CSCI 699 - ProbGen

Probabilistic and Generative Models

Willie Neiswanger

Lecture 4 - Approximate Inference

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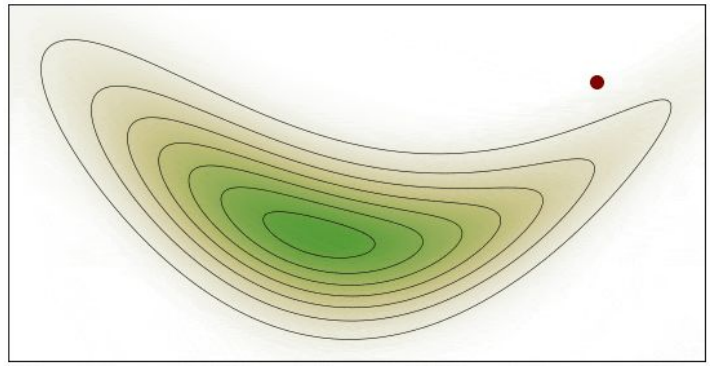
  - Gradient-based methods: Langevin Monte Carlo, Hamiltonian Monte Carlo.



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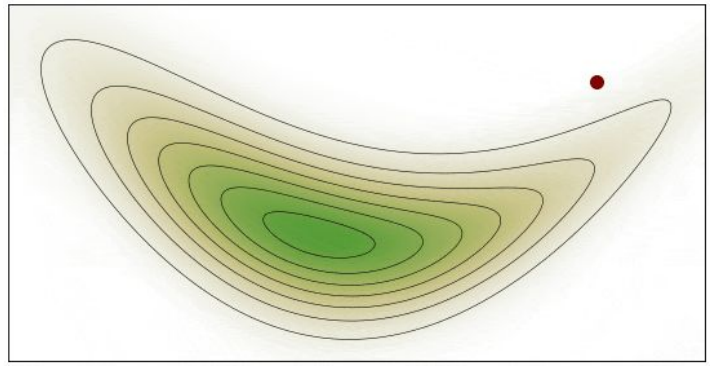

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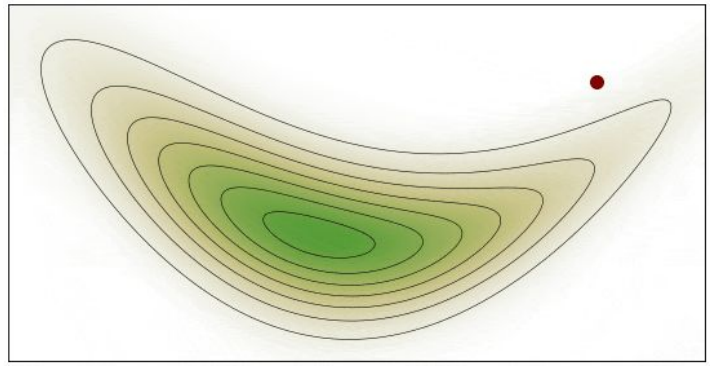

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After:

- Project Pitches #1: Groups 1-5

Review: Exact Inference in PGMs

Review — Last Class on Exact Inference

Lecture: Classic algorithms in probabilistic graphical models (PGMs) for exact and approximate inference & learning.

- Exact inference algorithms in PGMs.
- Variable Elimination algorithm.
- Belief Propagation algorithm (sum/max-product message passing).
- Famous algorithms: Forward-Backward & Viterbi.
- Expectation-Maximization (EM) algorithm.

Source: USC Viterbi Magazine, "The Viterbi Algorithm at 50"

Review — Last Class on Exact Inference

Variable elimination algorithm → for PGMs with discrete random variables.

Review — Last Class on Exact Inference

Variable elimination algorithm:

For each variable x_i,

(1) Form a product of all factors ϕ_i containing x_i.

(2) Marginalize out x_i to obtain a new factor τ.

(3) Replace the factors ϕ_i with τ.

A function of all other variables in factor.

⇒ Computationally efficient way of computing a marginal inference query.

Review — Last Class on Exact Inference

Variable elimination algorithm:

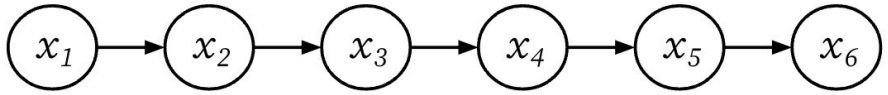
Showed examples on:

Markov chains

Variable Elimination — An Illustrative Example

Consider first the problem of marginal inference.

Suppose we are given this Markov chain PGM.



Joint PDF can be written:

Markovian property

$$p(x_1, \ldots, x_n) = p(x_1) \prod_{i=2}^{n} p(x_i \mid x_{i-1})$$

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Review — Last Class on Exact Inference

Variable elimination algorithm:

Showed examples on:

Student-grade-letter PGM

⇒ Eliminated: *d*, *i*, *s*, *g*
(to get marginal $p(l)$) .

Variable Elimination — General Form

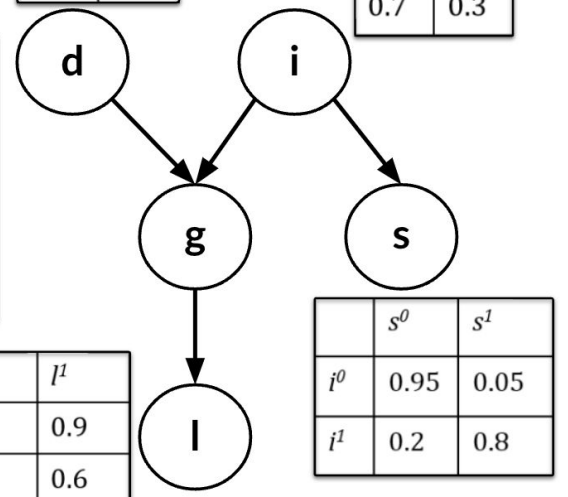
Recall the ***Student PGM*** from last class:

	g^1	g^2	g^3
i^0,d^0	0.3	0.4	0.3
i^0,d^1	0.05	0.25	0.7
i^1,d^0	0.9	0.08	0.02
i^1,d^1	0.5	0.3	0.2

d - Class difficulty.
i - Student's intelligence.
g - Student's grade in the class.
s - Student's SAT test score.
l - Professor's letter of recommendation.
(good vs bad letter)

d^0	d^1
0.6	0.4

i^0	i^1
0.7	0.3



	l^0	l^1
g^1	0.1	0.9
g^2	0.4	0.6
g^3	0.99	0.01

	s^0	s^1
i^0	0.95	0.05
i^1	0.2	0.8

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Review — Last Class on Exact Inference

Variable elimination algorithm:

Showed examples on:

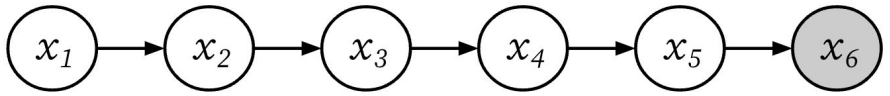
Extensions to conditional distributions (e.g., posterior distributions)

Variable Elimination — Extensions to Conditional Probabilities

We can extend this algorithm to conditional distributions (*e.g.*, posteriors)!

Suppose we have a joint probability $p(x_1, \ldots, x_n)$.

And our **goal** is to compute a given conditional probability, *e.g.*, $p(x_1 \mid x_n = 5)$.



Conditional PDF:

$$p(x_1 \mid x_n = 5) = \frac{p(x_1, x_n = 5)}{p(x_n = 5)}$$

Two marginal probabilities!

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Review — Last Class on Exact Inference

The **belief propagation** algorithm.

⇒ If you want to be able to answer *any* inference query.

(And not have to repeat belief propagation for each query).

Caveat: this is for *tree graph PGMs* … for general PGMs, need to use the Junction Tree algorithm, which we didn't cover in class.

Review — Last Class on Exact Inference

Definition. The **belief propagation** algorithm on tree graphs has two variants: *sum-product message passing*, and *max-product message passing*.

Sum-product message passing algorithm:

Used for marginal/conditional inference, *i.e.*, computing $p(x_i)$ or $p(x_i \mid x_k)$.

