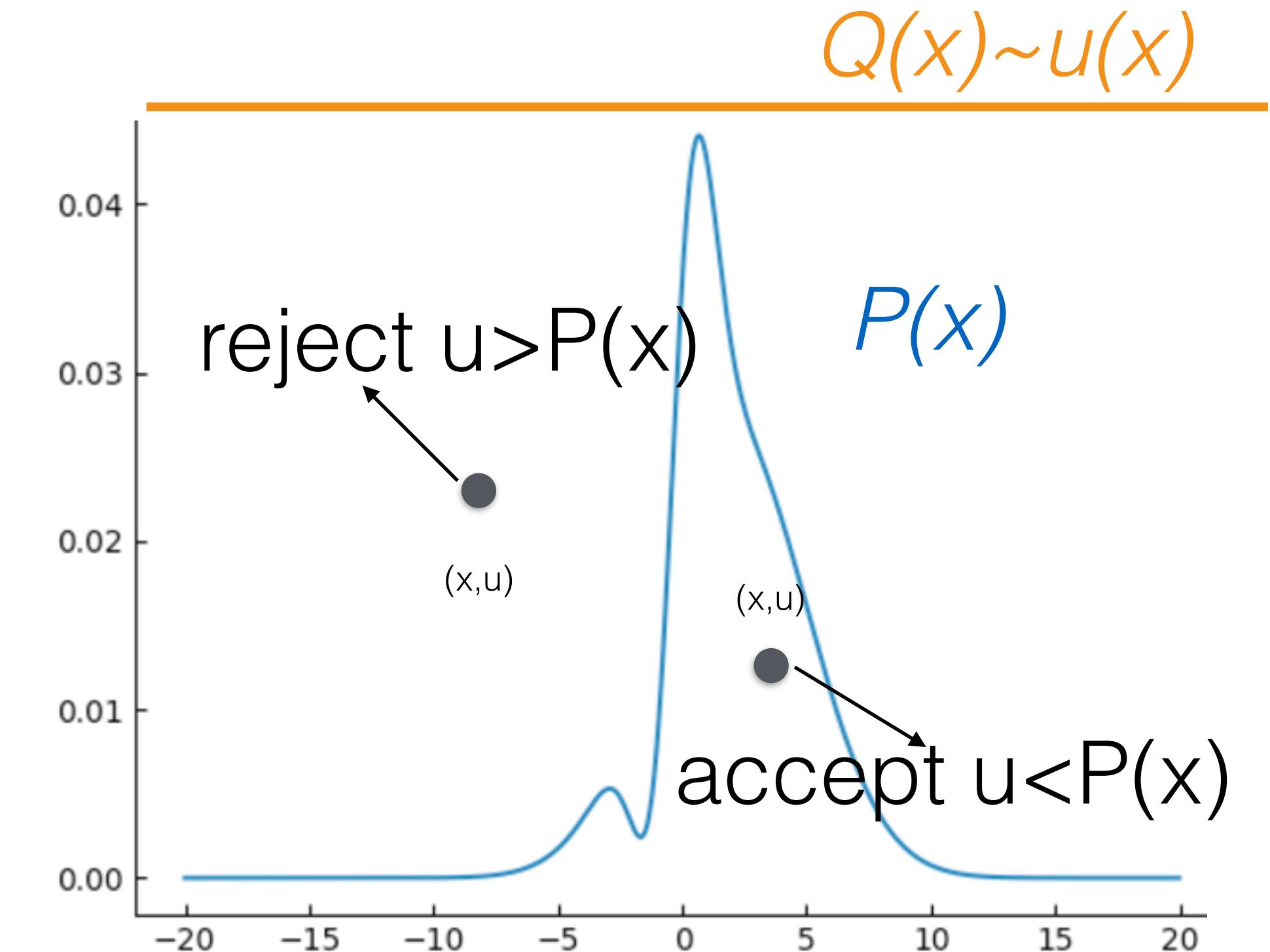
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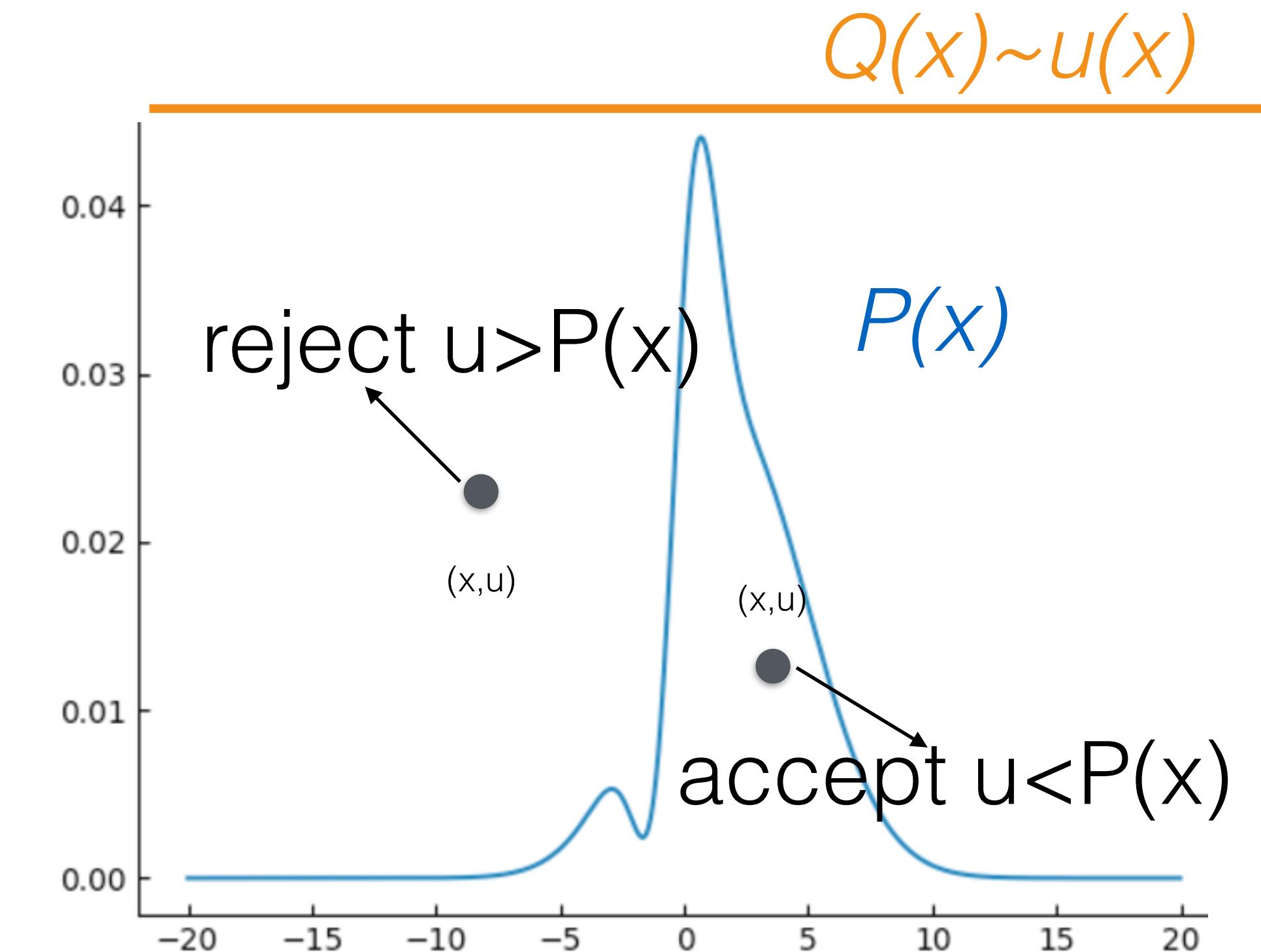


