Title: Numerical Methods Lecture

Speakers: Erik Schnetter

Collection: Numerical Methods 2023/24

Date: January 22, 2024 - 2:00 PM

URL: https://pirsa.org/24010017

Markov Chain Monte Carlo

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PSI Numerical Methods 2024

Borrowing heavily from Dan Foreman-Mackey's slides
https://speakerdeck.com/dfm/data-analysis-with-mcmc

These slides are available at
https://github.com/dstndstn/MCMC-talk

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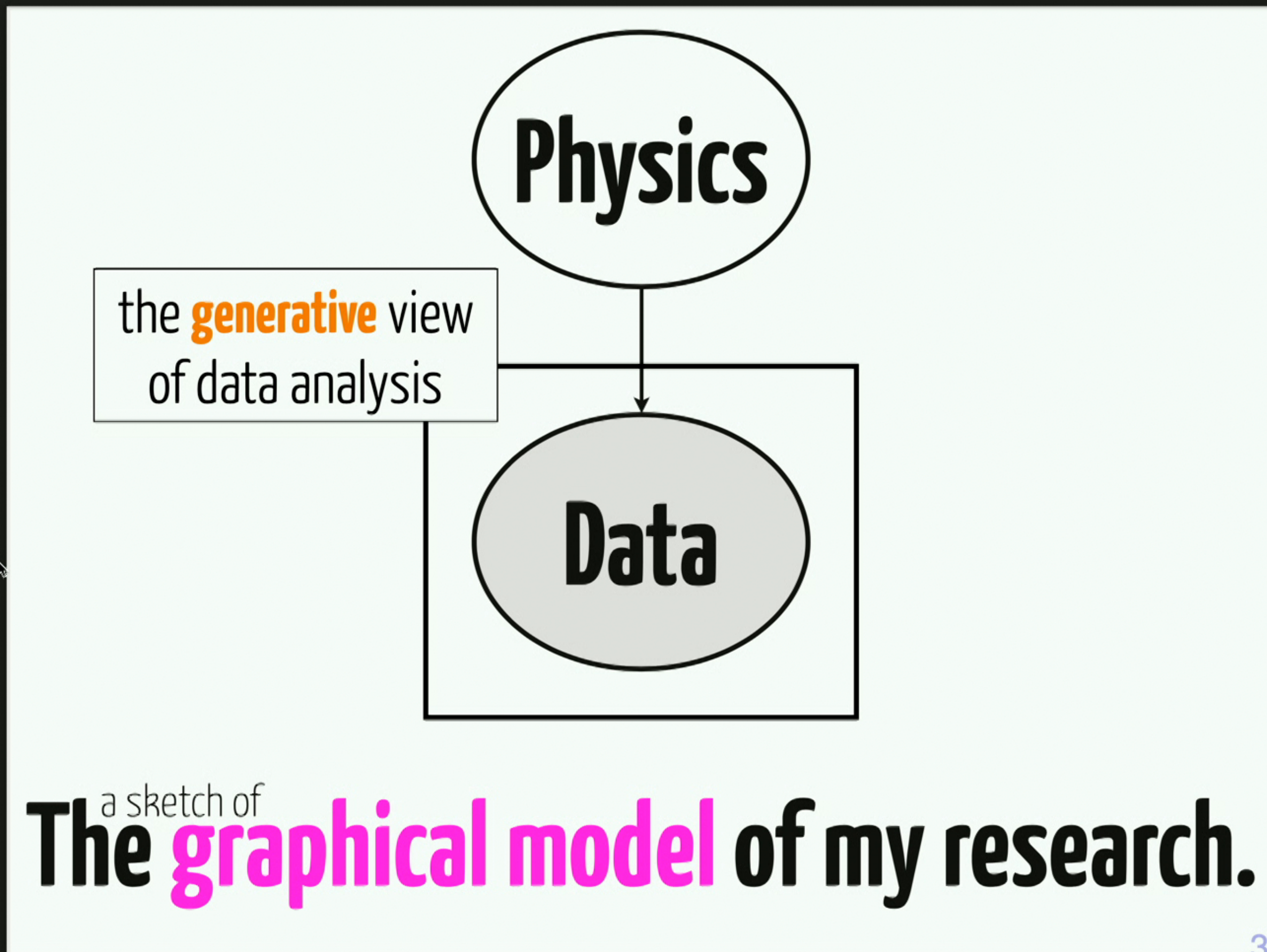
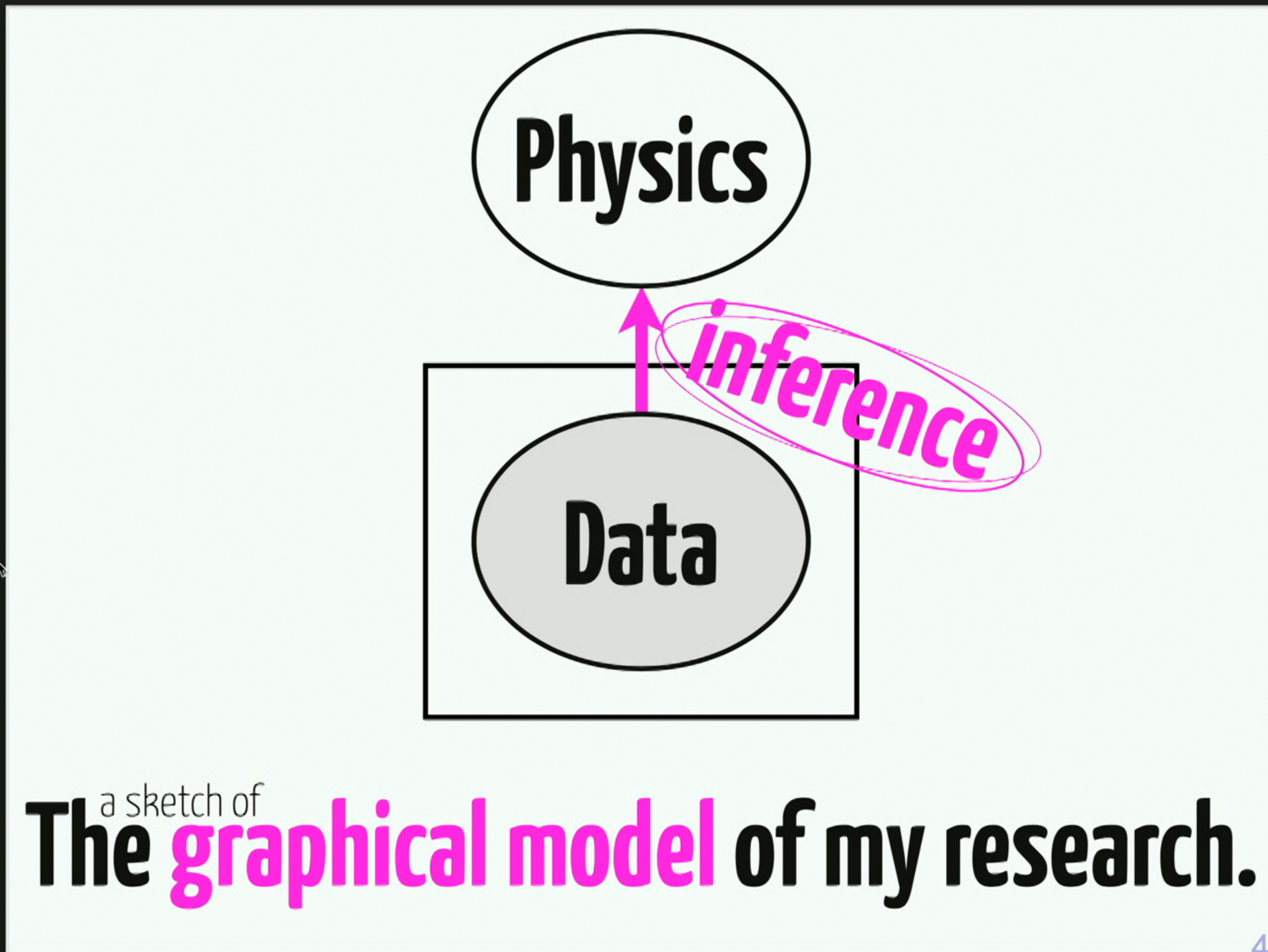
data analysis with

Markov chain Monte Carlo

Dan Foreman-Mackey
CCPP@NYU


Physics
the generative view of data analysis
Data
The a sketch of graphical model of my research.
3


Physics
inference
Data
The a sketch of graphical model of my research.
4

$$p(\text{data} \mid \text{physics})$$

likelihood function/generative model

↓

$$p(\text{physics} \mid \text{data}) \propto p(\text{physics})\, p(\text{data} \mid \text{physics})$$

posterior probability

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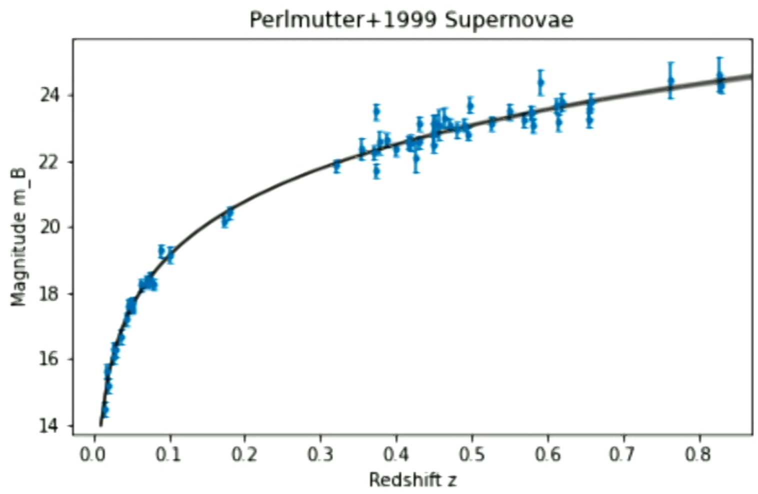
An example