Max-product message passing algorithm:

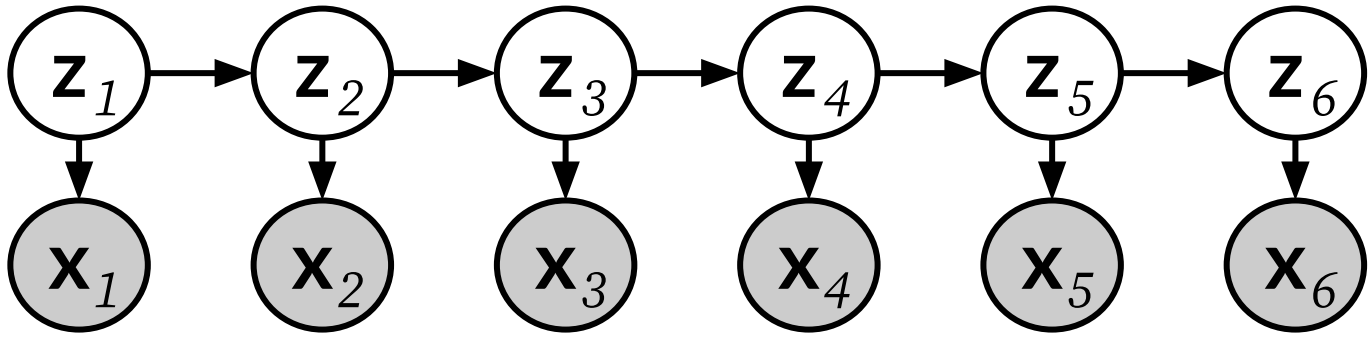
Used for MAP (*maximum a posteriori*) inference, *i.e.*, computing:

$$\max_{x_1,\ldots,x_n} p(x_1, \ldots, x_n) \quad \text{or} \quad \max_{x_i} p(x_i \mid x_k) \quad \text{or} \quad \arg\max_{x_i} p(x_i \mid x_k)$$

Review — Last Class on Exact Inference

Famous Example of Sum-Product Algorithm:

Forward-Backward Algorithm in HMMs!



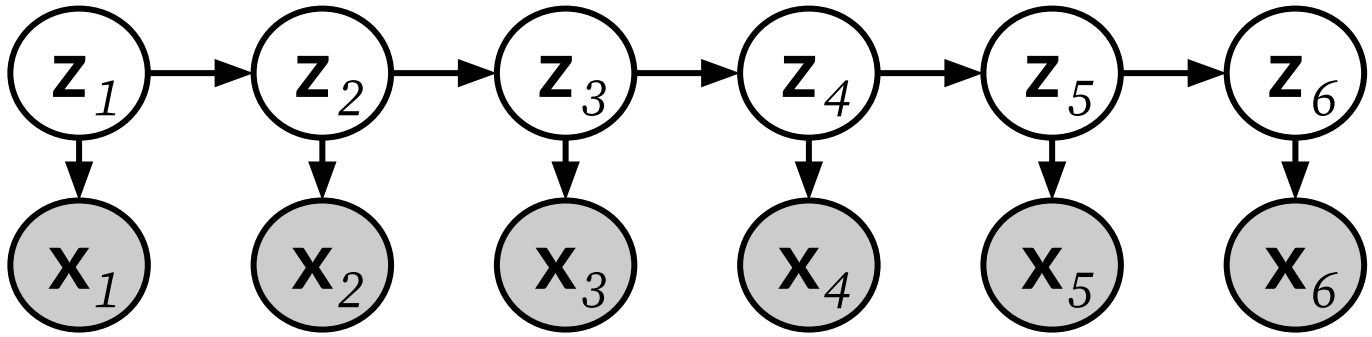
Suppose we want to query $p(z_i \mid x_1, \ldots, x_n)$ for all $z_i \in \{z_1, \ldots, z_n\}$.

Often called “smoothing”.

Review — Last Class on Exact Inference

Famous Example of Max-Product Algorithm:

Viterbi Algorithm in HMMs!



Suppose we want to query: $\max_{z_1,\ldots,z_n} p(z_1,\ldots,z_n \mid x_1,\ldots,x_n)$

MAP estimate of latent z's

Often called "Viterbi Path".

(Joint maximum over all)

Review — Last Class on Exact Inference

Then: Learning (parameter estimation) in PGMs.

Review — Last Class on Exact Inference

Then: Learning (parameter estimation) in PGMs.

Expectation maximization (EM) algorithm is a famous algorithm, which can be remembered as

Maximum likelihood estimation in models with latent variables.

Note: this is a key parameter estimation algorithm for PGMs — more general than inference/MAP in discrete-variable PGMs with tree structure.

(*E.g.*, which we assumed for belief propagation algorithms)

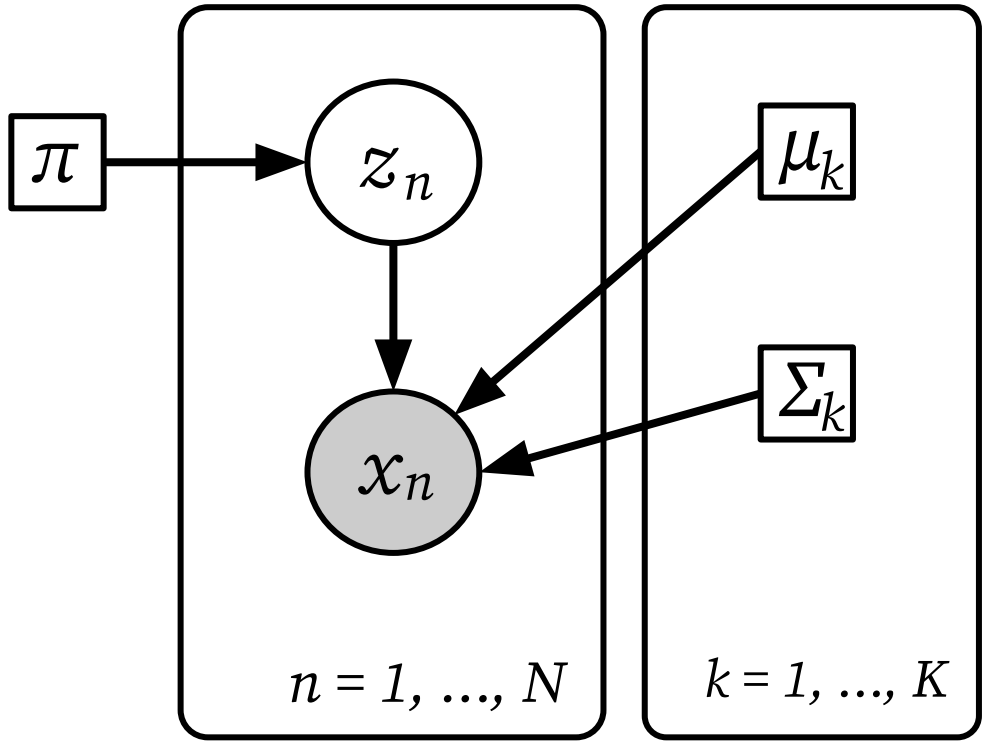
Review — Last Class on Exact Inference

Suppose we want to estimate the parameters: π, μ_k, Σ_k

Gaussian mixture model (GMM)

Chicken and egg problem!

- If we knew the parameters, then we could do inference to infer the latents.
- If we knew the latents, then we could run MLE (optimize) to estimate the parameters.



Review — Last Class on Exact Inference

Let's investigate the two steps of EM algorithm:

Step (1): "The E Step" — infer the latent variables: $z \sim p_\theta(z \mid x)$

So that you could compute this expected value:

$$\mathbb{E}_{z \sim p_\theta(z|x)} \left[\log p_\theta(x, z) \right]$$

⇒ The expected value of the (log) likelihood function, w.r.t. the conditional distribution of latents given observed (under current estimates of the parameters).

Review — Last Class on Exact Inference

Let's investigate the two steps of EM algorithm:

Step (2): "The M Step" — Run MLE to estimate the parameters:

$$\theta \leftarrow \arg\max_\theta \mathbb{E}_z \left[\log p_\theta(x, z)\right]$$

Objective: expectation from previous slide (optimizing over θ in the joint PDF)

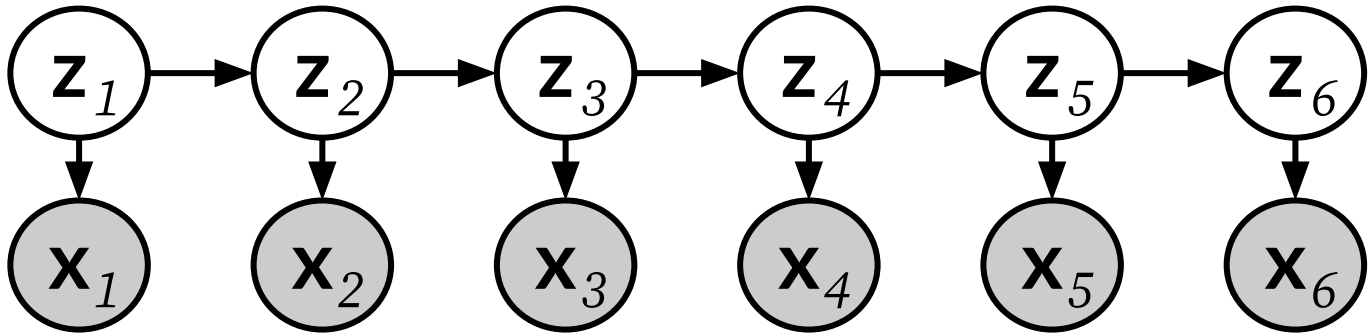
Given our expression for the expected log-likelihood (from the E-step), optimize as usual to get an estimate for the MLE.