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```
WHILE convergence: //  $P(x)$  is filled in
    draw a point  $x$  from  $Q(x)$ 
    calculate  $P(x)$ 
    draw a height  $u \sim \text{Uniform}[0, Q(x)]$ 
    IF :  $u <= P(x)$ 
        accept // point is sample of  $P(x)$ 
    ELSE :
        reject
```

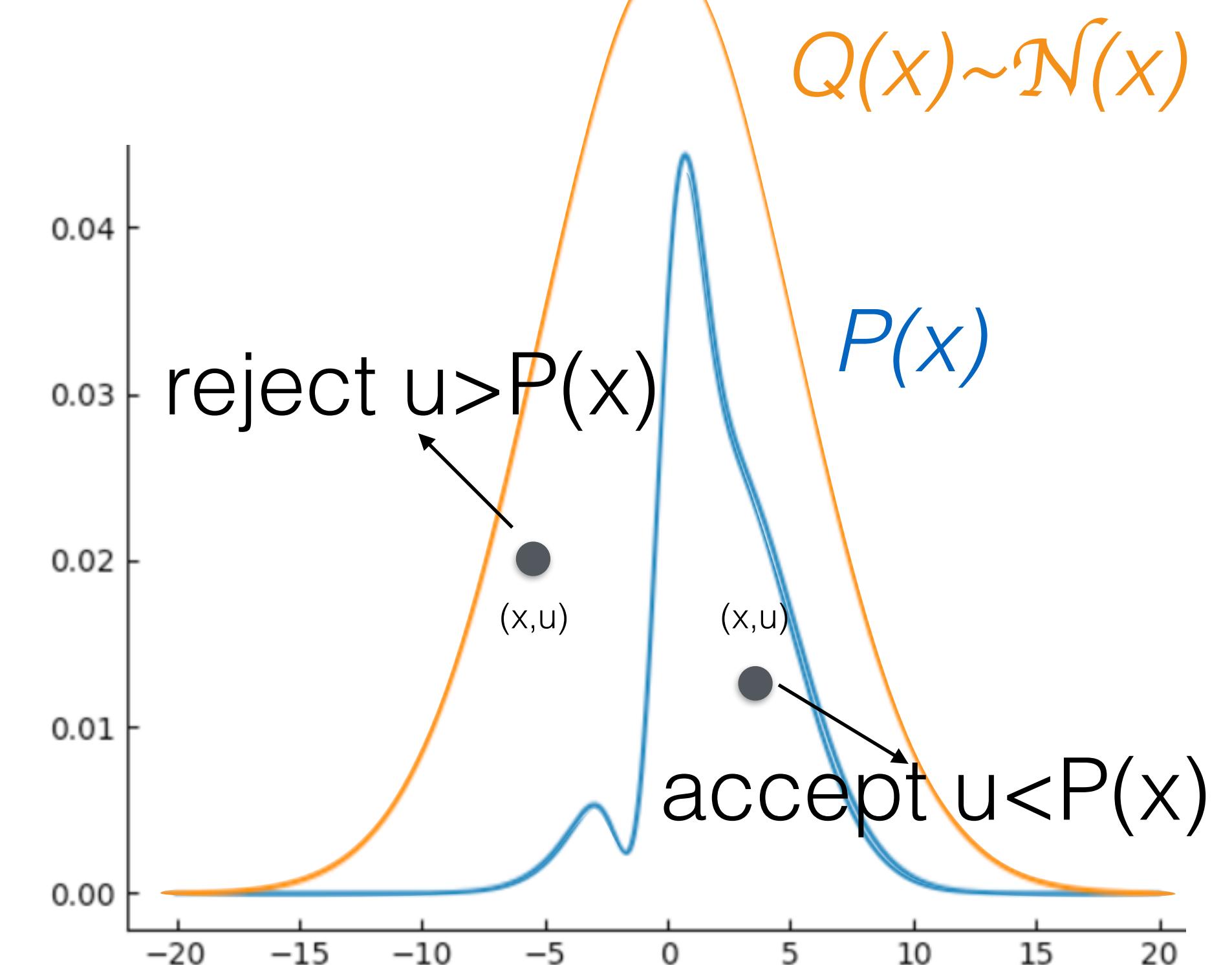


MC - Rejection Sampling

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***I dont know how to draw samples
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3. There exist distributions - $Q(x)$ - that are higher than the $P(x)$ at every x : e.g. *Gaussian distribution!*

```
WHILE convergence: //  $P(x)$  is filled in
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    calculate  $P(x)$ 
    draw a height  $u \sim \text{Uniform}[0, Q(x)]$ 
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```



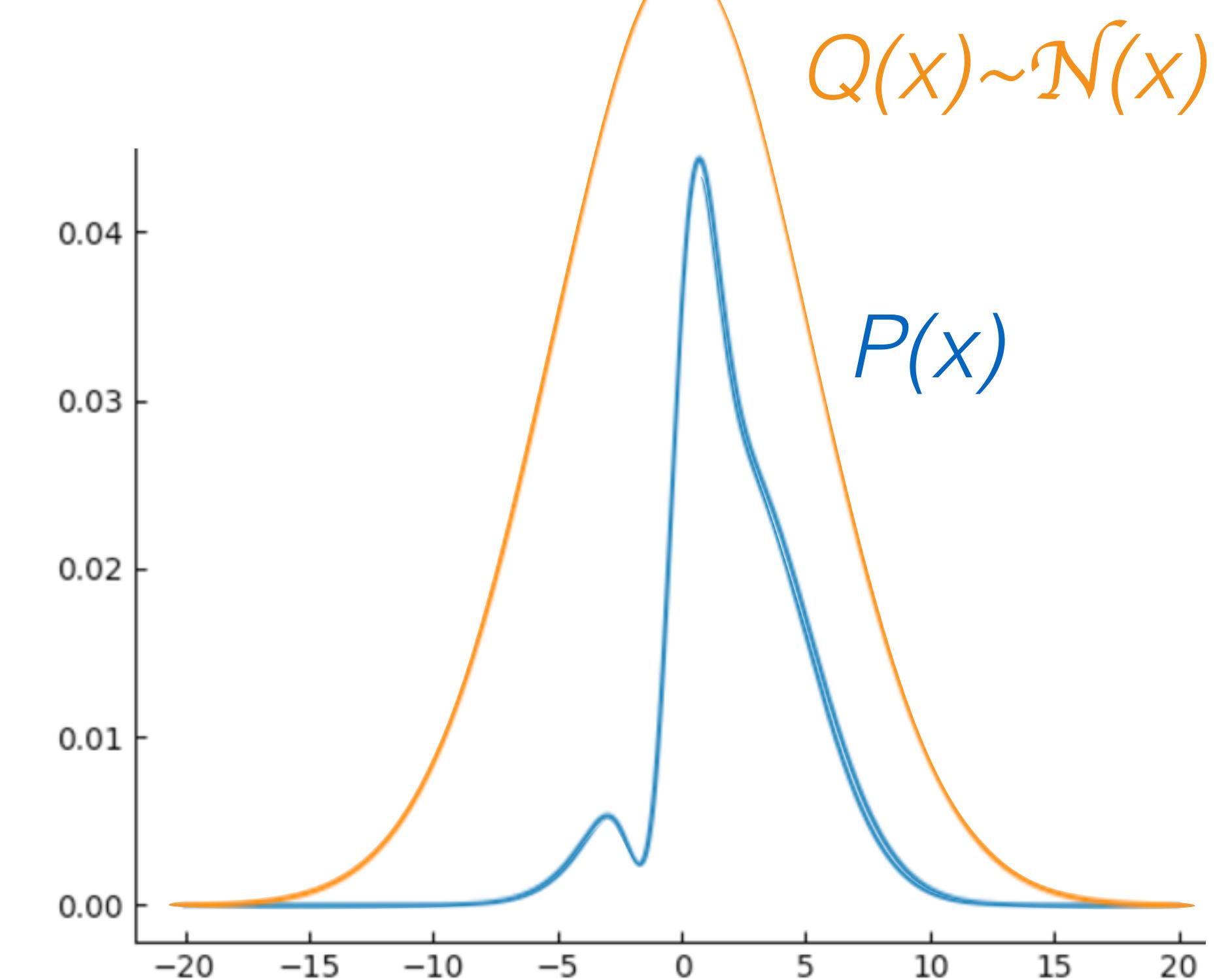
MC - Importance Sampling

SetUp 2:

1. I have a distribution described by some formula $P(x)$
2. The function *cannot* be (easily) integrated :
***I dont know how to draw samples
but I can calculate its value at every x***
3. There exist distributions - $Q(x)$

$$\begin{aligned}\int f(x)P(x)dx &= \int f(x)\frac{P(x)}{Q(x)}Q(x)dx, \quad (Q(x)>0 \text{ if } P(x)>0) \\ &\approx \frac{1}{S} \sum_{s=1}^S f(x_s) \frac{P(x_s)}{Q(x_s)}, \quad x(s) \sim Q(x)\end{aligned}$$

$Q(x) \Leftrightarrow P(x)$ guarantees that the integral does not diverge
choose $Q(x)$ s.t. $Q(x)$ is large where $f(x) P(x)$ is large



Markov Chain Monte Carlo



Markov Chain



Markov Chain

memory-less stochastic process:

make predictions for the future of the process based solely on its present state independently from the previous history;

i.e. the next state of the process is based on a chosen distribution (e.g. gaussian) with parameters that depend only on the current state (e.g. with mean at the current state)

Markov processes



Markov Chain

memory-less stochastic process:

e.g.:

Random Walk -> *next position is a stochastic perturbation over current position*