- Use Bayes' theorem to convert data likelihoods into contraints on the model parameters $\theta = \{\Omega_M, \Omega_\Lambda\}$
- $p(\theta \,|\, \mathrm{data}) \propto p(\theta)\, p(\mathrm{data} \,|\, \theta)$
- $p(\Omega_M, \Omega_\Lambda \,|\, \{\mathrm{mag}_i\}) \propto$
  $p(\Omega_M, \Omega_\Lambda) \prod_i \mathcal{N}(\mathrm{mag}_i \,|\, \mathrm{mag}_{\mathrm{int}} + D_L(z_i, \Omega_M, \Omega_\Lambda), \sigma_i^2)$



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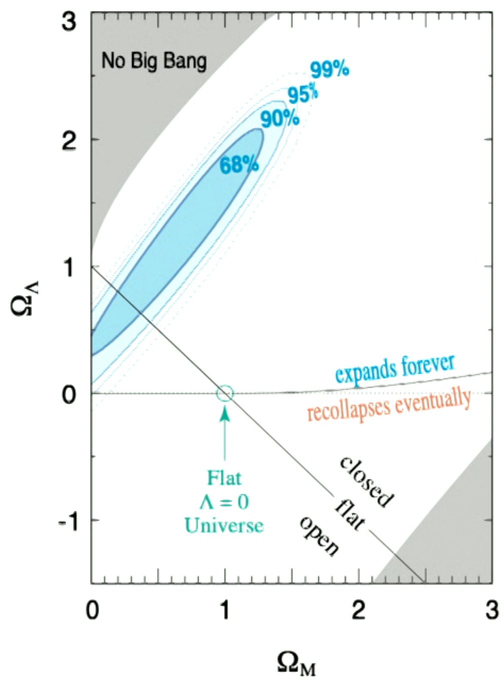
An example

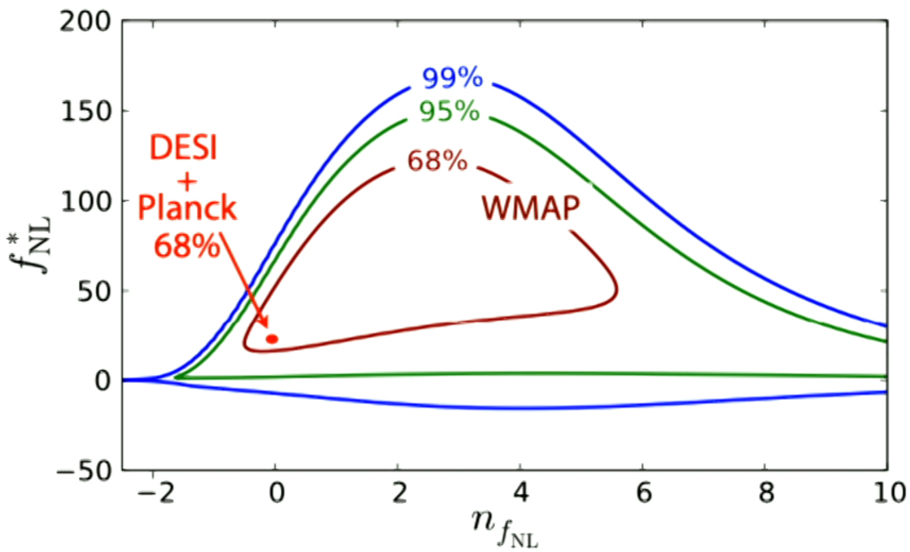
- Then they ran MCMC...
- Resulting parameter constraints (blue ellipse):



Why we often need MCMC

- Real-life models and likelihoods are often complex
- . . . so the resulting constraints have complicated distributions (not Gaussians!)
- . . . but we can represent them with samplings
- MCMC is used for drawing samples from probability distributions that we can compute numerically but cannot solve analytically

Samplings to represent constraints - examples



- From https://arxiv.org/abs/1611.00036

MCMC

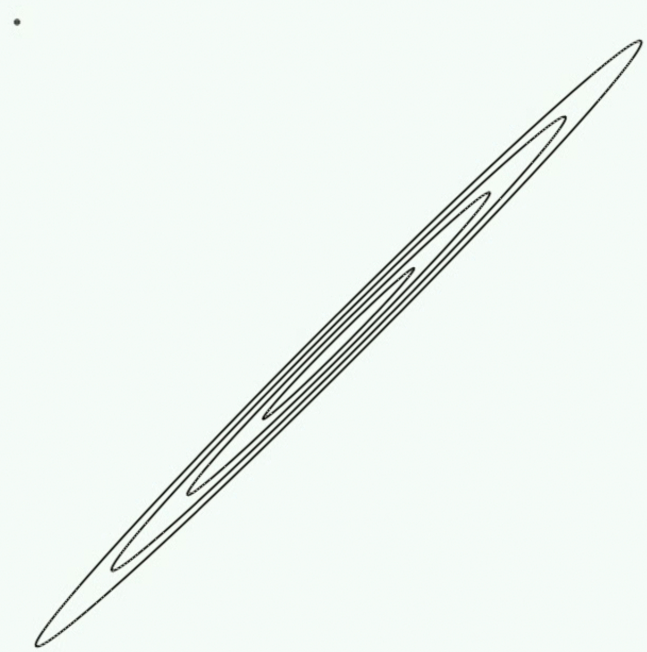
draws samples from a probability function