Review — Last Class on Exact Inference

Famous Example of EM Algorithm:

Baum–Welch Algorithm in HMMs!

Lloyd Welch is also USC affiliated :-).



Goal: estimate parameters of HMM (*i.e.*, parameters of: initial state distribution, transition distribution, and emission distributions).

Approximate Inference: Overview

Exact vs. Approximate Inference

In practice

- The probabilistic models that we use are often quite complex.
- Simple algorithms like variable elimination may be too slow.
- Many interesting classes of models do not admit tractable inference.
- ⇒ Much research effort is spent on *approximate inference* algorithms.

Main Approximate Inference Algorithms

At a high level: two popular "types" of approximate inference algorithms:

Markov chain Monte Carlo (MCMC)

E.g., Gibbs Sampling

Source: Jessica Stringham, Gibbs Sampling in Python

Variational Inference (VI)

E.g., black-box variational inference

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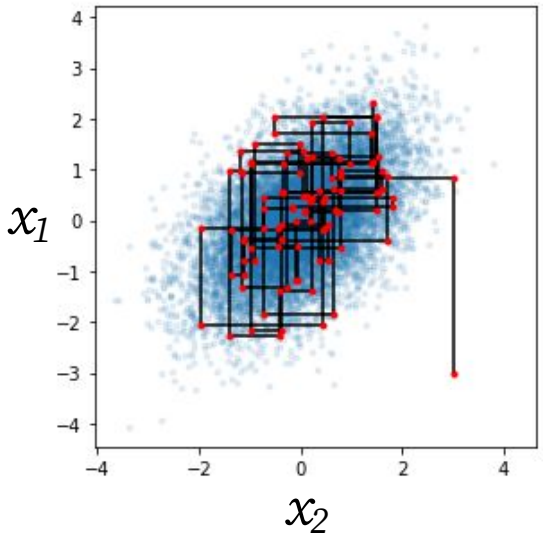

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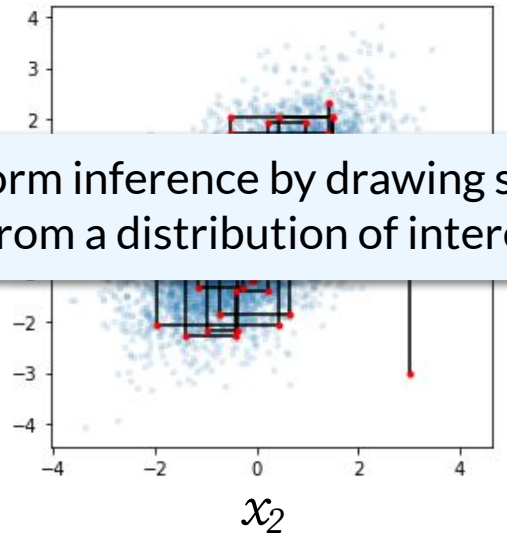

Perform inference by drawing samples from a distribution of interest.

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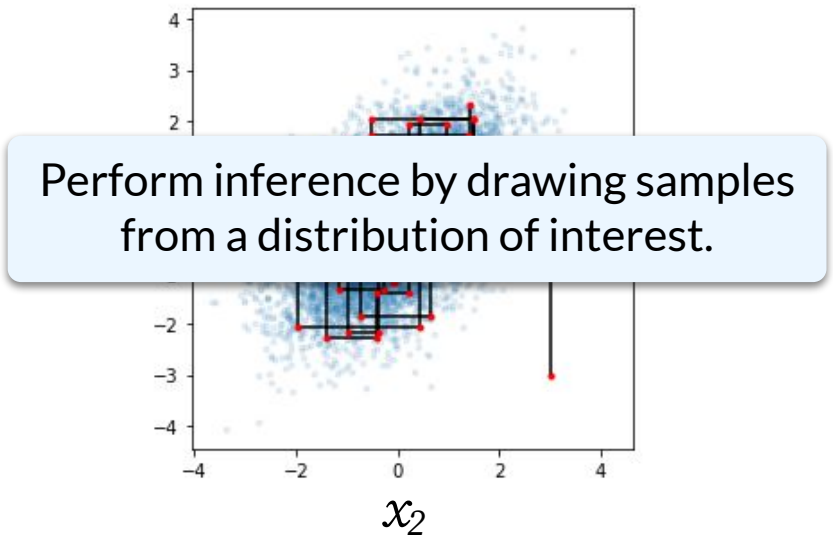

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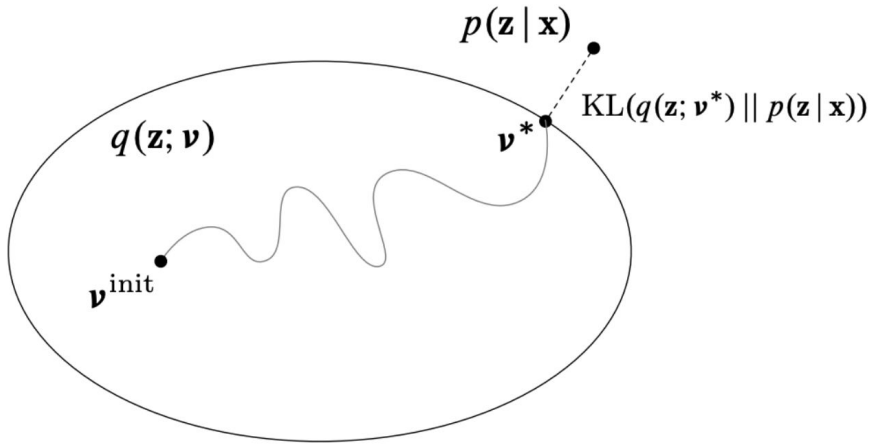

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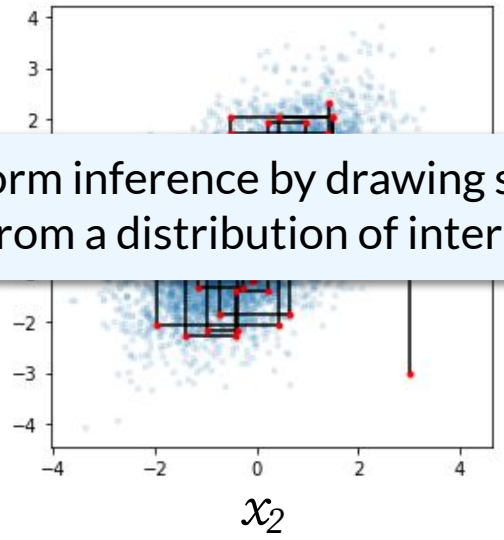

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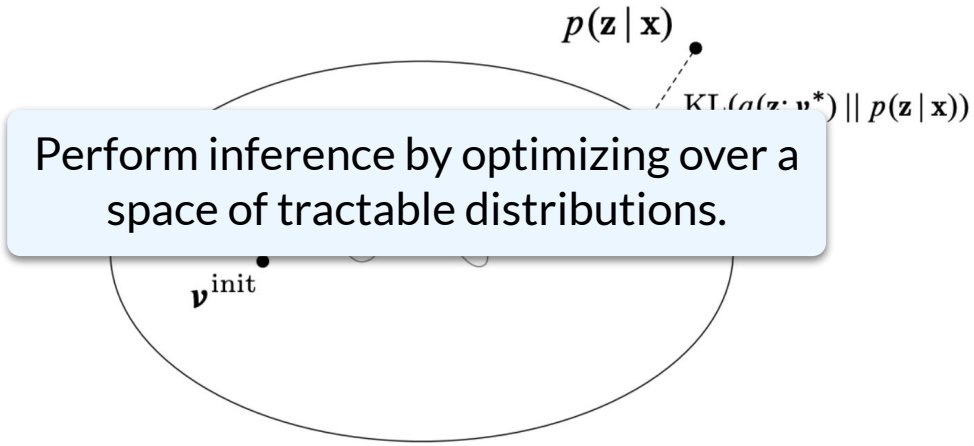

Perform inference by optimizing over a space of tractable distributions.

Source: Dave Blei, "Variational Inference"

Main Approximate Inference Algorithms

How are these methods used in probabilistic/generative modeling?

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Posterior Inference (⇒ inferring a conditional dist.)

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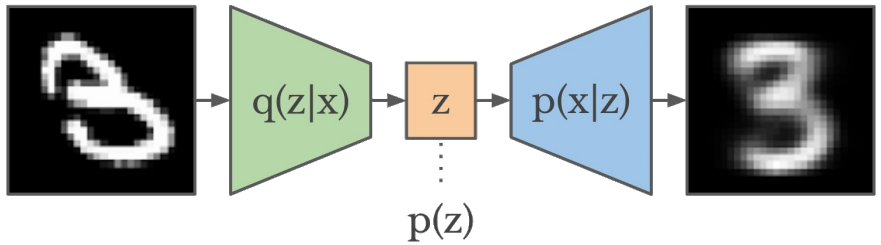
Posterior Inference (⇒ inferring a conditional dist.)