Gamblers' ruin

Waiting for upload.wikimedia.org...
...mito.ebilammiJiw.besoldu rot gnutifreibW

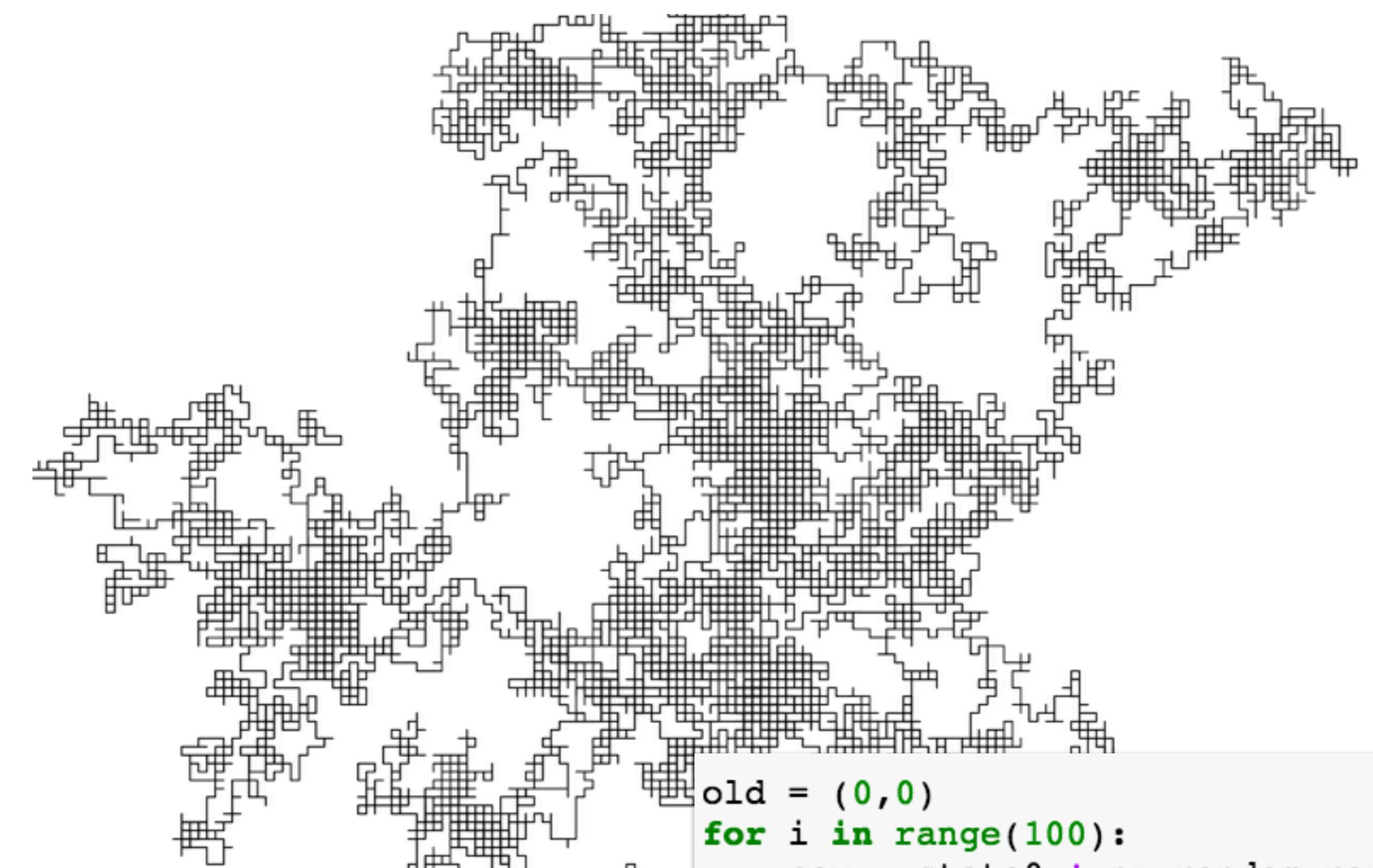
Markov processes

Markov Chain

memory-less stochastic process:

e.g.:

Random Walk -> choose next position as a gaussian perturbation over the current
Gamblers' ruin



```
old = (0,0)
for i in range(100):
    new = state0 + np.random.rand(2)
    old = new
```