and all you need to be able to do is

evaluate

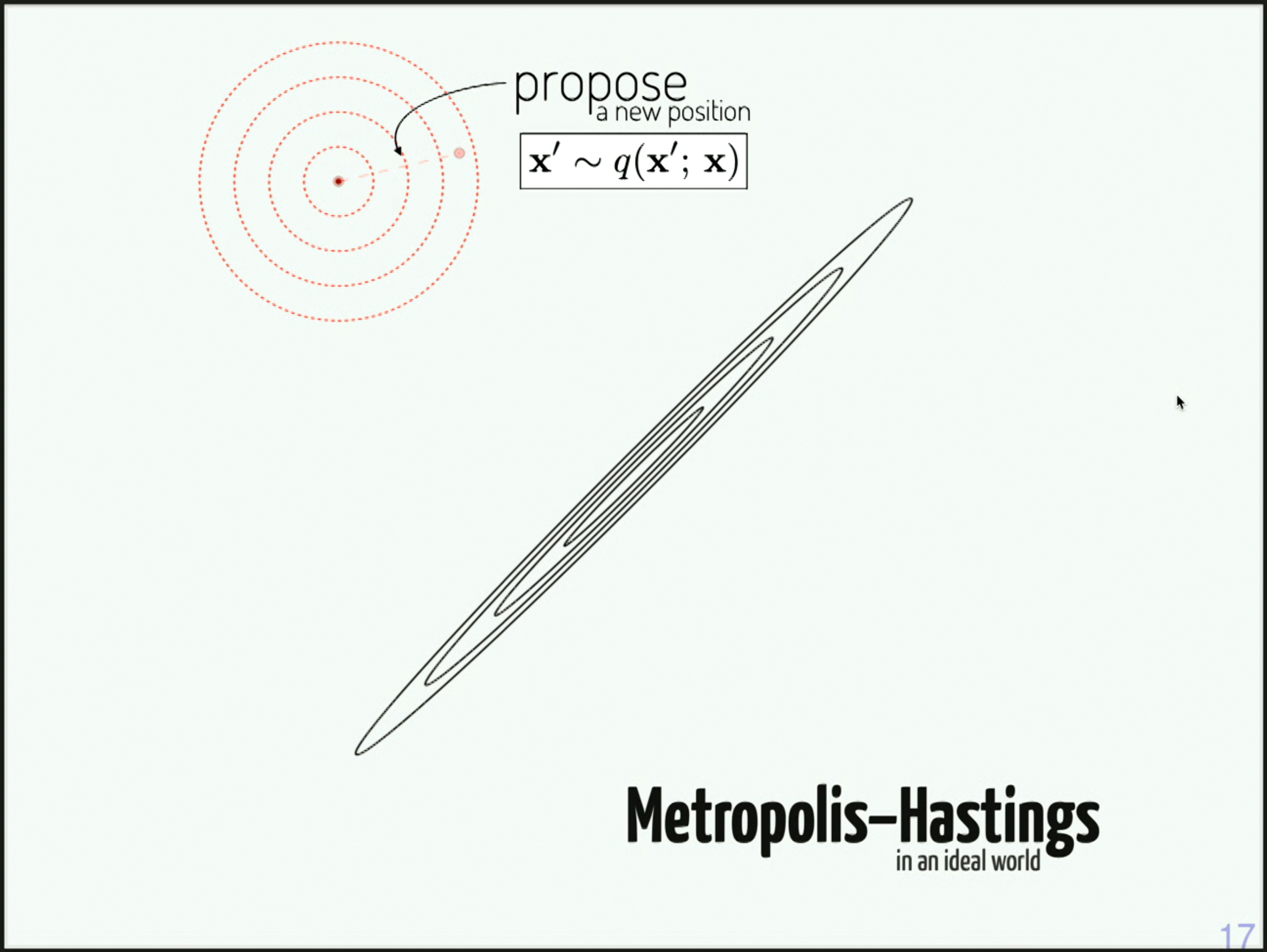
the function

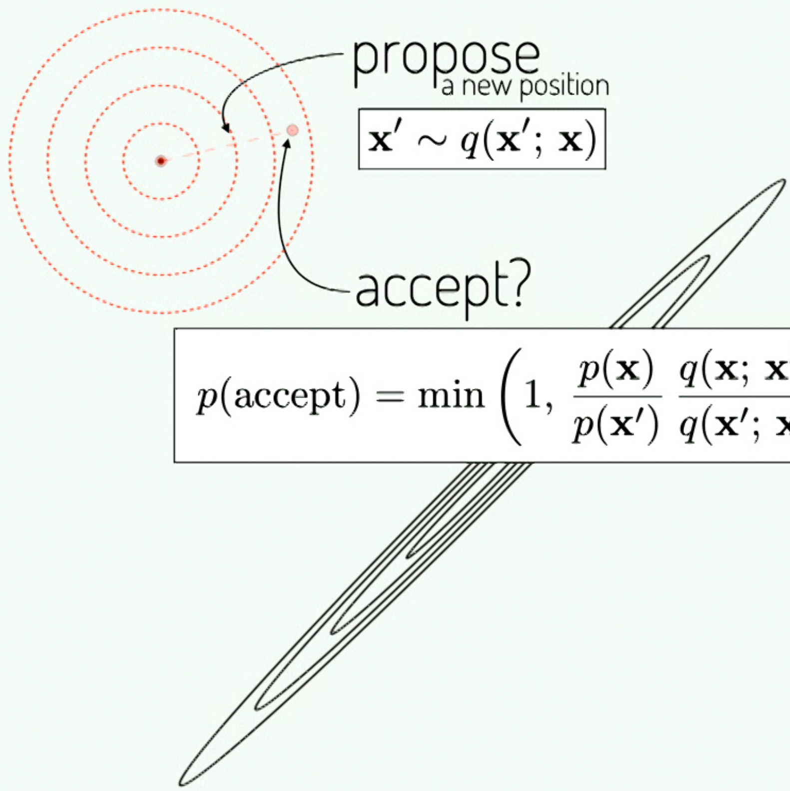
(up to a constant)



Metropolis–Hastings

14

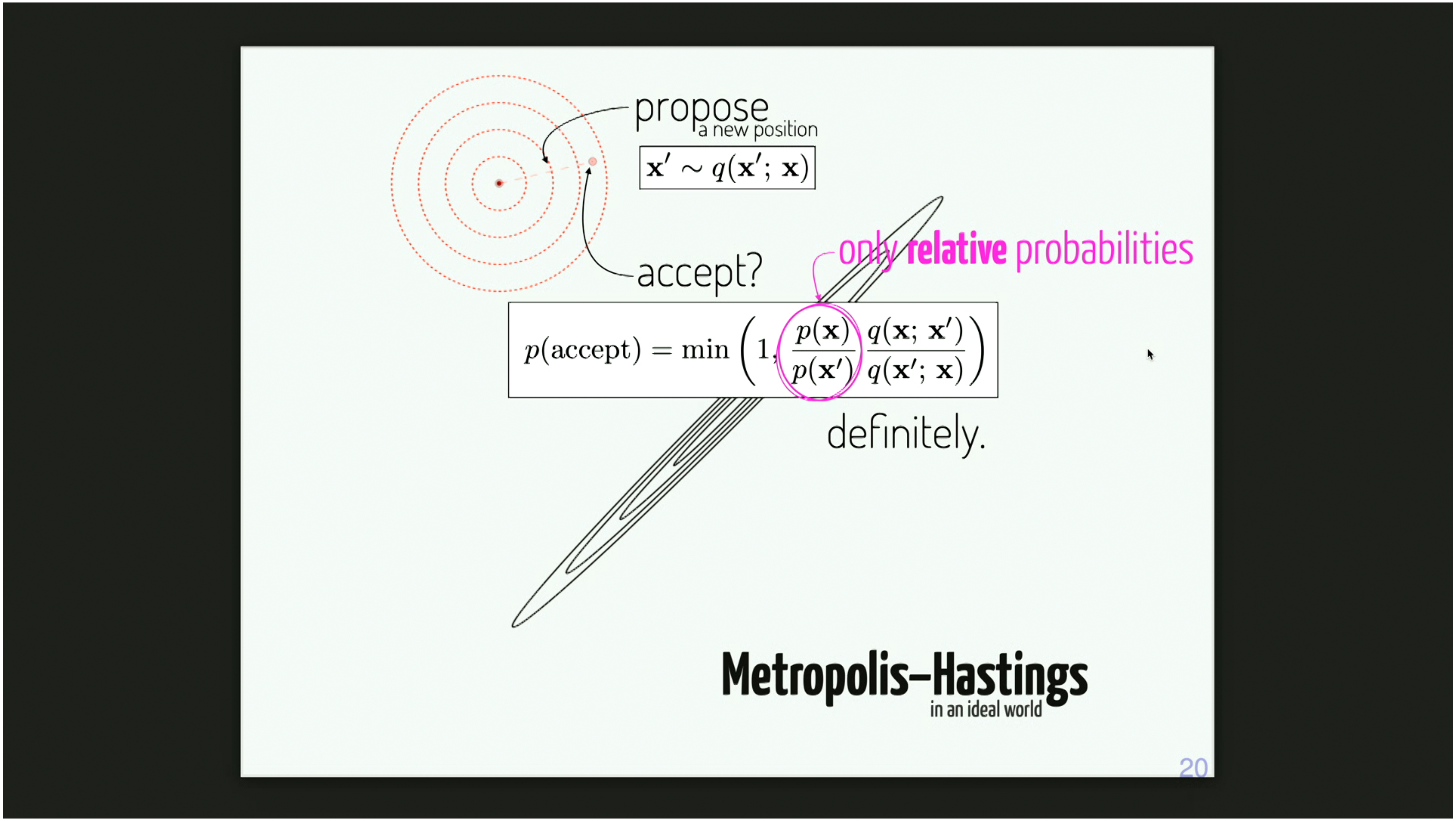

propose
a new position
$\mathbf{x}' \sim q(\mathbf{x}'; \mathbf{x})$
Metropolis–Hastings
in an ideal world
17



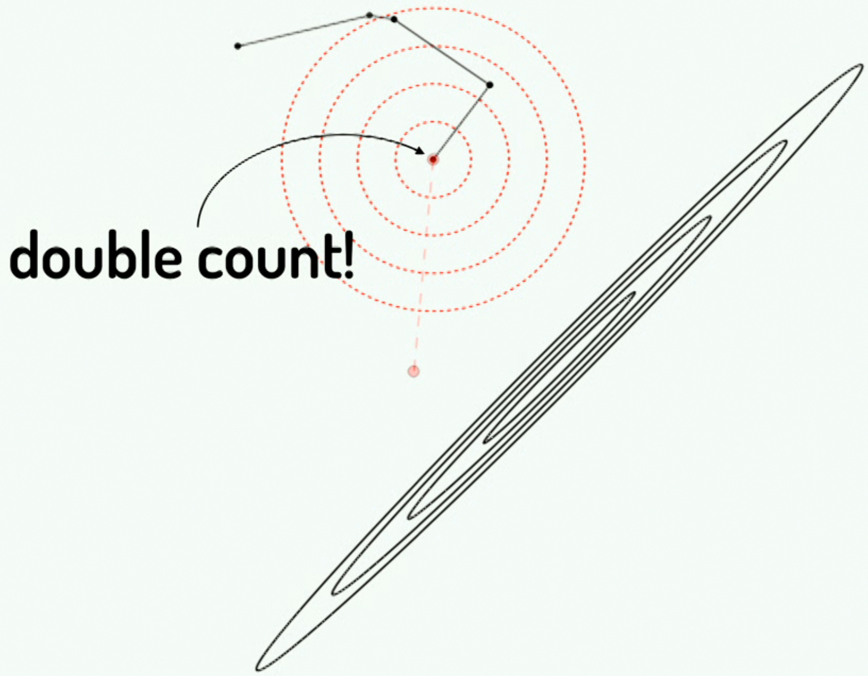
$$\mathbf{x}' \sim q(\mathbf{x}'; \mathbf{x})$$

$$p(\text{accept}) = \min\left(1, \frac{p(\mathbf{x})}{p(\mathbf{x}')} \frac{q(\mathbf{x}; \mathbf{x}')}{q(\mathbf{x}'; \mathbf{x})}\right)$$