- *E.g., Variational Inference Algorithms*
- ⇒ approximate posterior inference (conditional distribution of latent variables given observed variables) via an optimization procedure.



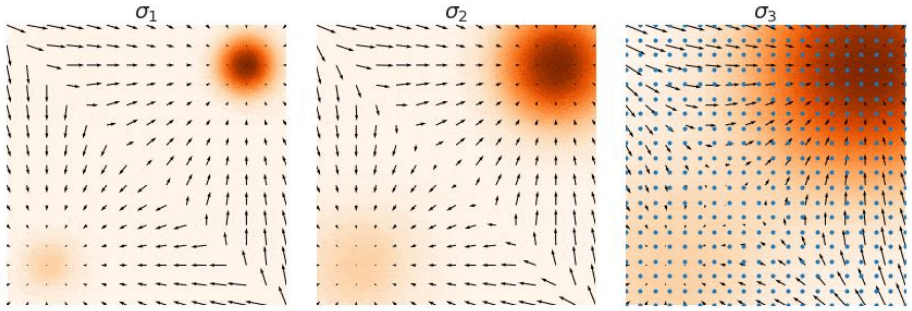
- VAE (Variational Autoencoder)
- DDPM (Denoising Diffusion Probabilistic Model)
- DDIM (Denoising Diffusion Implicit Model)
- Variational Inference in (Deep) Gaussian Processes

Main Approximate Inference Algorithms

How are these methods used in probabilistic/generative modeling?

Posterior Inference (⇒ inferring a conditional dist.)

- *E.g., Markov chain Monte Carlo (MCMC) Algorithms*
- ⇒ approximate posterior inference (conditional distribution of latent variables given observed variables)... *via sampling from conditional dist.*



- Score-based generative models.
- Bayesian neural networks.
- Energy-based deep generative models.
- Boltzmann Machines (RBMs, DBMs, and DBNs)

Sampling Methods: Monte Carlo and MCMC

Sampling Methods — Overview

Sampling approximate inference methods:

Produce answers by repeatedly generating random numbers from a distribution of interest.

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- Can compute various quantities of interesting, such as expectations $\mathbb{E}_{p(x)}\left[g(x)\right]$,
  - Where $g(x)$ is some "test function".
- Sampling methods have historically been most common approximate inference methods.
  - Though over the past ~15 years, variational methods have gained in popularity.
  - With primary advantages being speed, scale, and automation (ease of use).

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Sampling Methods — Overview

We will cover a progression of methods:

- Monte Carlo (MC)
- Markov chain Monte Carlo (MCMC)
  - Markov chains, stationary distributions
  - MCMC: Metropolis-Hastings, Gibbs sampling.
- Gradient-based Markov chain Monte Carlo (gradient-MCMC)
  - Langevin Monte Carlo (LMC), Hamiltonian Monte Carlo (HMC)
  - Also: stochastic-gradient-based Markov chain Monte Carlo (sg-MCMC)

Sampling from a Probability Distribution

As a warmup: consider how we might sample from a *categorical distribution*.

E.g., with k possible outcomes and associated probabilities: $\theta_1, \ldots, \theta_k$.

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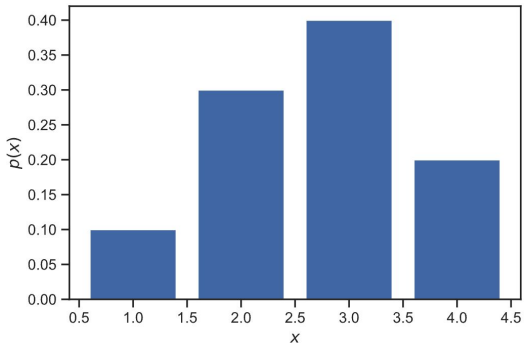
Recall: *categorical distribution*.

- A simple discrete distribution.
- With probability mass function:

$$X = \begin{cases} 1, & \text{with probability } \theta_1, \\ 2, & \text{with probability } \theta_2, \\ \vdots & \\ k, & \text{with probability } \theta_k. \end{cases}$$

... and $\sum_k \theta_k = 1$

For example:



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A deterministic sequence with statistical properties (*e.g.*, running averages) similar to that of a true random sequence.

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- Computers can only generate samples from simple distributions.
- *E.g.*, such as a uniform distribution over $[0, 1]$ ⇒ Even then, these are *pseudorandom!*
- ⇒ All (more-complex) sampling techniques involve calling some subroutine multiple times in a clever way.

A deterministic sequence with statistical properties (*e.g.*, running averages) similar to that of a true random sequence.

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For sampling from a categorical distribution:

Sampling from a Probability Distribution

As a warmup: consider how we might sample from a *categorical distribution*.

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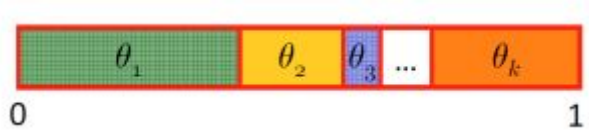
For sampling from a categorical distribution:

- Reduce it to sampling from a uniform distribution.
- Where we subdivide unit interval into k regions, with region i having size θ_i.
- Then we sample uniformly from $[0, 1]$, and return the region in which our sample falls.



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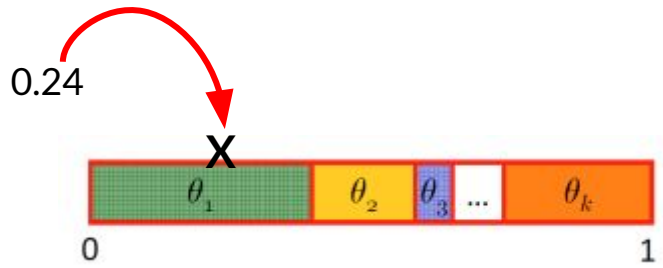

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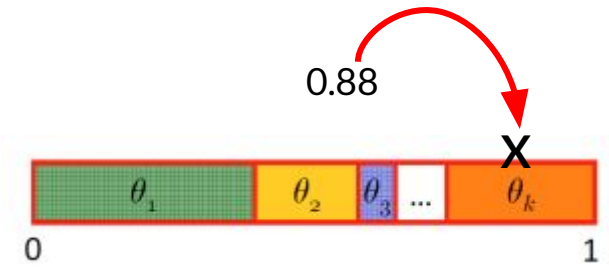
As a warmup: consider how we might sample from a *categorical distribution*.

E.g., with k possible outcomes and associated probabilities: $\theta_1, \ldots, \theta_k$.

For sampling from a categorical distribution:

- Reduce it to sampling from a uniform distribution.
- Where we subdivide unit interval into k regions, with region i having size θ_k.
- Then we sample uniformly from $[0, 1]$, and return the region in which our sample falls.



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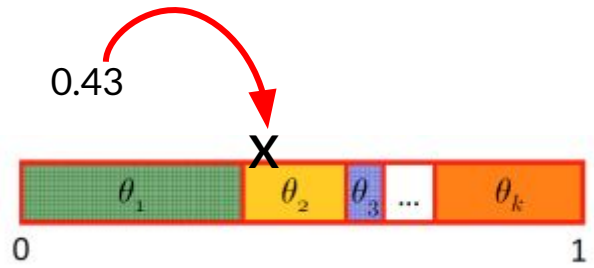

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Forward Sampling from Joint PDF — For a given a PGM

How about if we have a more-complex, higher dimensional PDF? (*E.g.*, as a PGM).

Suppose we want to sample from this distribution (*i.e.*, joint PDF).

Can we take advantage of the PGM structure?