Markov Chain Monte Carlo



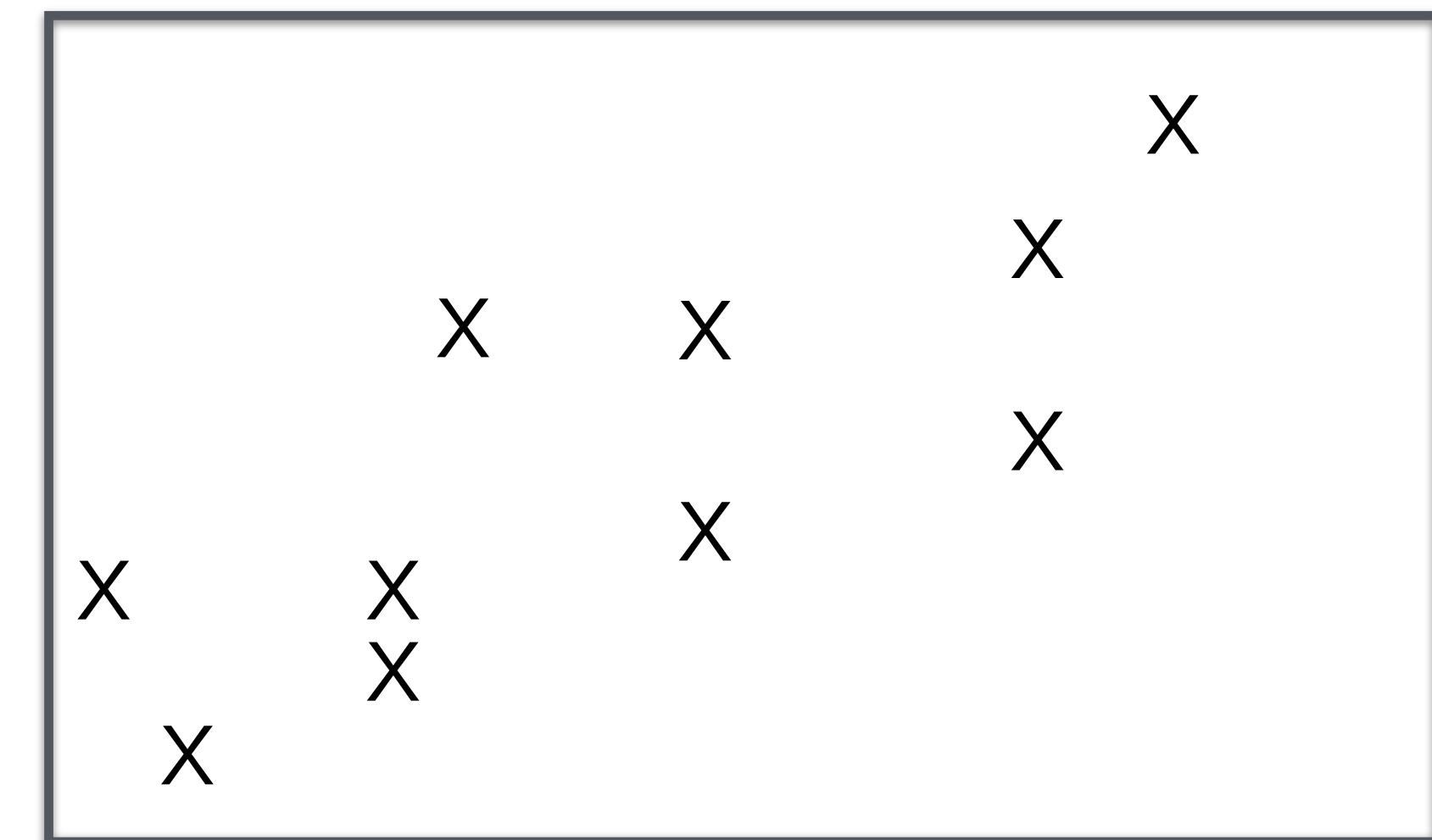
MCMC - motivation

I have a model and I want to find the best parameters to describe my data

Data D

Model - some function $f(\theta)$

Parameters θ

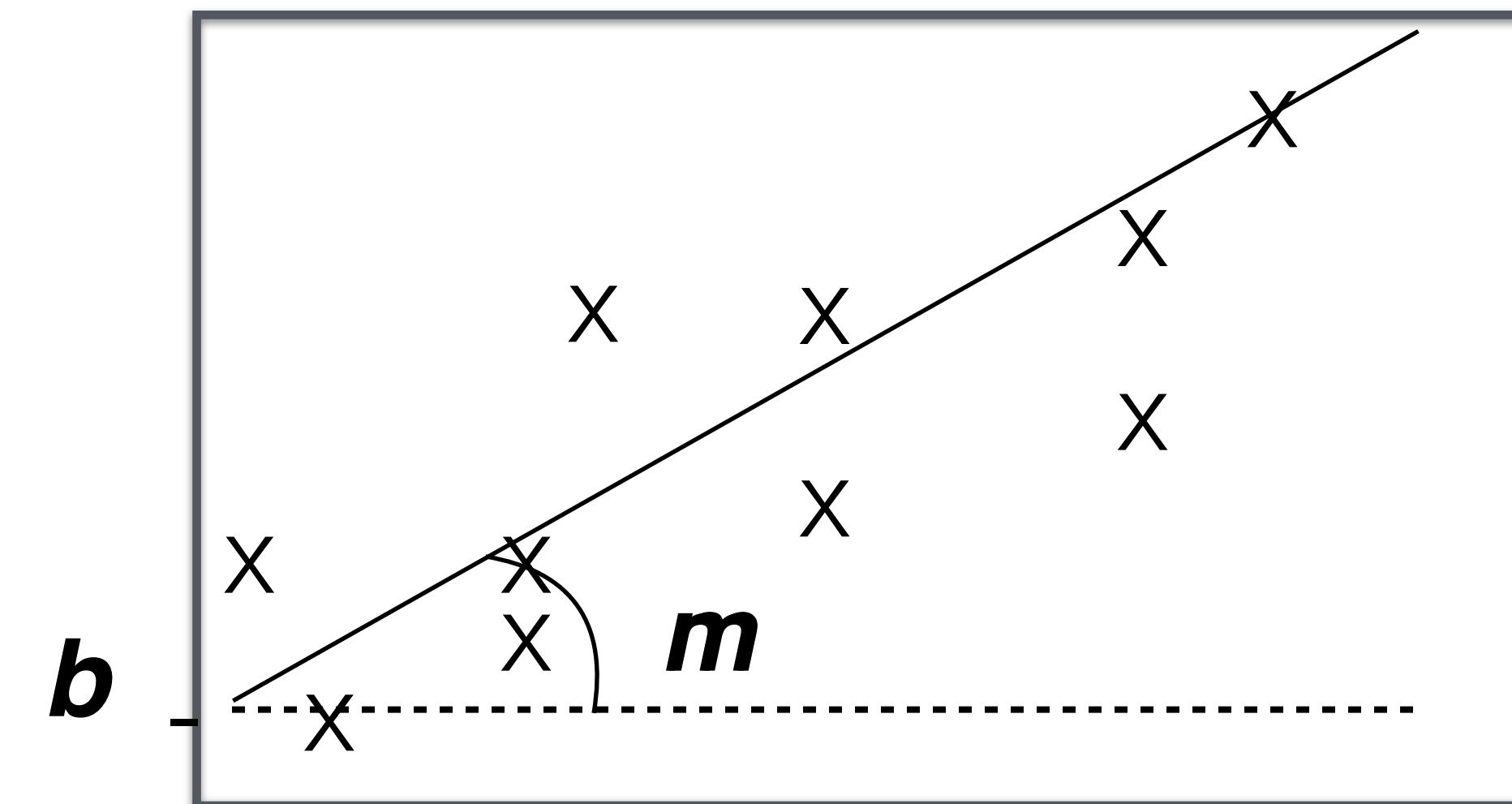


I have a model and I want to find the best parameters to describe my data

Data \mathcal{D}

Model $f(\mathbf{m}, \mathbf{b}) = mx + b$

Parameters $\theta = (\mathbf{m}, \mathbf{b})$



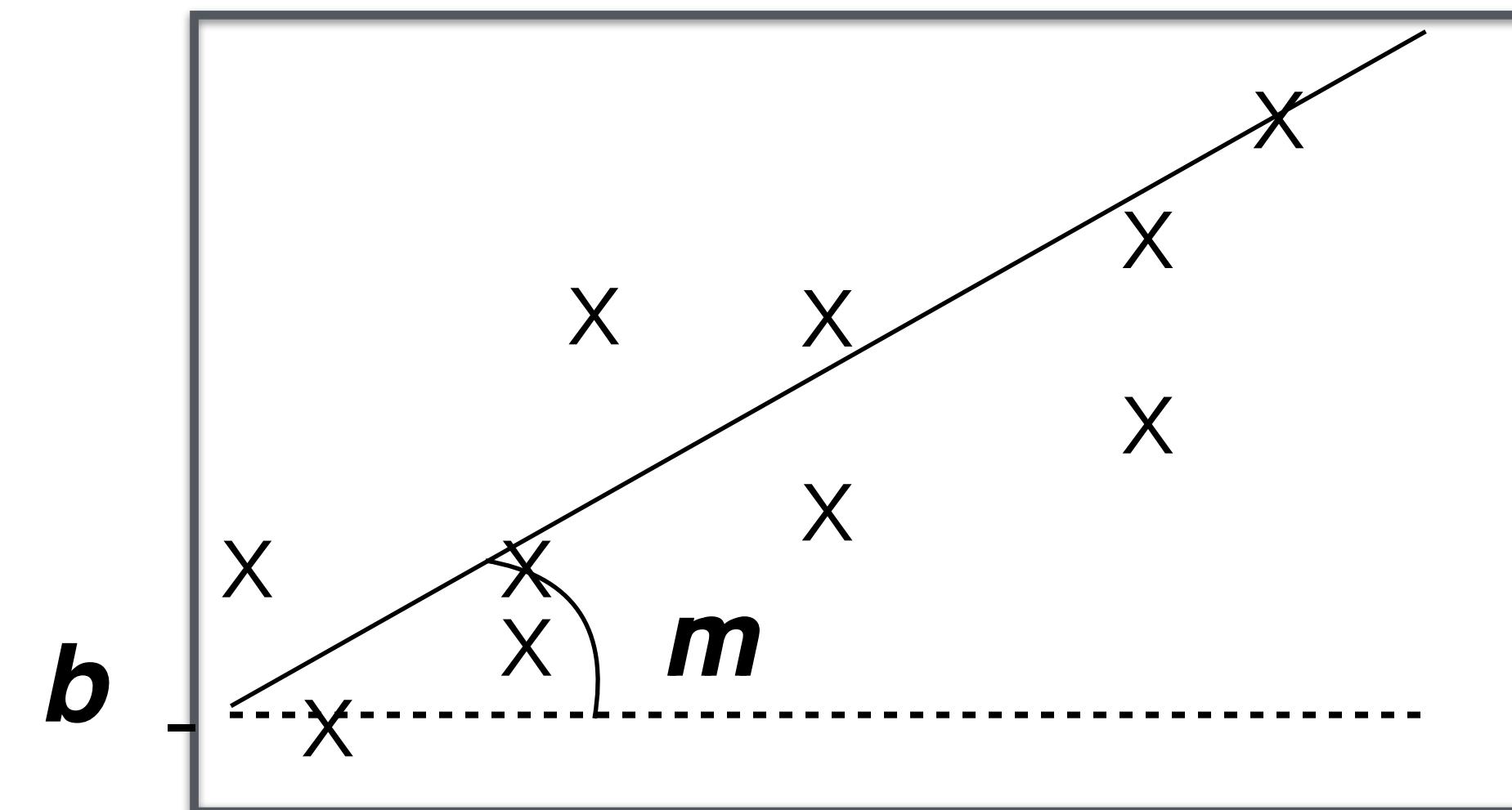
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Data D

Model $f(\mathbf{m}, \mathbf{b}) = mx + b$

Parameters $\theta = (\mathbf{m}, \mathbf{b})$



To find the best model parameters:
maximize likelihood: **θ such that $P(D|\theta)$ is max**

https://github.com/fedhere/PUI2016_fb55/blob/master/HW6_fb55/building_nrg_solution.ipynb