Metropolis–Hastings
in an ideal world



propose
a new position
$\mathbf{x}' \sim q(\mathbf{x}'; \mathbf{x})$
accept?
only relative probabilities
$p(\text{accept}) = \min\left(1, \frac{p(\mathbf{x})}{p(\mathbf{x}')} \frac{q(\mathbf{x}; \mathbf{x}')}{q(\mathbf{x}'; \mathbf{x})}\right)$
definitely.
Metropolis–Hastings
in an ideal world
20



Metropolis–Hastings
in an ideal world

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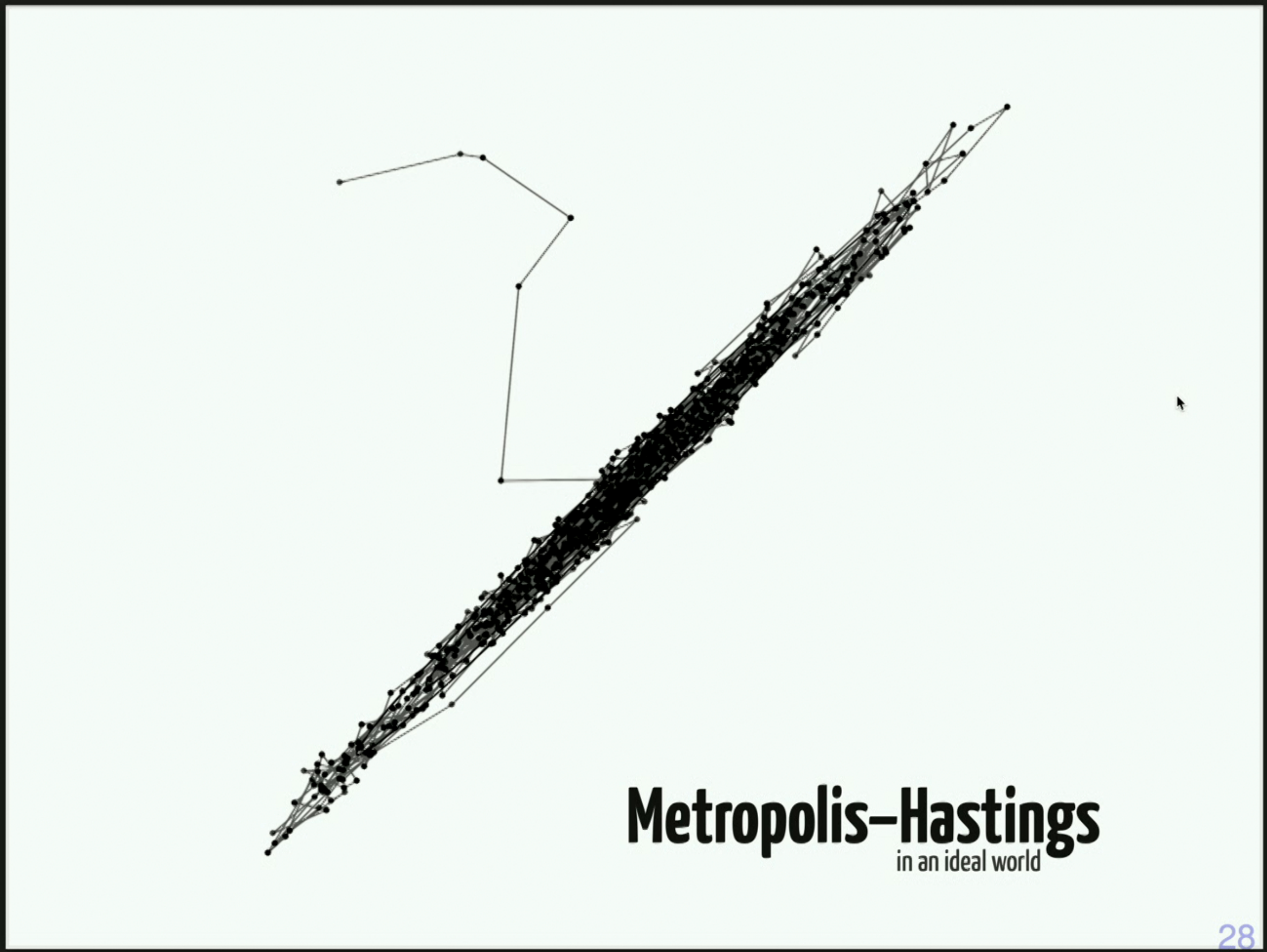

Metropolis–Hastings
in an ideal world
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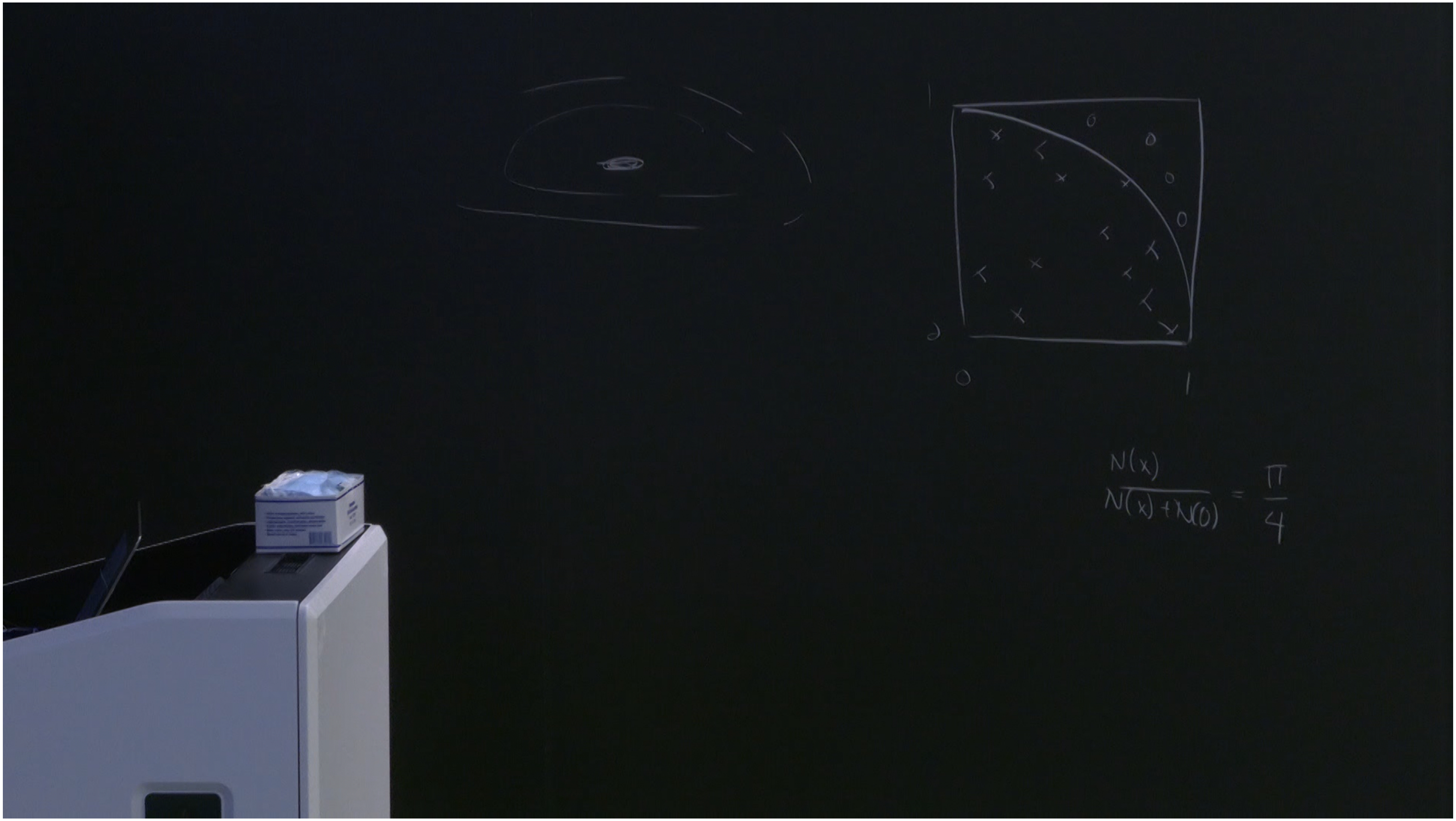
About the name

- Monte Carlo: a reference to the famous Monte Carlo Casino in Monaco, alluding to the randomness used in the algorithm
- Markov Chain: a list of samples, where each one is generated by a process that only looks at the previous one.
- Markov: a 19th-centure Russian mathematician and impressive-moustache-haver with an extensive list of things named after him
- Metropolis–Hastings: lead authors of 1953 and 1970 papers (resp.) giving the algorithm with symmetric and general proposal distributions (resp.)