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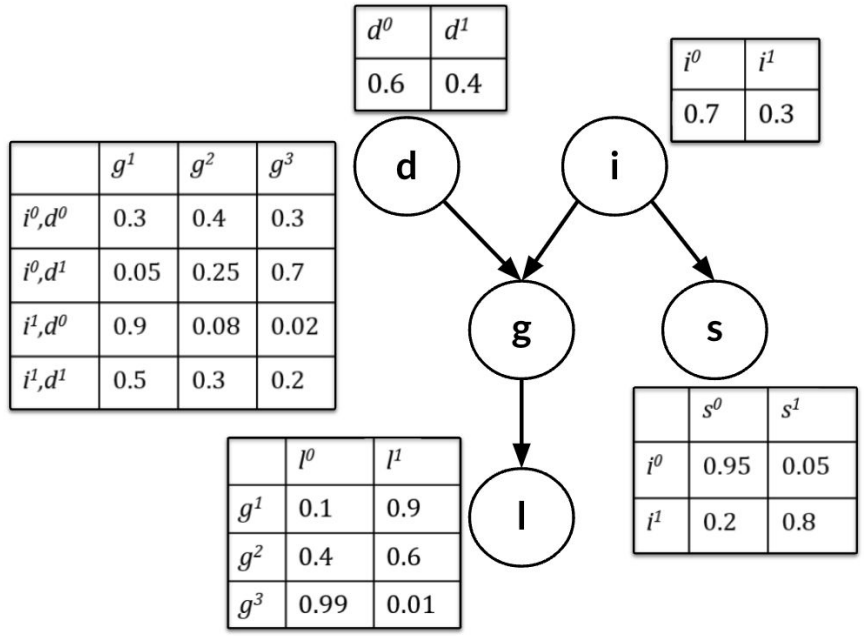

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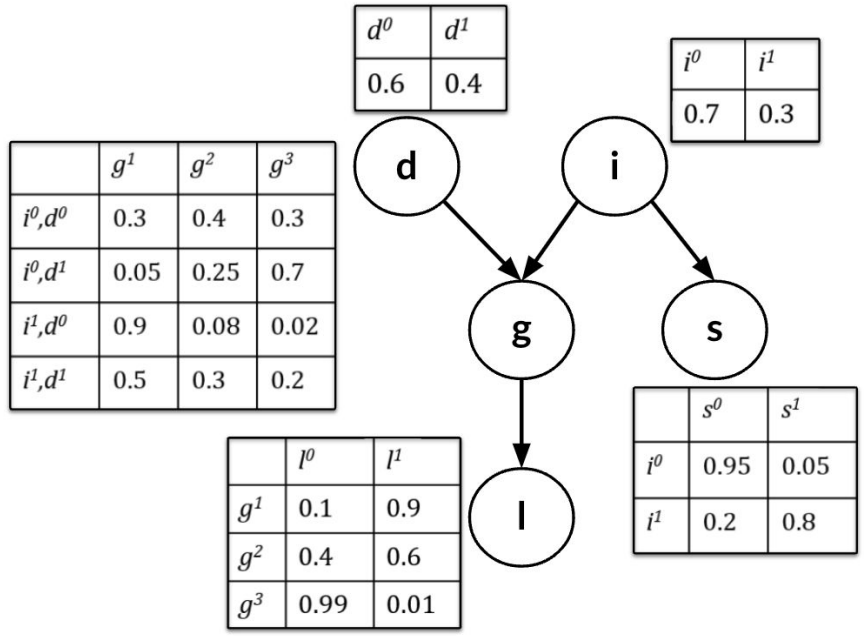

Joint PDF:

$$p(l, g, i, d, s) = p(d)\ p(i)\ p(s \mid i)\ p(g \mid i, d)\ p(l \mid g)$$

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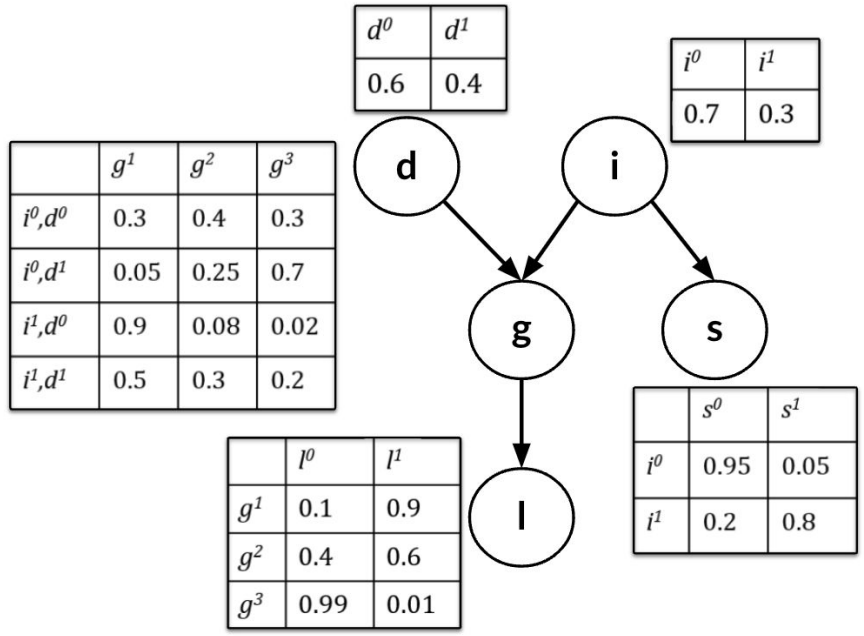
- Sample from each conditional probability distribution in turn (*i.e.*, follow generative process).
- At each step, conditioning on the sampled values of the previous step.



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Monte Carlo (MC) Estimation

Why do we want these samples and what do we typically do with them?

Monte Carlo (MC) Estimation

Samples from a distribution allow us to estimate expectations/integrals of the form:

$$\mathbb{E}_{x \sim p(x)}\left[g(x)\right] = \int_{\mathcal{X}} g(x)p(x)dx$$

$g(x)$ is some arbitrary "test function".

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Instead, we can approximate it with a large number of samples from $p(x)$.

⇒ Algorithms such as this are referred to as **Monte Carlo methods.**

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Monte Carlo (MC) Estimation

Backstory —

Source: Wikipedia

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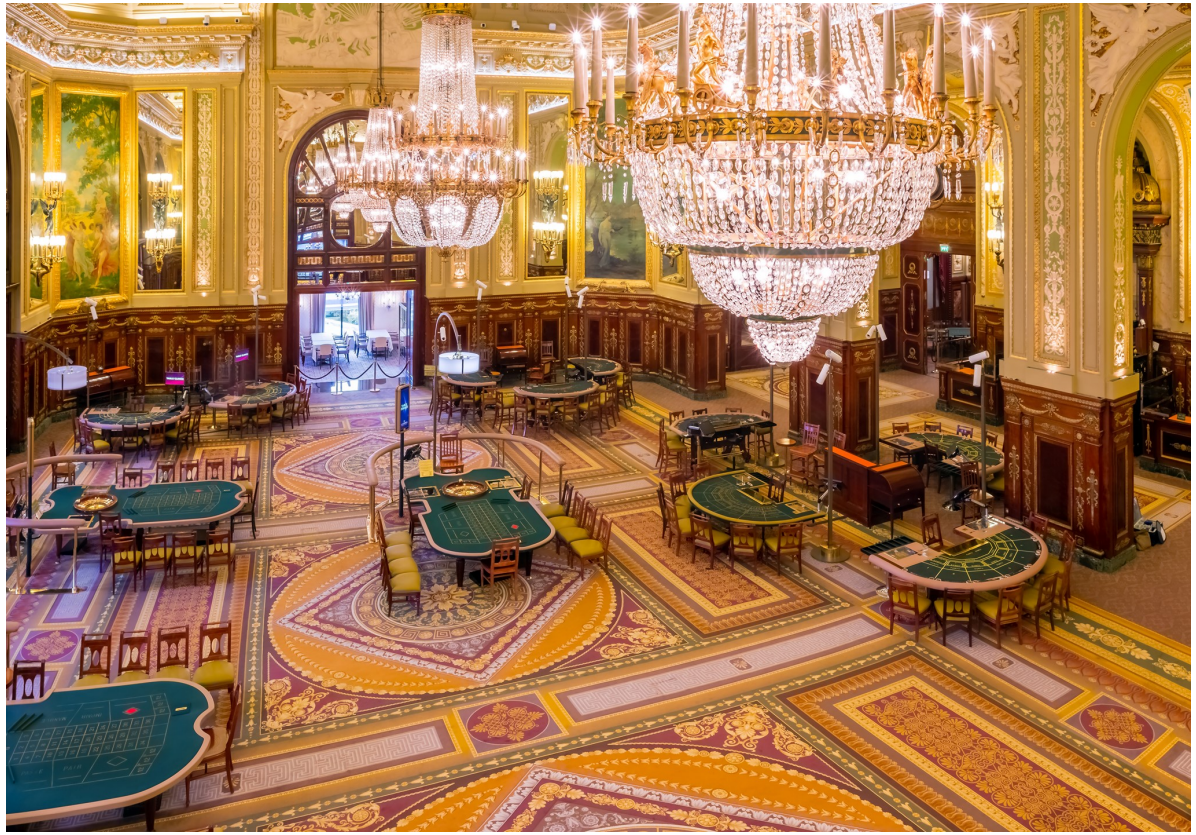