I have a model and I want to find the best parameters to describe my data

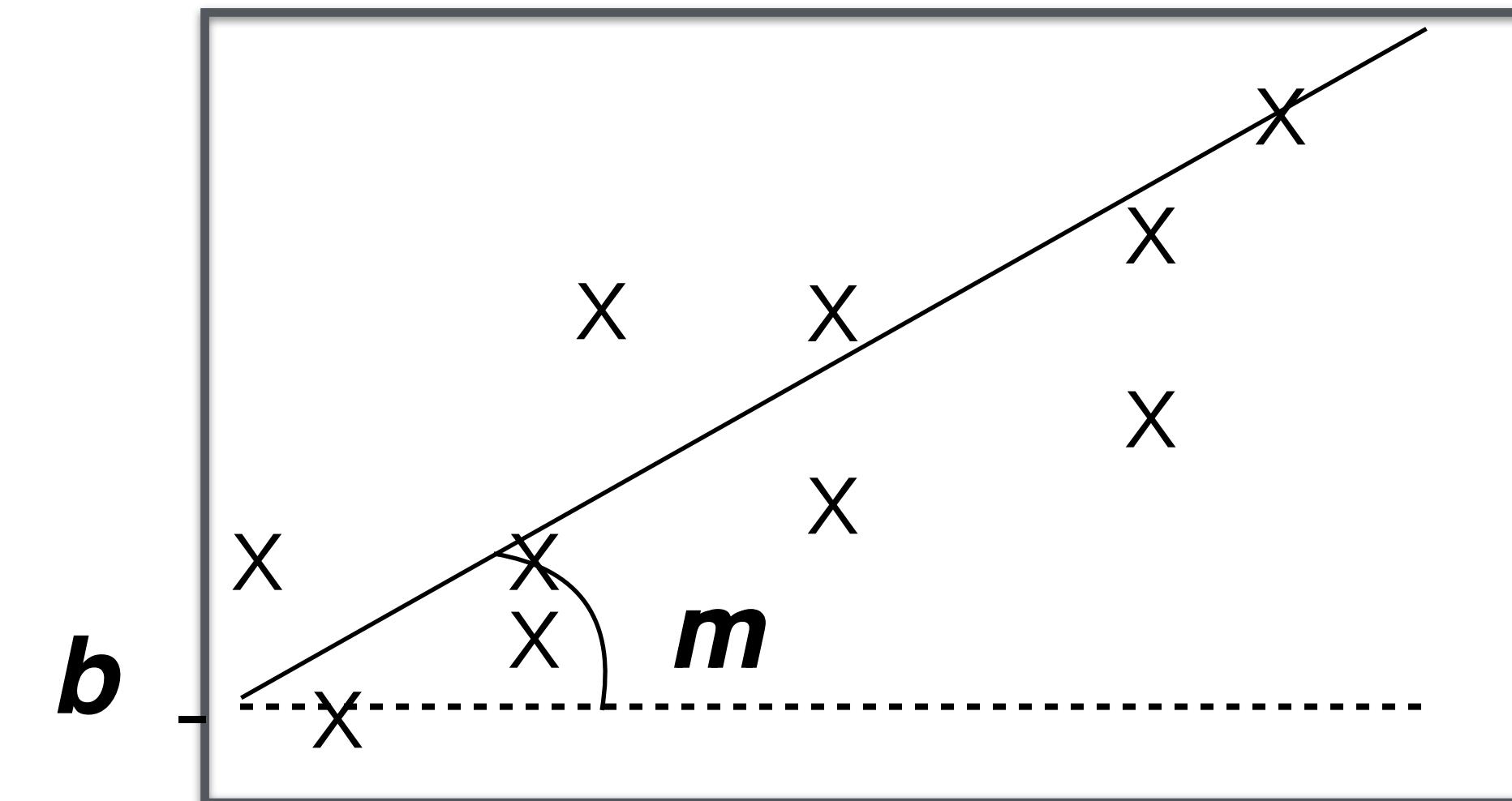
Data \mathcal{D}

Model $f(\mathbf{m}, \mathbf{b}) = mx + b$

Parameters $\theta = (\mathbf{m}, \mathbf{b})$

Refresher about *likelihood*:

- The likelihood of a distribution has the same form as its PDF
- the likelihood of a Gaussian distribution is:



$$L \equiv P(D|N, \mu, \sigma) = \frac{1}{\sqrt{2\pi} \sigma} \prod_{i=1}^N \exp\left(-\frac{(\mu-x)^2}{2\sigma^2}\right)$$

- generally we like to work in log space with likelihoods because they can be very large numbers and finding the maximum is equivalent to finding a 0 in log space

$$\log(L) = -\frac{1}{2} \sum_{i=1}^N \log(2\pi) - \sum_{i=1}^N \log(\sigma^2) - \frac{1}{2} \sum_{i=1}^N \frac{(\mu-x)^2}{\sigma^2} = C - \frac{1}{2} \chi^2$$

MCMC - motivation

I have a model and I want to find the best parameters to describe my data

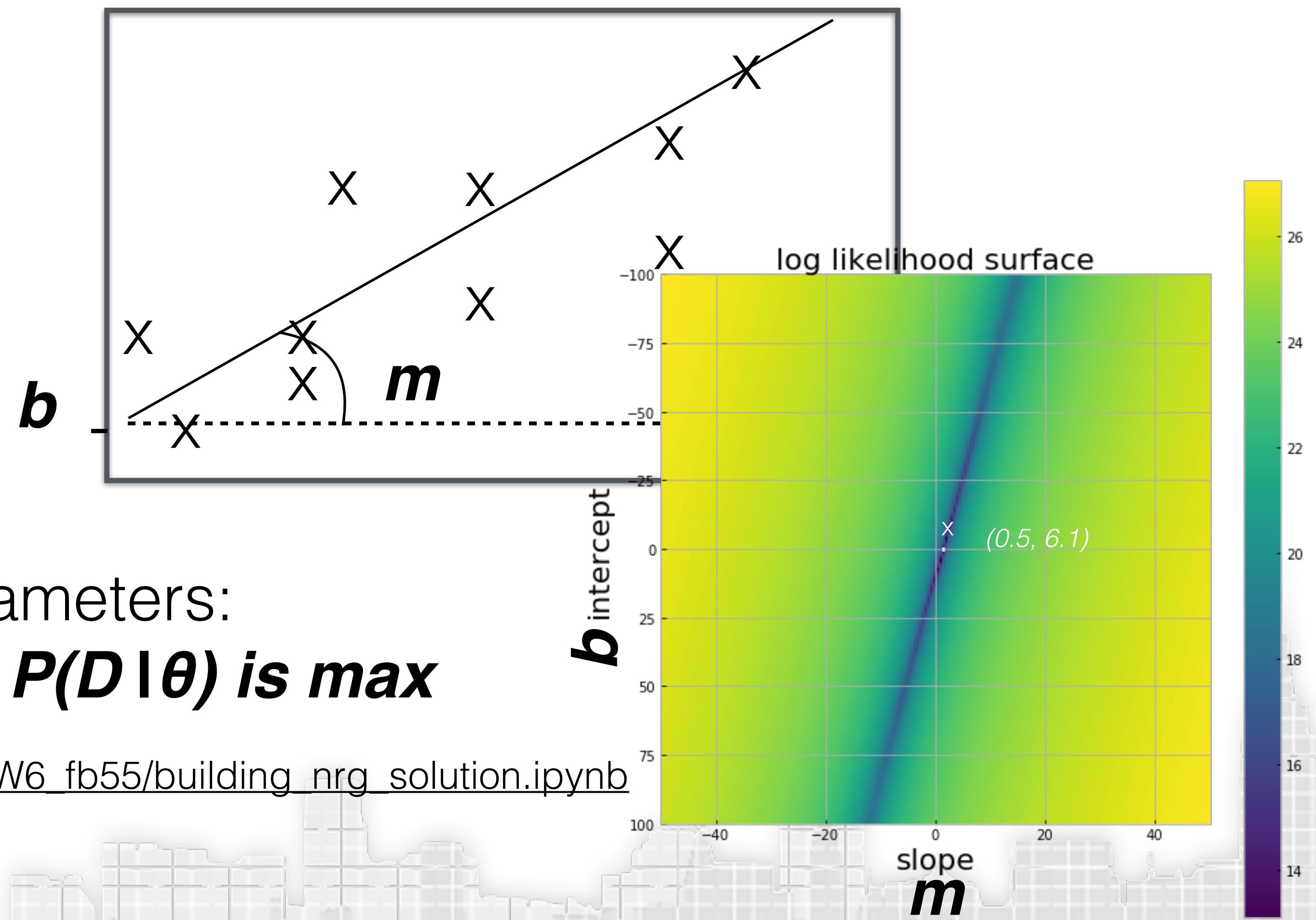
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Bayes theorem:

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

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Definitions:

posterior: joint probability distribution of a parameter set (m, b) condition upon some data D and a model hypothesis f

Bayes theorem:

$$P(\theta|D,f) = \frac{P(D|\theta,f)P(\theta,f)}{P(D|f)}$$

Definitions:

posterior

posterior: joint probability distribution of a parameter set (m, b) condition upon some data D and a model hypothesis f

Bayes theorem:

$$P(\theta|D,f) = \frac{P(D|\theta,f)P(\theta,f)}{P(D|f)}$$

likelihood prior
posterior evidence

Definitions:

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Bayes theorem:

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posterior **prior**

Definitions:

posterior: joint probability distribution of a parameter set (m, b) condition upon some data D and a model hypothesis f

prior: “intellectual” knowledge about the model parameters

Bayes theorem:

$$P(\theta|D,f) = \frac{P(D|\theta,f)P(\theta,f)}{P(D|f)}$$

posterior **prior**

Definitions:

posterior: joint probability distribution of a parameter set (m, b) condition upon some data D and a model hypothesis f

prior: “intellectual” knowledge about the model parameters

e.g.: energy consumption increased w number of units: $m > 0$

Bayes theorem:

$$P(\theta|D,f) = \frac{P(D|\theta,f)P(\theta,f)}{P(D|f)}$$

posterior

prior

evidence

Definitions:

posterior: joint probability distribution of a parameter set (m, b) condition upon some data D and a model hypothesis f

prior: “intellectual” knowledge about the model parameters

evidence: marginal likelihood of data under the model

$$P(D|f) = \int P(D|\theta,f)P(\theta|f)d\theta$$

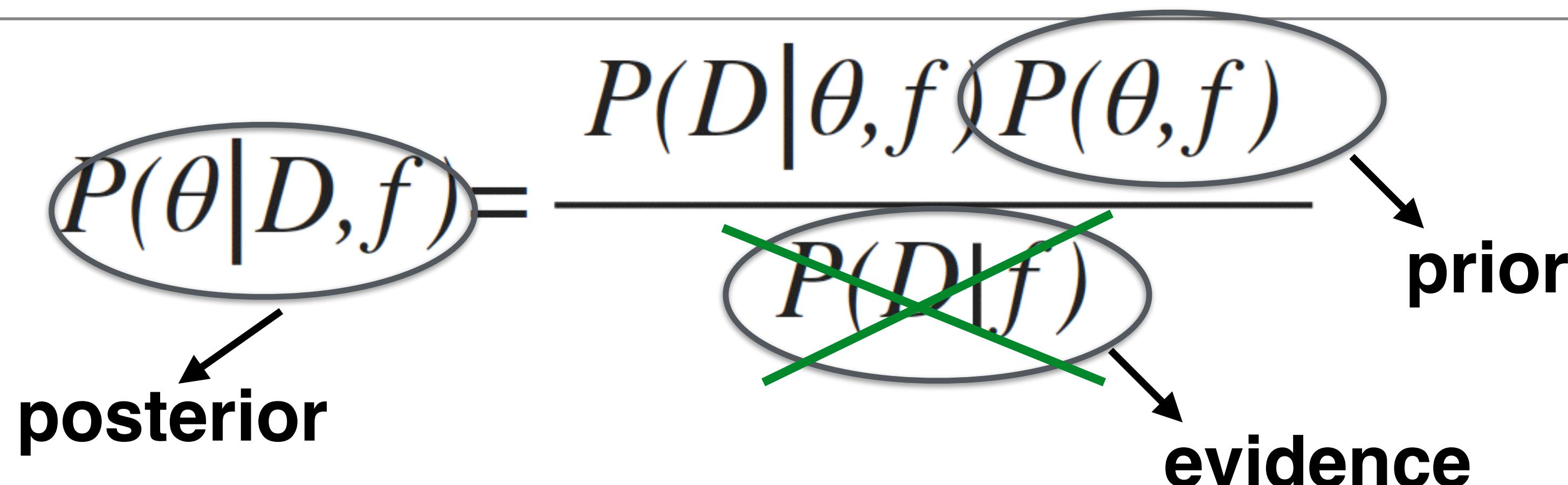
Bayes theorem:

$$P(\theta|D,f) = \frac{P(D|\theta,f)P(\theta,f)}{\cancel{P(D|f)}}$$

posterior

prior

evidence



Definitions:

posterior: joint probability distribution of a parameter set (m, b) condition upon some data D and a model hypothesis f

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its constant in θ so we can ignore it $P(D|f) = \int P(D|\theta,f)P(\theta|f)d\theta$

Bayes theorem:

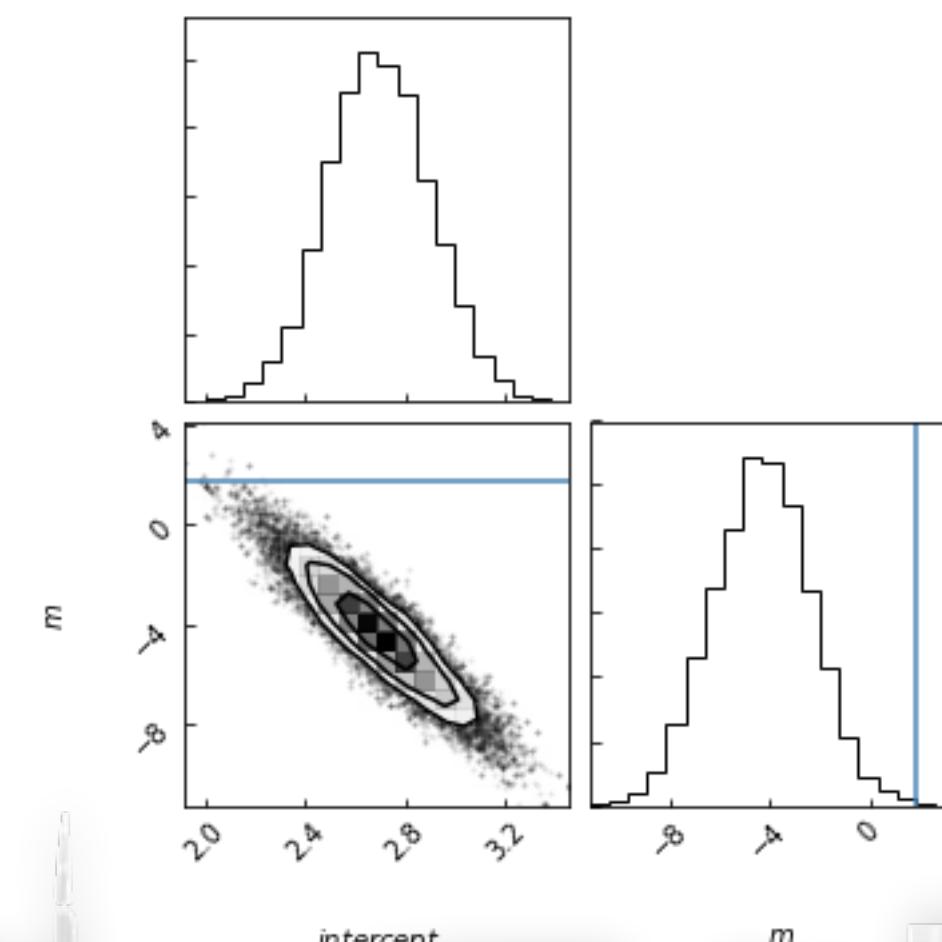
$$P(\theta|D,f) \propto P(D|\theta,f)P(\theta,f)$$

Definitions:

posterior

posterior: joint probability distribution of a parameter set (m, b) condition upon some data D and a model hypothesis f

triangle plot



MCMC - Metropolis Hastings algorithm

Bayes theorem:

$$P(\theta|D,f) \propto P(D|\theta,f)P(\theta,f)$$

Goal: sample the posterior distribution

[A nice tutorial on MCMC](#) by Thomas Wiecki (Quantopian)

While My MCMC Gently Samples

Bayesian modeling, Computational Psychiatry, and Python

choose a starting point **current = $\theta_0 = (m,b)$**

WHILE convergence criterion is met:

calculate current posterior **post_curr = $P(D|\theta,f)$**

*/*proposal*/*
choose a new set of parameters **new = $\theta_{new} = (m,b)$**

calculate the new posterior **post_new = $P(D|\theta_{new},f)$**

IF **post_new > post_curr:**

current = new

ELSE:

*/*accept with probability $P(D|\theta_{new},f) / P(D|\theta,f)$ */*

r = random uniform number [0,1]

 IF **r < post_new / post_orig:**

current = new

 ELSE:

pass //do nothing

Bayes theorem:

$$P(\theta|D,f) \propto P(D|\theta,f)P(\theta,f)$$

Goal: sample the posterior distribution

Questions:

1. how do I choose the next point?

choose a starting point **current = $\theta_0 = (m,b)$**

WHILE convergence criterion is met:

 calculate current posterior **post_curr = $P(D|\theta,f)$**

*/*proposal*/*

 choose a new set of parameters **new = $\theta_{new} = (m,b)$**

 calculate the new posterior **post_new = $P(D|\theta_{new},f)$**

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MCMC - Metropolis Hastings algorithm

Bayes theorem:

$$P(\theta|D,f) \propto P(D|\theta,f)P(\theta,f)$$

Goal: sample the posterior distribution

Questions:

1. how do I choose the next point?