0
1
N(x) / N(x) + N(0) = π / 4

The Algorithm (1)

```
function mcmc(prob_func, propose_func, initial_pos, nsteps)
    p = initial_pos
    prob = prob_func(p)
    chain = []
    for i in 1:nsteps
        # propose a new position in parameter space
        # ...
        # compute probability at new position
        # ...
        # decide whether to jump to the new position
        if # ...
            # ...
            # ...
        end
        # save the position
        append!(chain, p)
    end
    return chain
end
```

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The Algorithm (2)

```
function mcmc(prob_func, propose_func, initial_pos, nsteps)
    p = initial_pos
    prob = prob_func(p)
    chain = []
    for i in 1:nsteps
        # propose a new position in parameter space
        p_new = propose_func(p)
        # compute probability at new position
        prob_new = prob_func(p_new)
        # decide whether to jump to the new position
        if prob_new / prob > uniform_random()
            p = p_new
            prob = prob_new
        end
        # save the position
        append!(chain, p)
    end
    return chain
end
```

The Algorithm (3)

```
function mcmc(logprob_func, propose_func, initial_pos, nsteps)
    p = initial_pos
    logprob = logprob_func(p)
    chain = []
    for i in 1:nsteps
        # propose a new position in parameter space
        p_new = propose_func(p)
        # compute probability at new position
        logprob_new = logprob_func(p_new)
        # decide whether to jump to the new position
        if exp(logprob_new - logprob) > uniform_random()
            p = p_new
            logprob = logprob_new
        end
        # save the position
        append!(chain, p)
    end
    return chain
end
```

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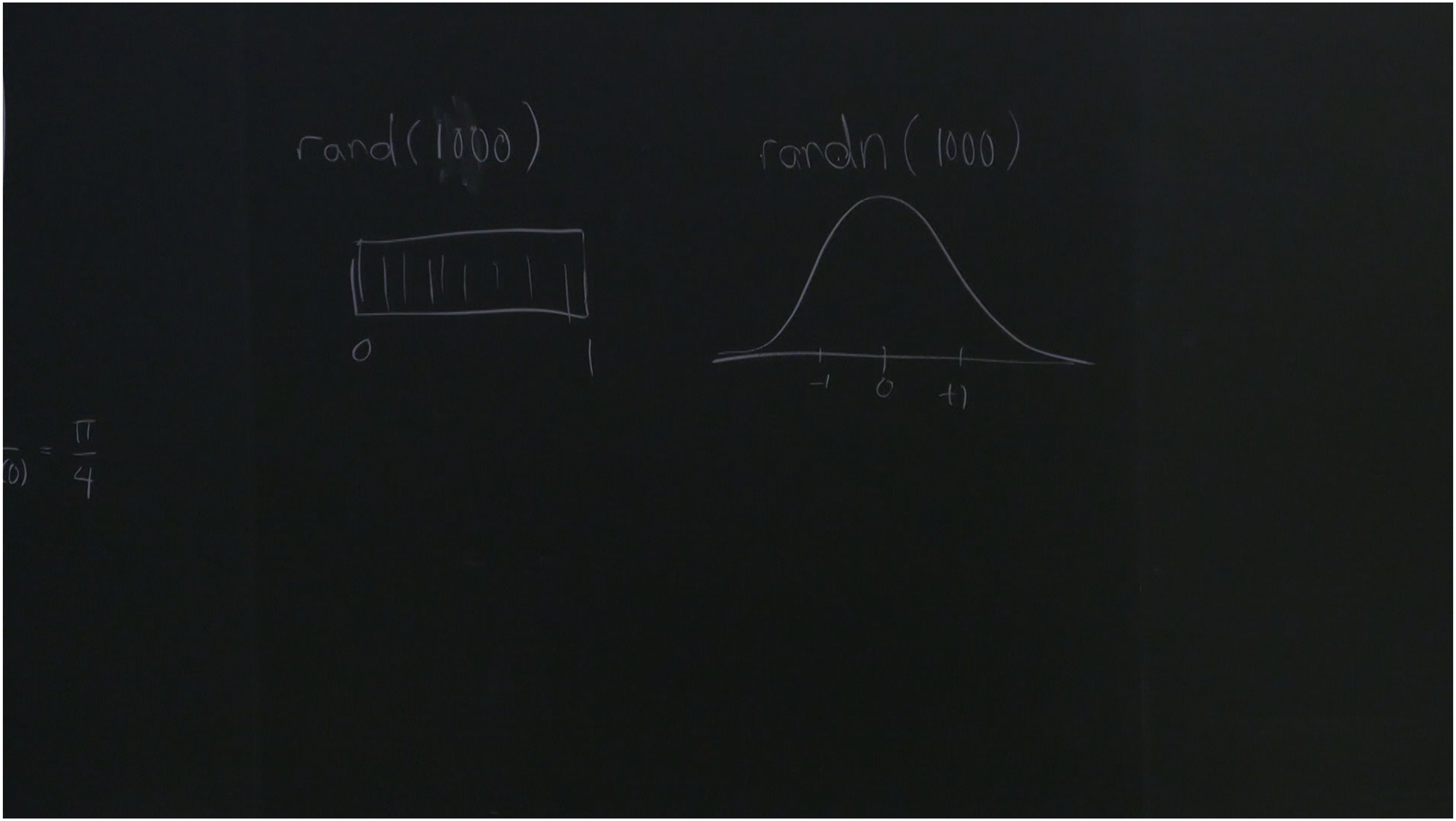
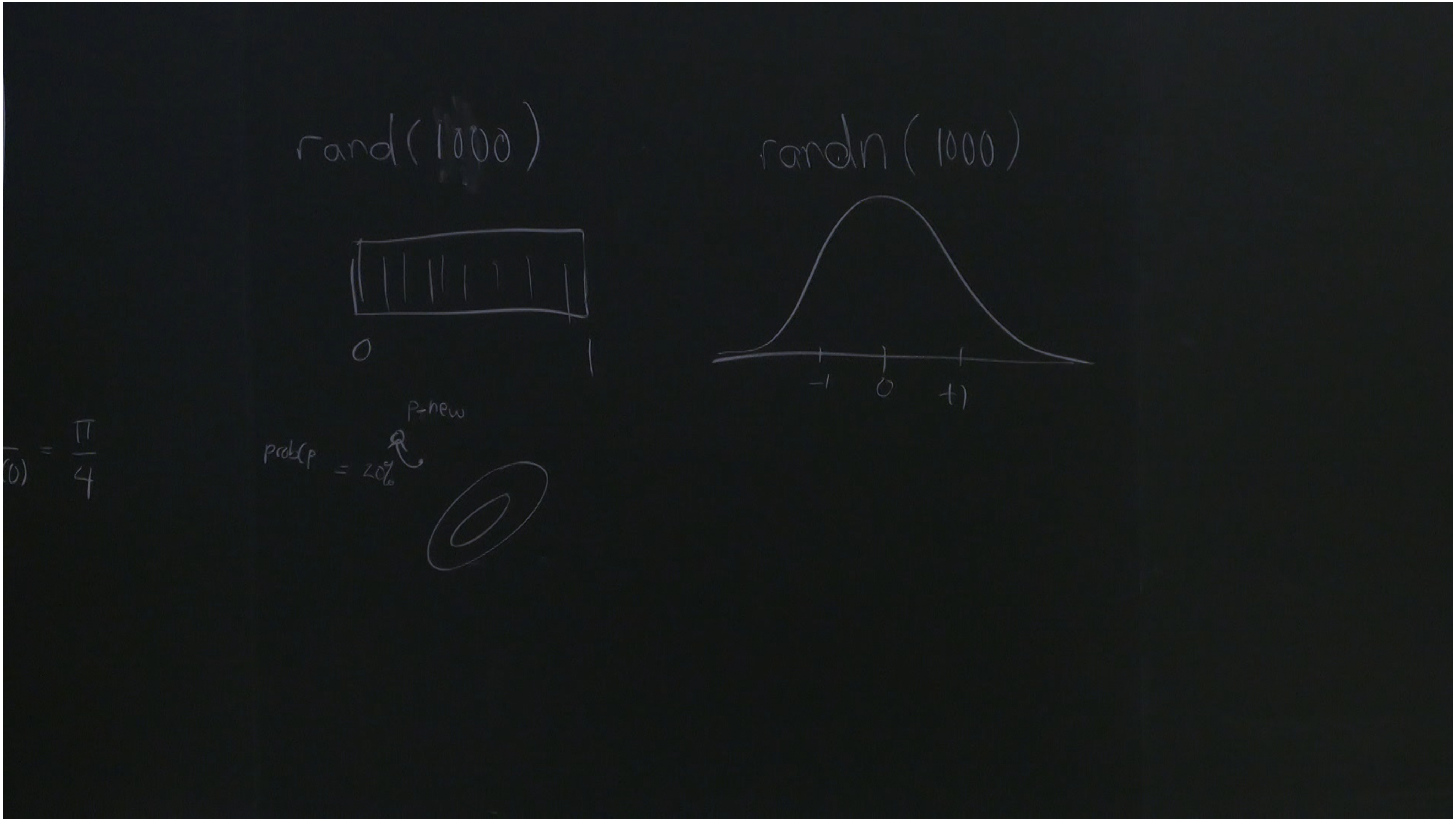
The Algorithm (4)