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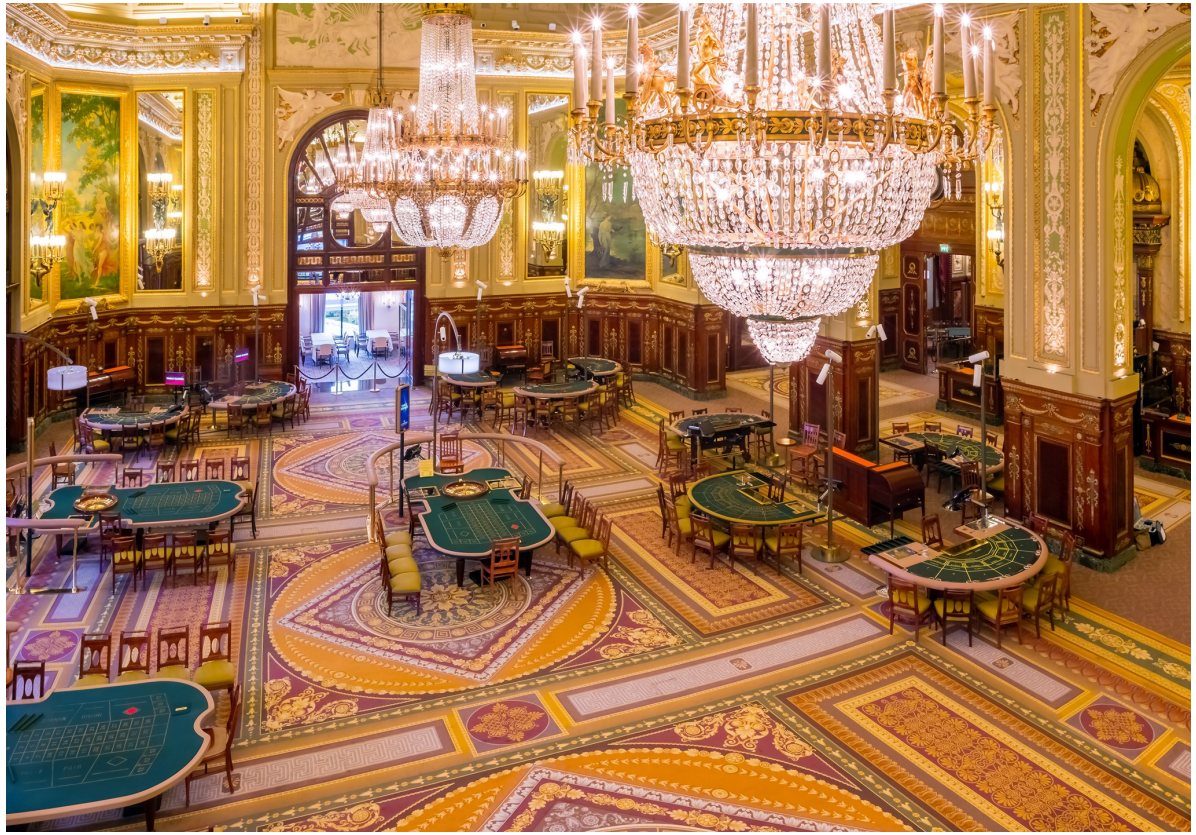

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Also a professor at USC! (*briefly!*)

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where samples $x^{(1)},\ldots,x^{(T)} \sim p(x)$ are drawn i.i.d. from the distribution $p(x)$.

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⇒ Variance can be made arbitrarily small

⇒ the *sample average* approaches the expectation as $T \to \infty$.

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Rejection Sampling

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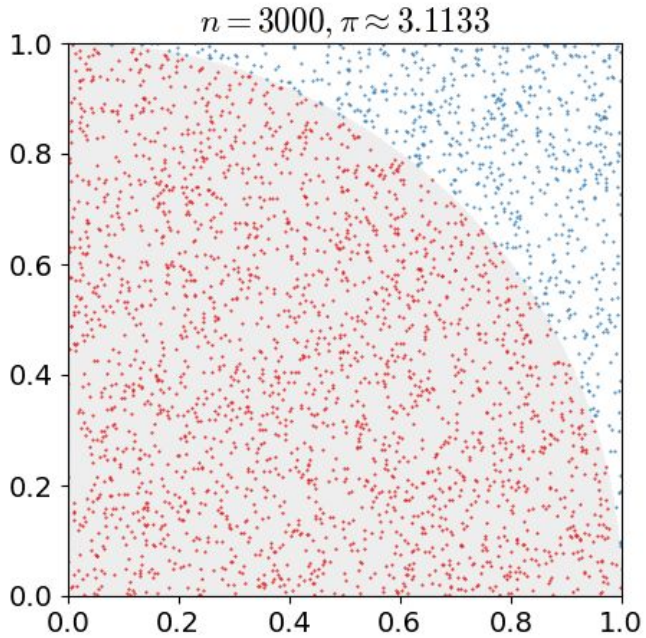
E.g., Approximating π: $(\pi r\text{^}2)/4$ vs $r\text{^}2$ →

Approximating π



Rejection Sampling

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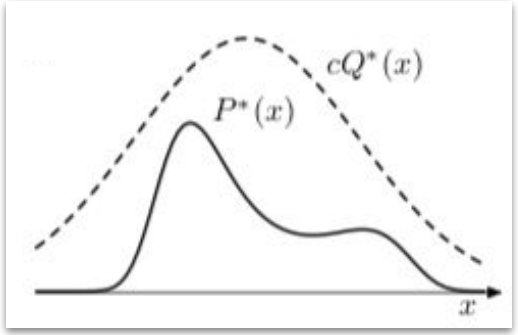
More formally:

Suppose we have a (potentially) complex PDF, written $p(x) = \frac{1}{Z}\tilde{p}(x)$.

We can propose, and sample from, a (more tractable) *proposal density*, denoted $q(x)$, if we assume that we know a value of a constant c such that:

$$cq(x) > \tilde{p}(x), \quad \forall x$$



Source: Jesse Bettencourt, Probabilistic Machine Learning

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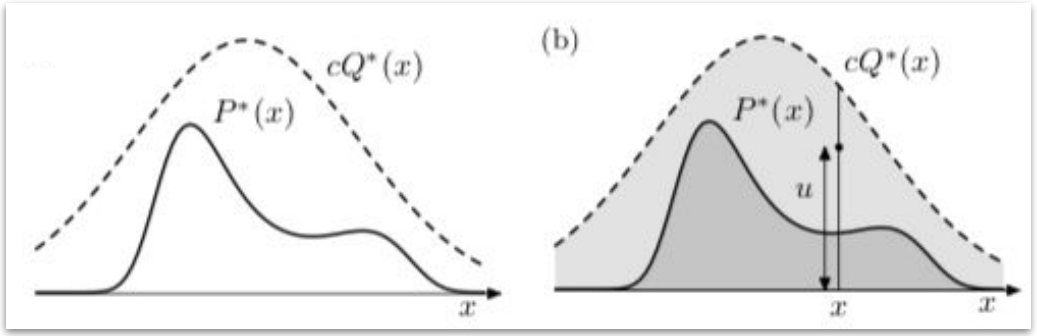

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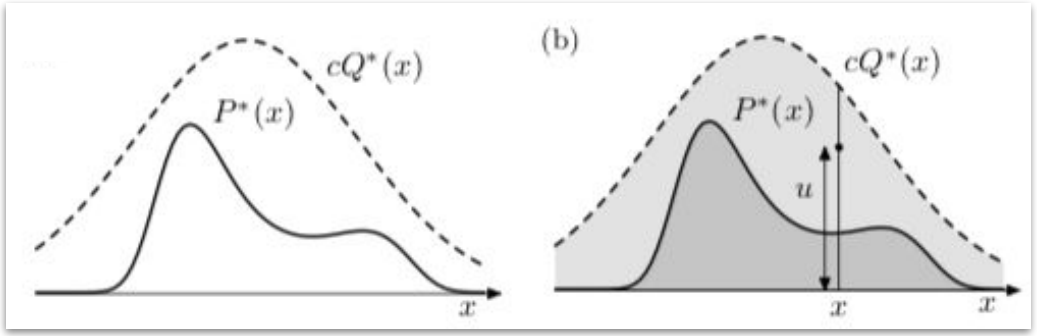

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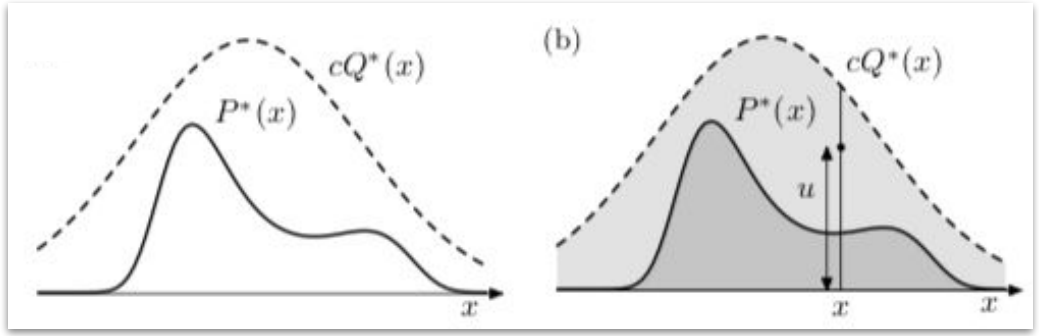