Any Markovian process

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*/*proposal*/*

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Any *Markovian* process

Any *ergodic* process
(with enough time all locations will be explored)

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CN: detailed balance

detailed balance $\pi(x_1)p(x_2|x_1)=\pi(x_2)p(x_1|x_2)$

Metropolis Rosenbluth Rosenbluth Teller 1953 - Hastings 1970

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DYI_MCMC.ipynb

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Questions:

1. how do I choose the next point?

Gibbs sampling:

Metropolis Hastings proposal distribution with
change *along a single direction at a time =>*
always accept
must know the integral $P(D|f)$ along that direction

detailed balance $\pi(x_1)p(x_2|x_1)=\pi(x_2)p(x_1|x_2)$

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1. how do I choose the next point?

Other options:

- simulated annealing (good for multimodal)
- parallel tempering (good for multimodal)
- differential evolution (good for covariant spaces)

detailed balance $\pi(x_1)p(x_2|x_1)=\pi(x_2)p(x_1|x_2)$

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Questions:

1. how do I choose the next point?

Other options:

affine invariant : [EMCEE package](#)

detailed balance $\pi(x_1)p(x_2|x_1)=\pi(x_2)p(x_1|x_2)$

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MCMC - EMCEE



0:29

federica bianco - Monte Carlo methods

MCMC - convergence

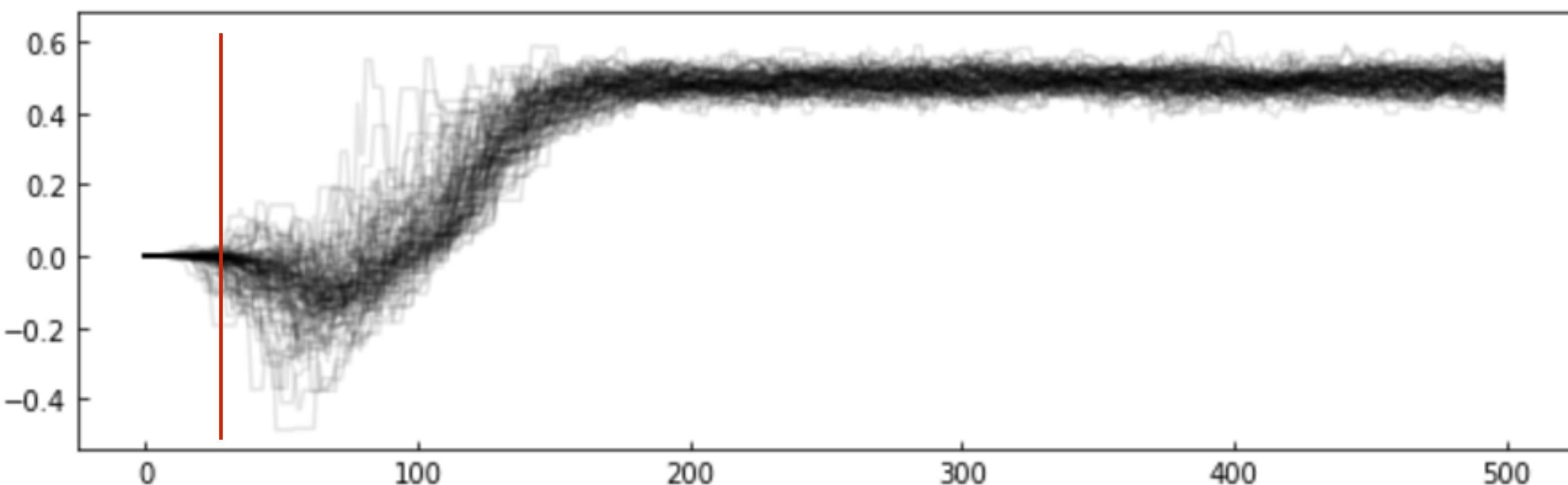
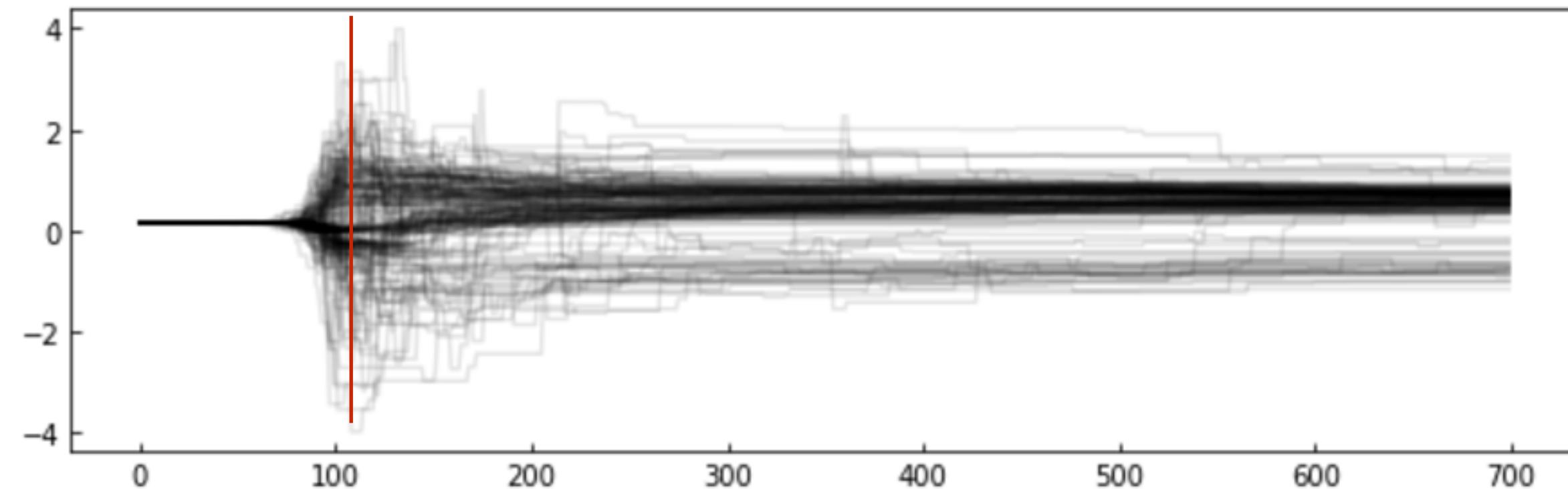
Bayes theorem:

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Goal: sample the posterior distribution

Questions:

1. how do I choose the next point?
2. when have I sampled the posterior adequately?
has your chain *burned-in* ?



Bayes theorem:

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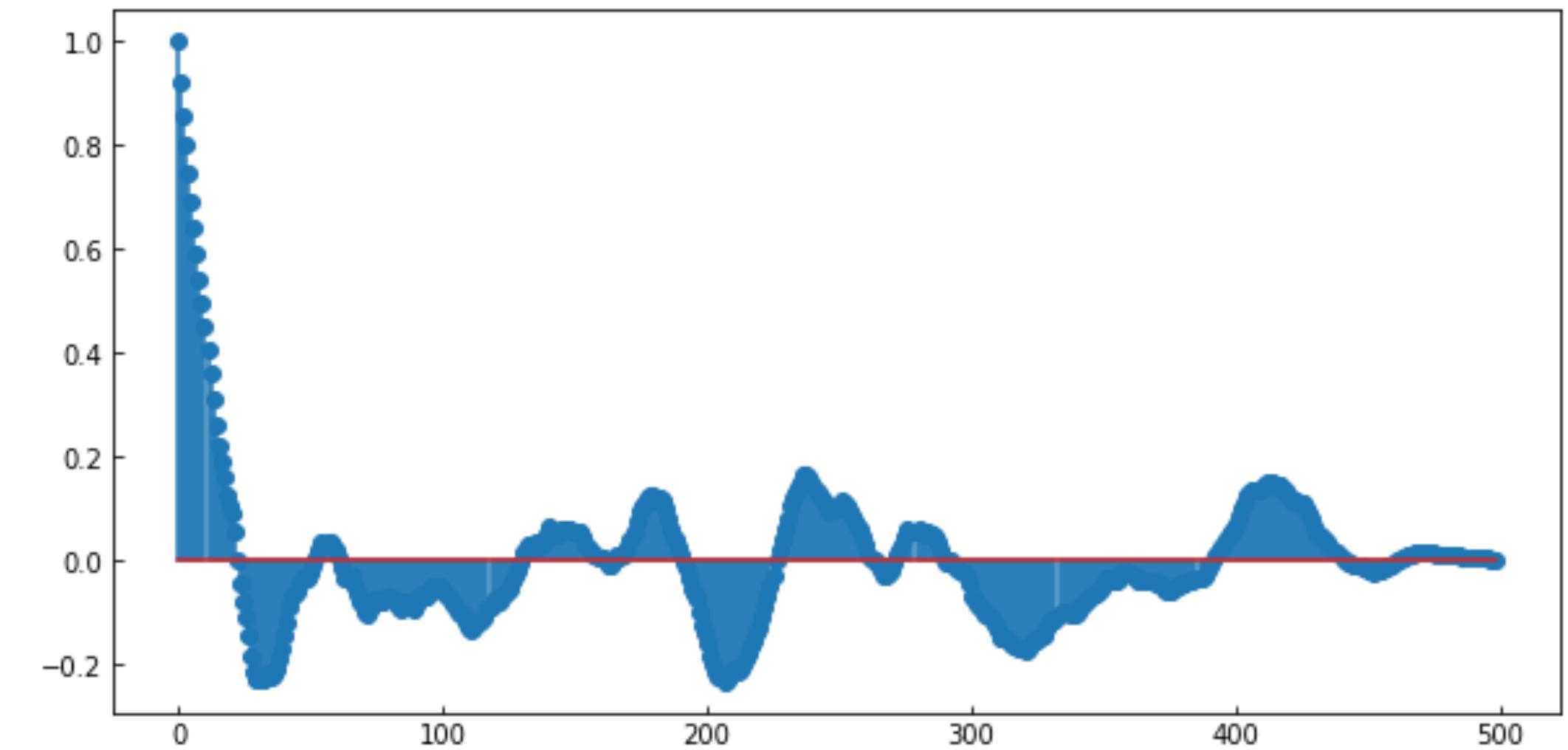
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a. **check autocorrelation within a chain (*Raftery*)**