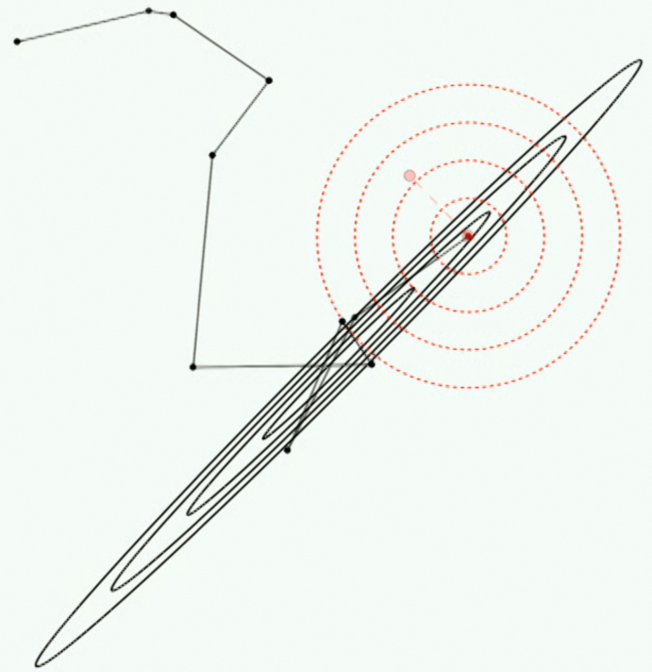
```
function mcmc(logprob_func, propose_func, initial_pos, nsteps)
    p = initial_pos
    logprob = logprob_func(p)
    chain = []
    naccept = 0
    for i in 1:nsteps
        # propose a new position in parameter space
        p_new = propose_func(p)
        # compute probability at new position
        logprob_new = logprob_func(p_new)
        # decide whether to jump to the new position
        if exp(logprob_new - logprob) > uniform_random():
            p = p_new
            logprob = logprob_new
            naccept += 1
        end
        # save the position
        append!(chain, p)
    end
    return chain, naccept/nsteps
```


rand(1000)
0
1
randn(1000)
-1
0
+1
= π/4


rand(1000)
randn(1000)
0
1
-1
0
+1
p-new
= 20%
π
4

Practicalities

- How do I choose a proposal distribution?
- How many steps do I have to take?



Metropolis–Hastings

in the real world

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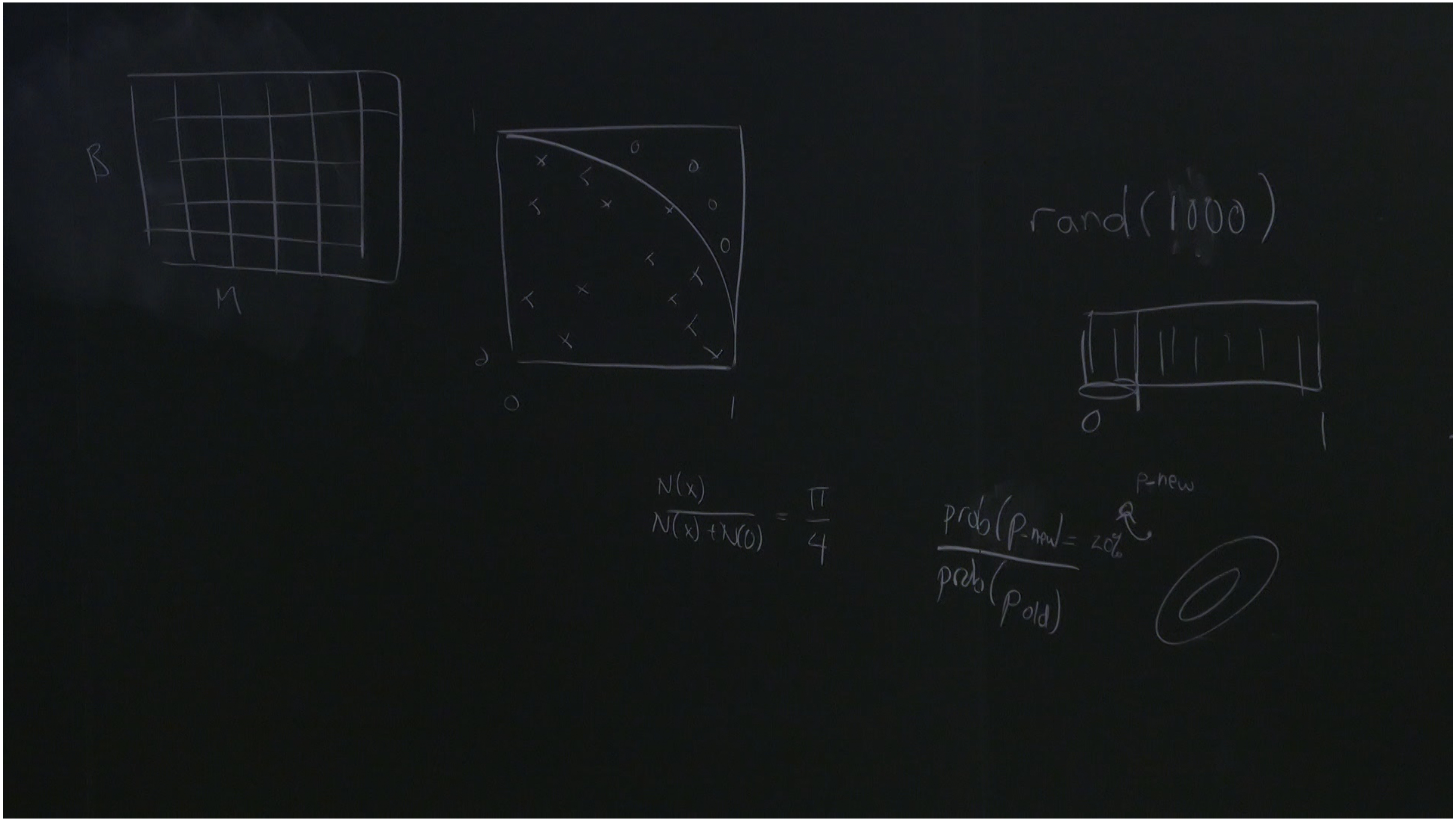
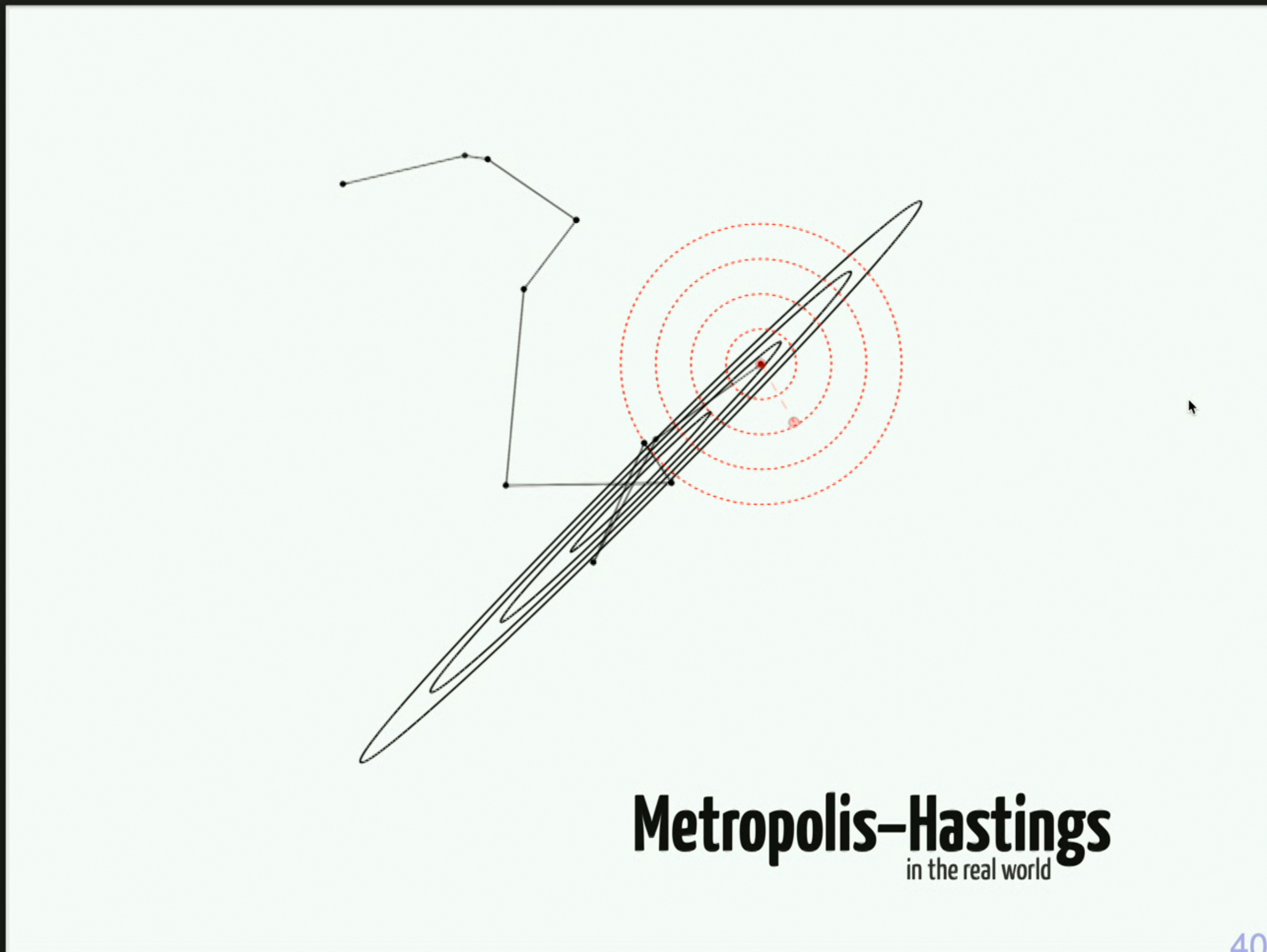
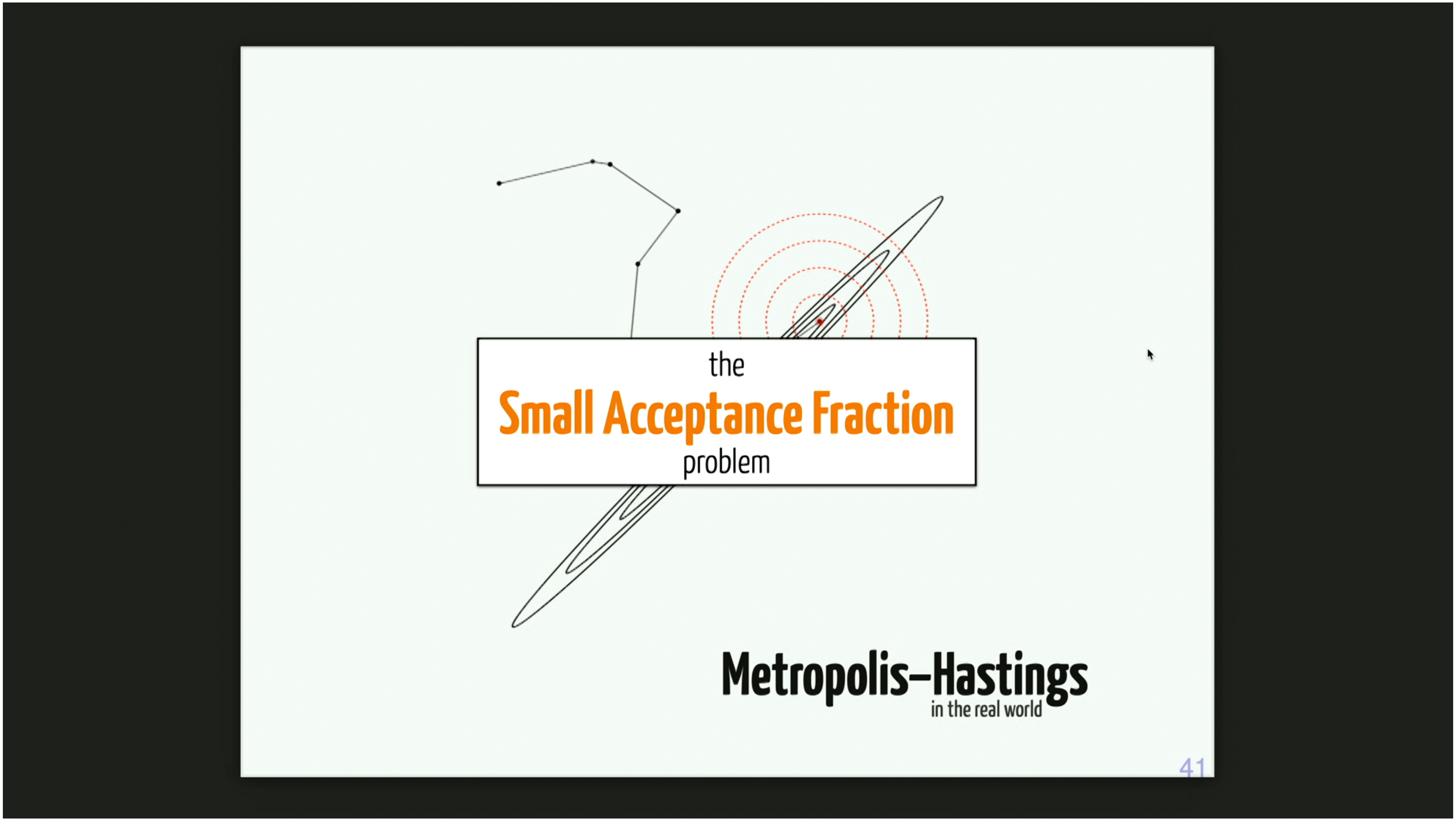