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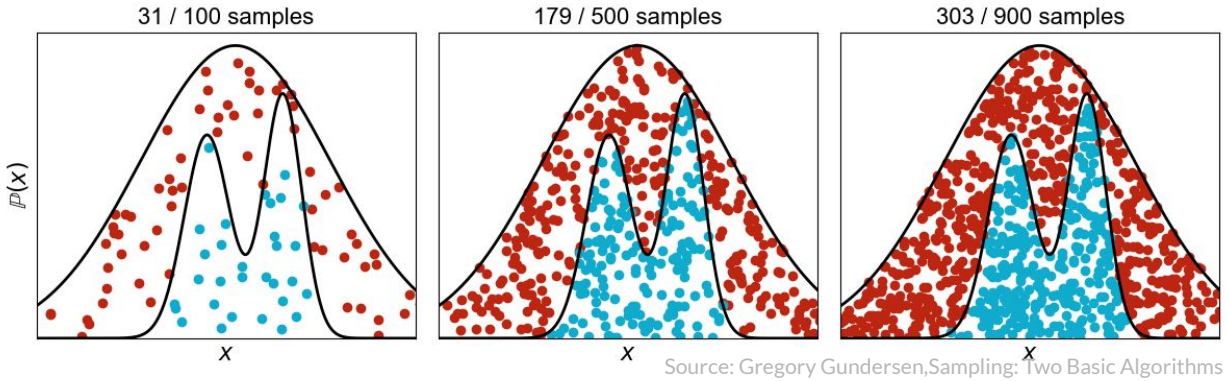

Source: Gregory Gundersen,Sampling: Two Basic Algorithms

This samples uniformly over AUC ⇒ x is drawn proportional to PDF!

Rejection Sampling

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Suppose we have a Bayes Net over the set of (discrete) variables $X = Z \cup E$.

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⇒ draw many samples from p and keep the fraction that are consistent with E=e.

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Rejection $\rightarrow$ Importance Sampling

Unfortunately, rejection sampling can be very wasteful (especially in higher dims).

E.g., if $p(E = e)$ equals 1% mass of joint, then we will discard 99% of all samples.

Rejection → Importance Sampling

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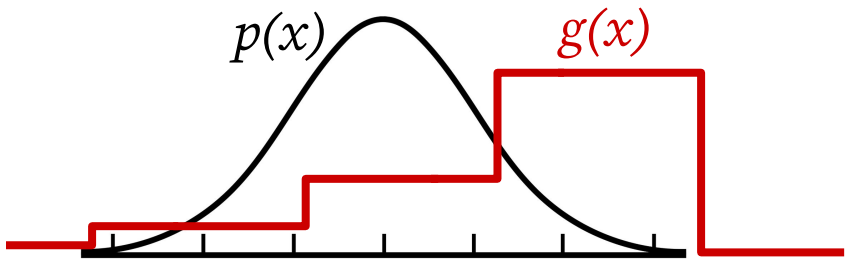
A more efficient method of MC method for expectations ⇒ **importance sampling**.

Main idea:

- 1. Sample from a proposal distribution $q(x)$ (ideally with $q(x)$ roughly proportional to $g(x) \cdot p(x)$.
- 2. Reweight the samples (in a principled way), so that their sum still approximates the desired integral.



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We can rewrite this expectation as:

(Assuming discrete RVs, but same argument holds for continuous RVs.)

$$\mathbb{E}_{x \sim p(x)}[g(x)] = \sum_x g(x)p(x)$$

$$= \sum_x g(x)\frac{p(x)}{q(x)}q(x)$$

$$= \mathbb{E}_{x \sim q(x)}[g(x)w(x)], \quad \text{where } w(x) = \frac{p(x)}{q(x)}$$

$$\approx \frac{1}{T}\sum_{t=1}^{T} g(x^{(t)})w(x^{(t)}), \quad \text{where } x^{(1)}, \ldots, x^{(T)} \overset{\text{iid}}{\sim} q(x)$$

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Definition of expected value

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Multiply by *1* = *q(x)/q(x)*

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Rewrite as expectation *w.r.t. q(x)*

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MC Estimate!

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Sometimes referred to as an *IS estimate.*

MC Estimate!

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Importance Sampling

The variance of this new random variable is:

Importance Sampling

Recall: $\mathrm{Var}\left[X\right] = \mathbb{E}\left[X^2\right] - \mathbb{E}\left[X\right]^2$

The variance of this new random variable is:

$$\mathrm{Var}_{x\sim q(x)}\left[g(x)w(x)\right] = \mathbb{E}_{x\sim q(x)}\left[g^2(x)w^2(x)\right] - \mathbb{E}_{x\sim q(x)}\left[g(x)w(x)\right]^2 \geq 0$$

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

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In practice: this is not constructive → the denominator is the quantity we want!

However, it gives intuition for what we want: high where both $g(x)$ and $p(x)$ are high.

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

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→ Recall that in rejection sampling, we simply throw away all samples from $p(x)$ where the variables in E did not take a value of e.

$$p(E = e) = \mathbb{E}_{x \sim p}[\mathbb{I}(E = e)]$$

"draw many samples from p and keep the fraction that are consistent with the value of the marginal."

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Definition of joint/conditional

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Multiply by 1, switch arguments in expectation (same as in RS)

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Monte Carlo estimate!

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Unlike rejection sampling, this uses all of the samples when computing the estimate!

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Markov Chain Monte Carlo (MCMC)

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Suppose we want to sample from more complex distribution!

Markov chain Monte Carlo (**MCMC**) gives us a way to do this.

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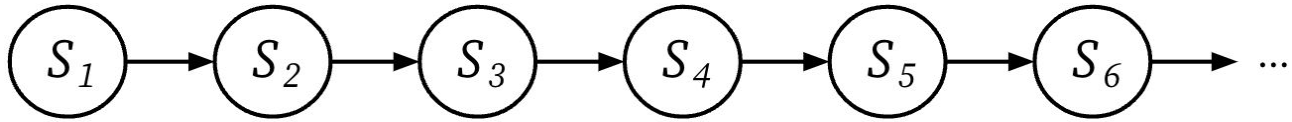

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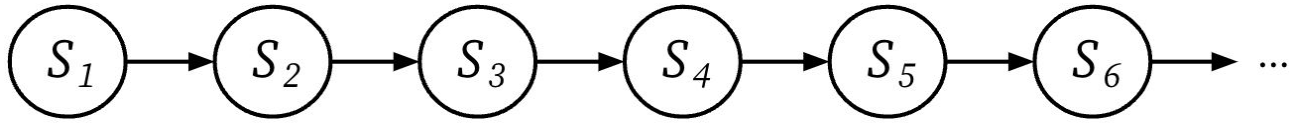

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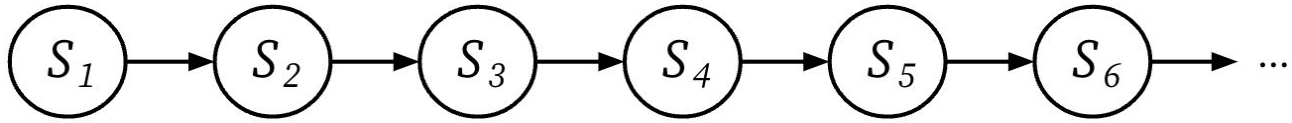

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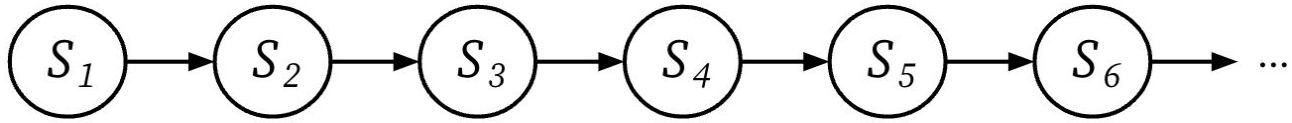

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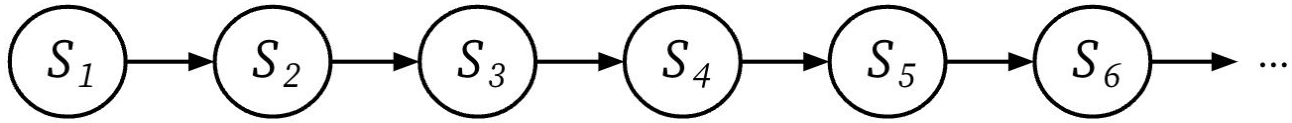

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- Note that the conditional probability is same for each i …
- ⇒ the transition probabilities at any time depend only on the given state and not on the history of how we got there (“Markov assumption”).