- b. check that all chains converged to same region (a stationary distribution *GelmanRubin*)
- c. mean at beginning = mean at end (*Geweke*)
- d. check that entire chain reached stationary distribution (or a final fraction of the chain, *Heidelberg-Welch* using Cramer-von-Mises statistic)



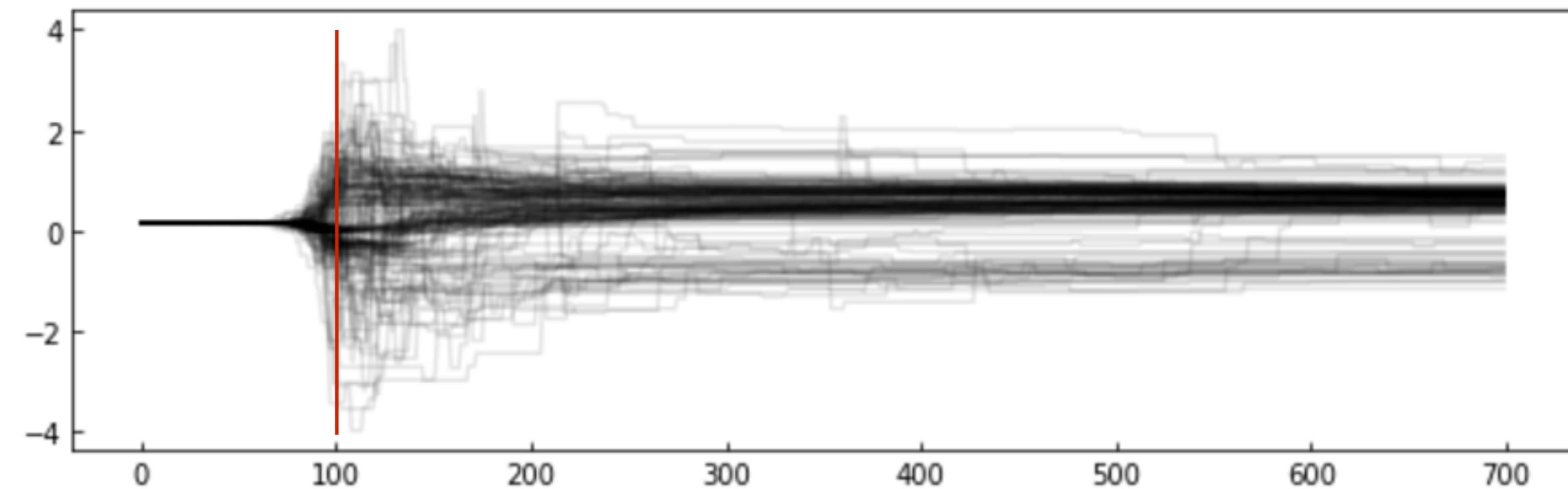
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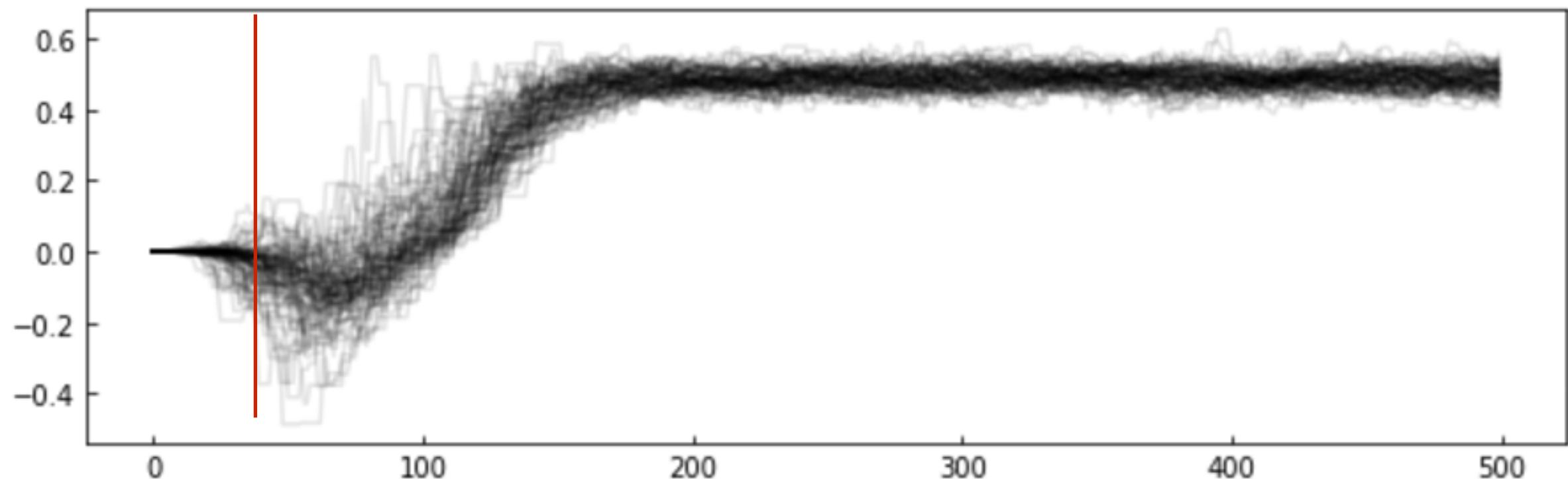
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Questions:

1. how do I choose the next point?
2. when have I sampled the posterior adequately?
3. how can it be-the samples are *not independent!*

good point!...

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Resources Markov Chain Monte Carlo

Information Theory, Inference, and Learning Algorithms

David J.C. MacKay, 2003

Numerical Recipes

Bill Press+ 1992 (+)

Ensemble samplers with affine invariance

Jonathan Goodman and Jonathan Weare 2010

Resources Markov Chain Monte Carlo

Slides on sampling from distributions

Paul E. Johnson 2015

EMCEE readme

provides high level discussion, references, suggestion on parameter choices
D. Foerman-Mackey, D. Hogg, D. Lang, J. Goodman+ 2012

Bill Press (Numerical Recipes) Video

proving how Metropolis-Hastings satisfied Detail Balance

Quick Glossary

- **Stochastic**: random, following any distribution
- **PDF**: probability distribution function $P(x)$ describes the *relative* likelihood of sample x compared
- **CDF**: cumulative distribution function - the probability that a value drawn from a distribution will be smaller than x $F(x) = \int_{-\infty}^x P(x)$
- **Marginalize**: integrate along a dimension
- **Gaussian distribution**: a distribution with PDF $N(\mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{\sigma^2}}$
- **Chi Squared χ^2** : a model fitting method based on the provable fact that (under proper assumption) the function follows a χ^2 distribution $\sum_{i=1}^N \frac{(M-D)^2}{\sigma^2} \sim \chi^2_{DOF}$
- **Likelihood**: in Bayes theorem: the term indicating the probability of the data under the model for a choice of parameters. More generally it can be thought of the probability of the parameters given the data
- **Posterior**: the probability of data given model calculated by Bayes theorem as likelihood * prior / evidence
- **Evidence**: the probability of the data given a model marginalized over all parameters
- **Prior**: prior, or otherwise obtained, knowledge about the problem which indicates how likely the model parameters are for any value
- **Markovian process** - a process whose next stage depends stochastically on the current state only