B
M
rand(1000)
N(x)
N(x) + N(0) = π/4
p_new
prob(p_new = 20%
prob(p_old)


Metropolis–Hastings
in the real world
40


the
Small Acceptance Fraction
problem
Metropolis–Hastings
in the real world
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Metropolis–Hastings
in the real world
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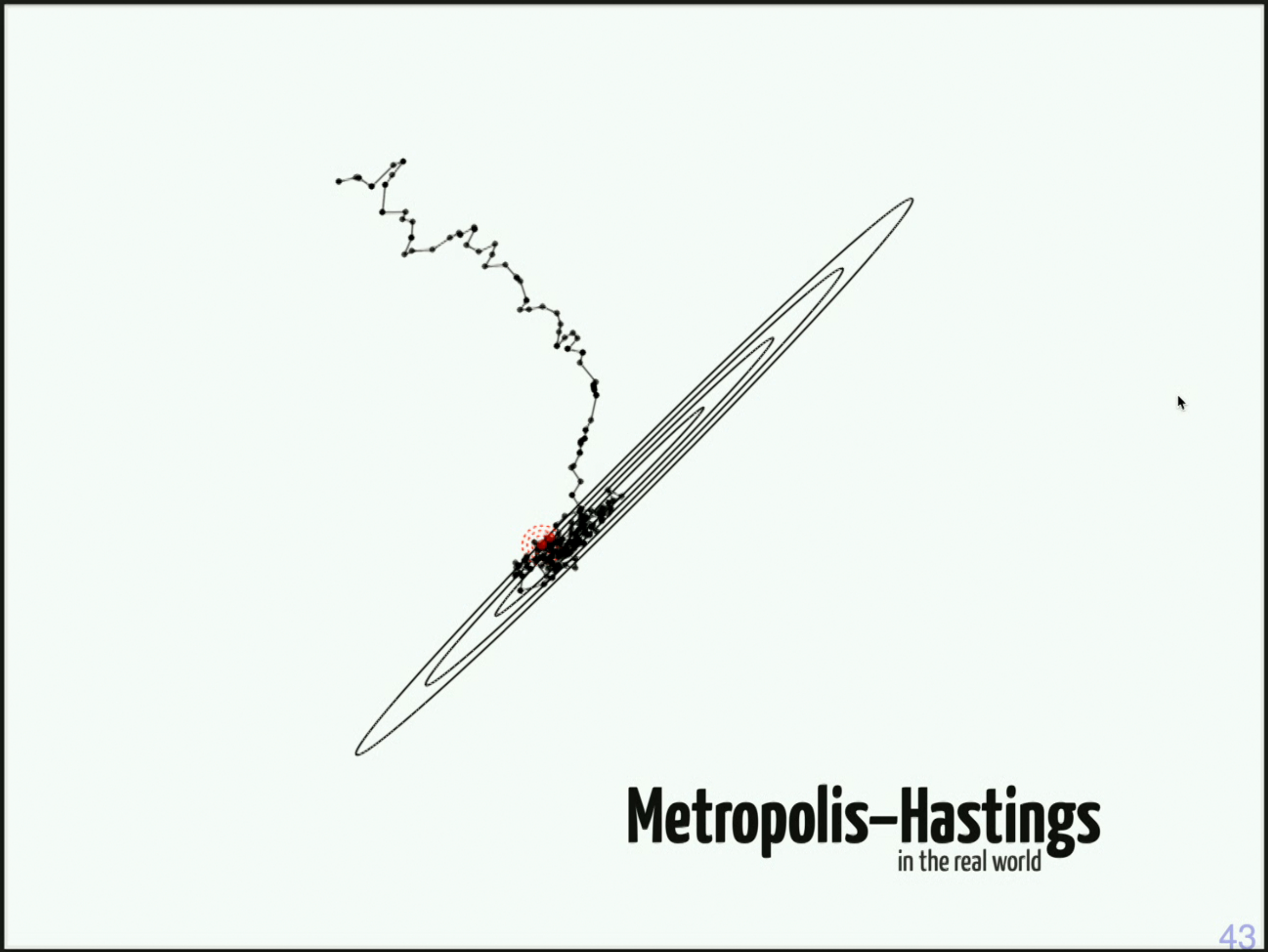
Metropolis–Hastings
in the real world
43


the
Huge Acceptance Fraction
problem
Metropolis–Hastings
in the real world
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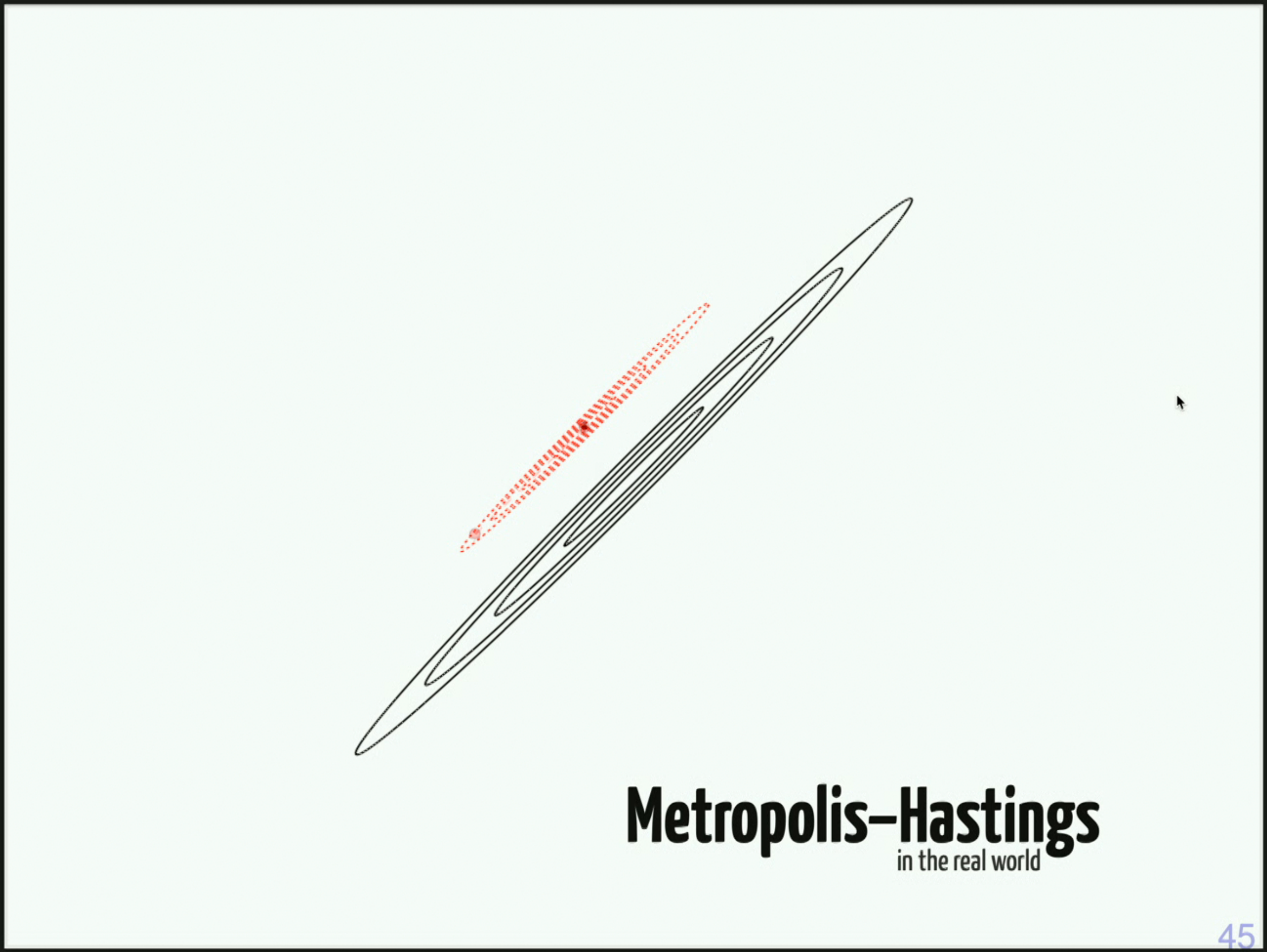
Metropolis–Hastings
in the real world
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that's D(D+1)/2 tuning parameters
Metropolis–Hastings
in the real world
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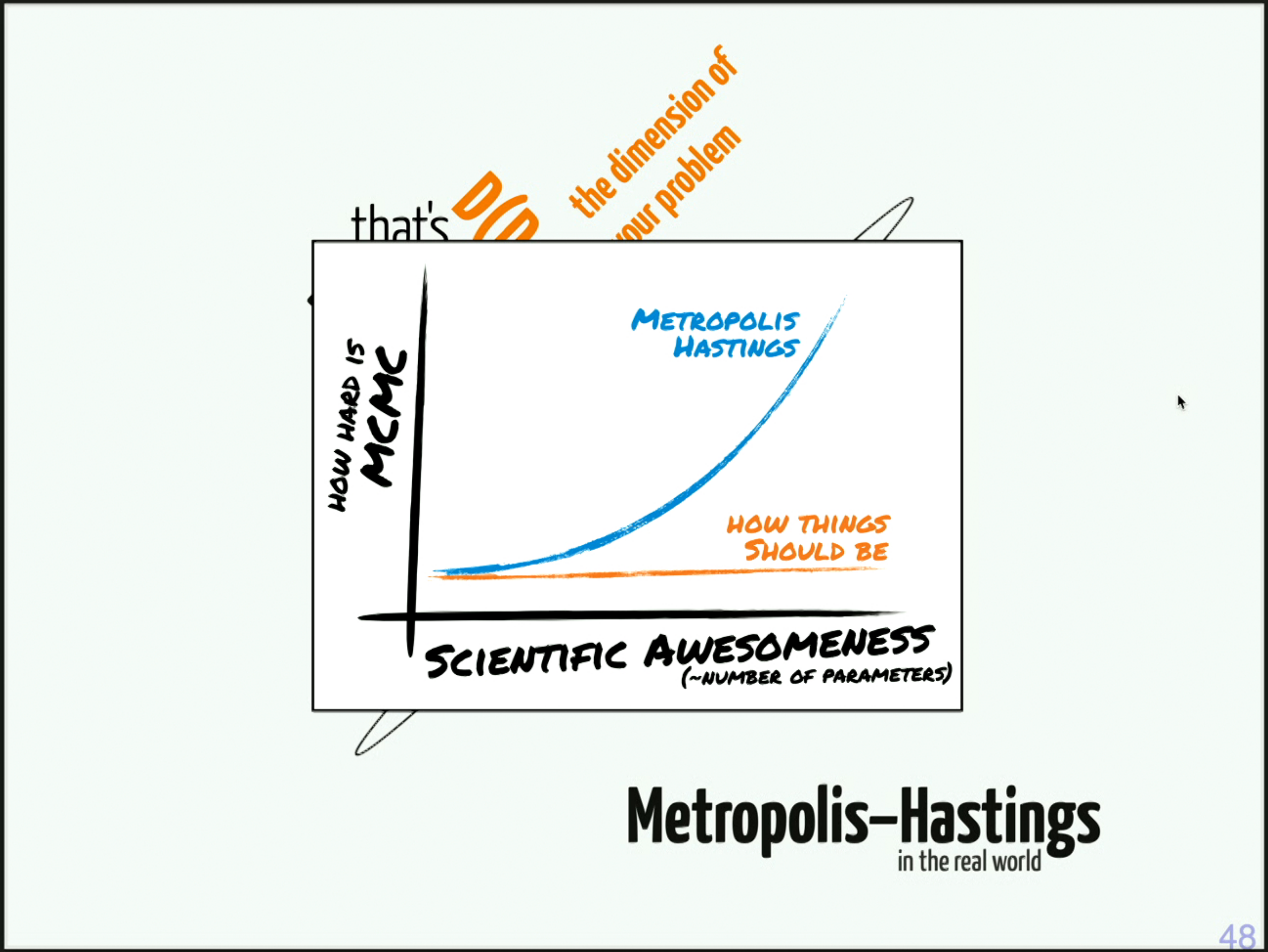

that's
the dimension of
your problem
METROPOLIS HASTINGS
HOW HARD IS MCMC
HOW THINGS SHOULD BE
SCIENTIFIC AWESOMENESS
(~NUMBER OF PARAMETERS)
Metropolis–Hastings
in the real world
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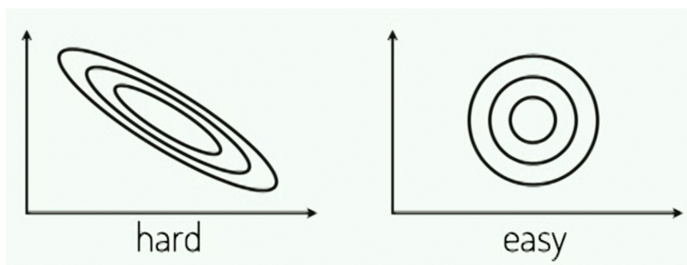
A connection to symmetries

- In Metropolis–Hastings MCMC, the *proposal distribution* needs tuning parameters, especially as dimensionality increases
- Can be seen as a lack of symmetry in the algorithm—the algorithm is sensitive to the parameterization of the problem
- For example, it's not invariant to an affine transformation
- Next lecture, I'll show you an alternative algorithm that does have affine invariance



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How many samples do I need?

- Burn-in — skip the first N samples
- *Has my chain converged?*
- MCMC produces correlated samples, so
  - How correlated are my samples?
    - Can measure the *autocorrelation time* τ
    - Keep $1/\tau$ of the MCMC samples
    - eg *https://github.com/dfm/acor*
  - How many uncorrelated samples do I need?
    - No easy general answer to this question!
    - "How many can you afford?"

Conclusions

- MCMC remains an essential tool for probabilistic inference
- For science: lets us contrain model parameters based on data (Bayesian inference)
- Beguilingly simple algorithm, but difficult practicalities
- MCMC has beautiful theoretical guarantees... as compute time $\to \infty$