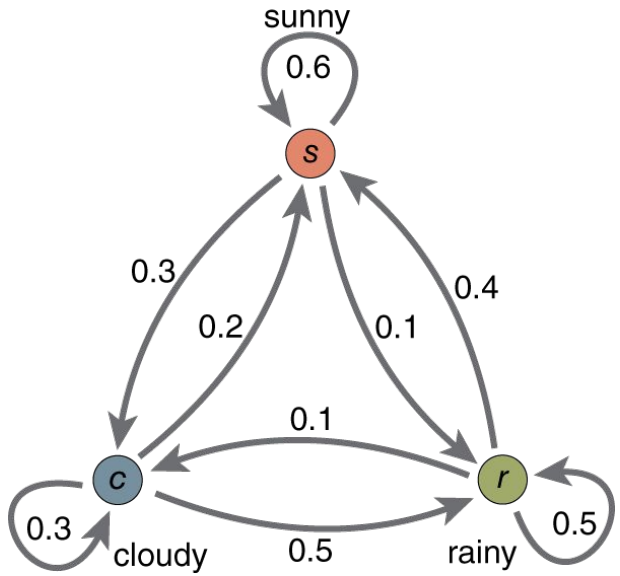
“Given the present, the future does not depend on the past”

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Markov Chain Monte Carlo (MCMC) — Markov Chains

Example: Markov chain with discrete random variables.

⇒ Each random variable $S_i \in \{1, 2, \ldots, d\}$ taking one of d possible values.



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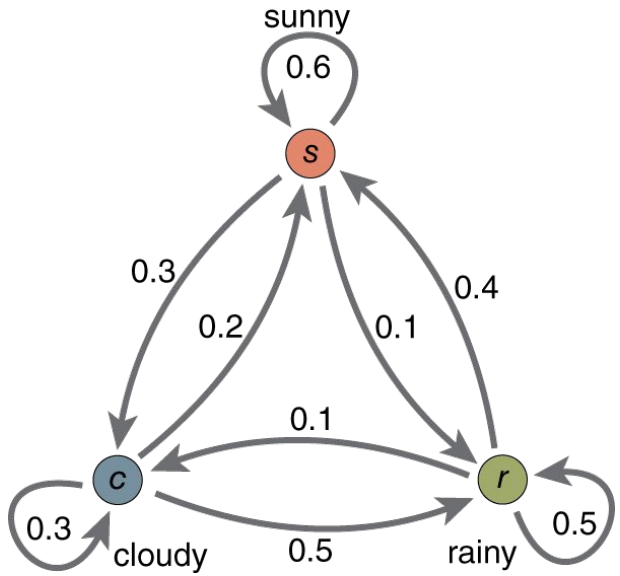

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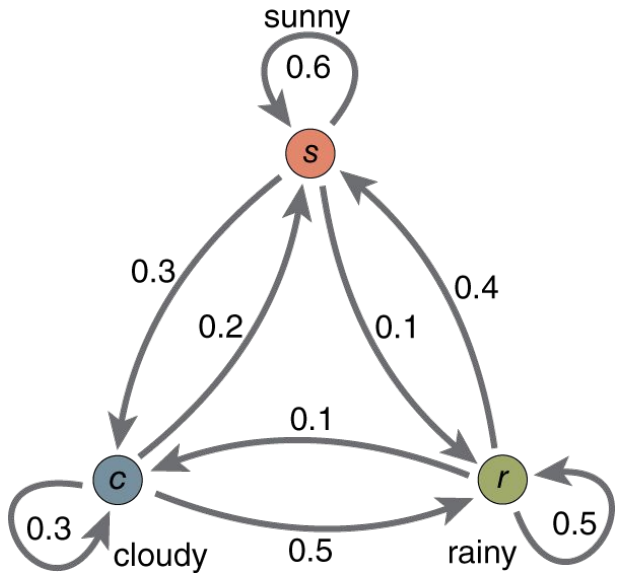

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Suppose we write the initial state distribution $p(S_0)$ as a vector p_0.

⇒ We can write the probability p_t of ending up in a given state as:

$$p_t = T^t p_0$$

T^t is a matrix power (*i.e.*, apply the matrix operator t times)

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Markov Chain Monte Carlo (MCMC) — Markov Chains

Stationary Distributions

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Below we will construct Markov chains with the same stationary distribution for any initial distribution p_0.

⇒ So we often refer to it as ***the*** stationary distribution of the Markov chain.

Markov Chain Monte Carlo (MCMC) — Markov Chains

Detailed Balance

Markov Chain Monte Carlo (MCMC) — Markov Chains

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(Part of) a sufficient condition for π to be a stationary distribution is a property called *detailed balance*:

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Markov Chain Monte Carlo (MCMC) — Markov Chains

Also holds for **continuous** random variable MCs (w/ *transition distributions*)

Detailed Balance

(Part of) a sufficient condition for $\pi(x)$ to be a stationary distribution is a property called *detailed balance*:

$$\pi(x')T(x \mid x') = \pi(x)T(x' \mid x) \quad \text{for all } x$$

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Ergodicity

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  - It is possible to get from any state to any other state with probability > 0, in a finite number of steps.
- *Aperiodicity*:
  - It is possible to return to any (previously sampled) state at any time.

In continuous variable MC's these conditions are often referred* to as *ergodicity*.

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- *Aperiodicity*: "Avoids transitioning between sets of states in a cycle"
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⇒ then we can sample from this Markov chain, and iteratively get closer to samples from the probability distribution (as we approach stationary distribution).

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Thus, in an MCMC algorithm you typically perform the following two steps:

(Given as input: a transition matrix/distribution T, and an initial assignment of variables, x_0).

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Assuming that B is sufficiently large, the latter set of N samples will approximately be drawn from $p(x)$.

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Markov Chain Monte Carlo (MCMC) — Algorithms

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Markov Chain Monte Carlo (MCMC) — Algorithms

We'll review through a few different MCMC algorithms following these steps:

- Metropolis-Hastings (MH) — a "core" MCMC algorithm
- Gibbs Sampling — can be viewed as a special case of MH.
- Langevin Monte Carlo — can be viewed as a *gradient-based* case of MH.
- Hamiltonian Monte Carlo — can be viewed as a *better gradient-based* case of MH.

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Metropolis-Hastings (MH)

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The **Metropolis Hastings Algorithm** constructs a transition distribution $T(x' \mid x)$ using two components:

- A user-specified *transition kernel* $Q(x' \mid x)$.
- An *acceptance probability* for moves proposed by Q, specified by the algorithm as:

$$A(x' \mid x) = \min\left(1, \frac{p(x')Q(x \mid x')}{p(x)Q(x' \mid x)}\right).$$

Often called the *acceptance ratio.*

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At each step of the MH, we sample $x' \sim Q(x' \mid x)$ and then we either *accept* it with probability $\alpha = A(x' \mid x)$ or reject it and remain at our previous state.

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Important: $p(x)$, $p(x')$ can be unnormalized PDF! ⇒ easier to apply.

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Metropolis-Hastings (MH)

Intuition:

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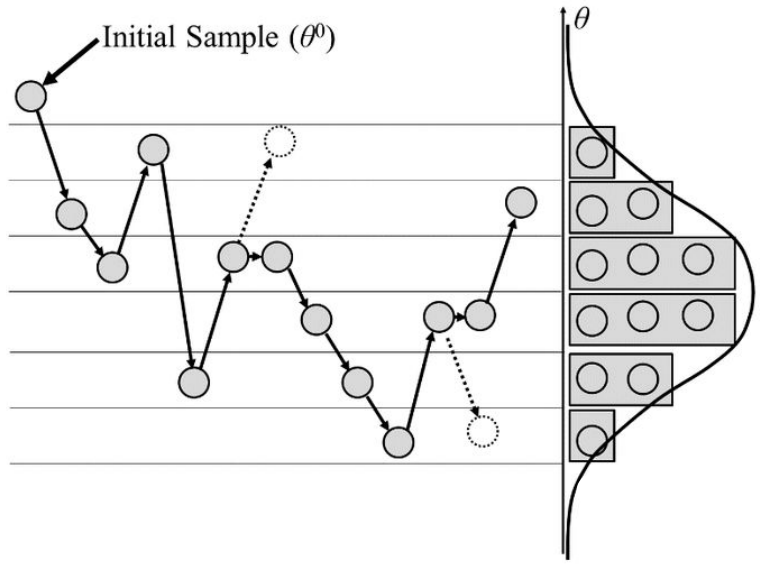
The acceptance probability encourages us to move towards more-likely (higher-mass) regions of the distribution $p(x)$.

When Q suggests we move into a low-probability region, we follow that move only a fraction of the time.



Source: Wikipedia, "Metropolis-Hastings Algorithm"

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Note that when $Q(x' \mid x) = Q(x \mid x')$, a symmetric distribution (*e.g.*, Gaussians), then the acceptance ratio simplifies to:

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Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Metropolis-Hastings (MH)

Intuition:

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⇒ *Metropolis* Algorithm (symmetric proposals)

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This variant of the algorithm (*Metropolis Algorithm*) originally published in 1953!

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

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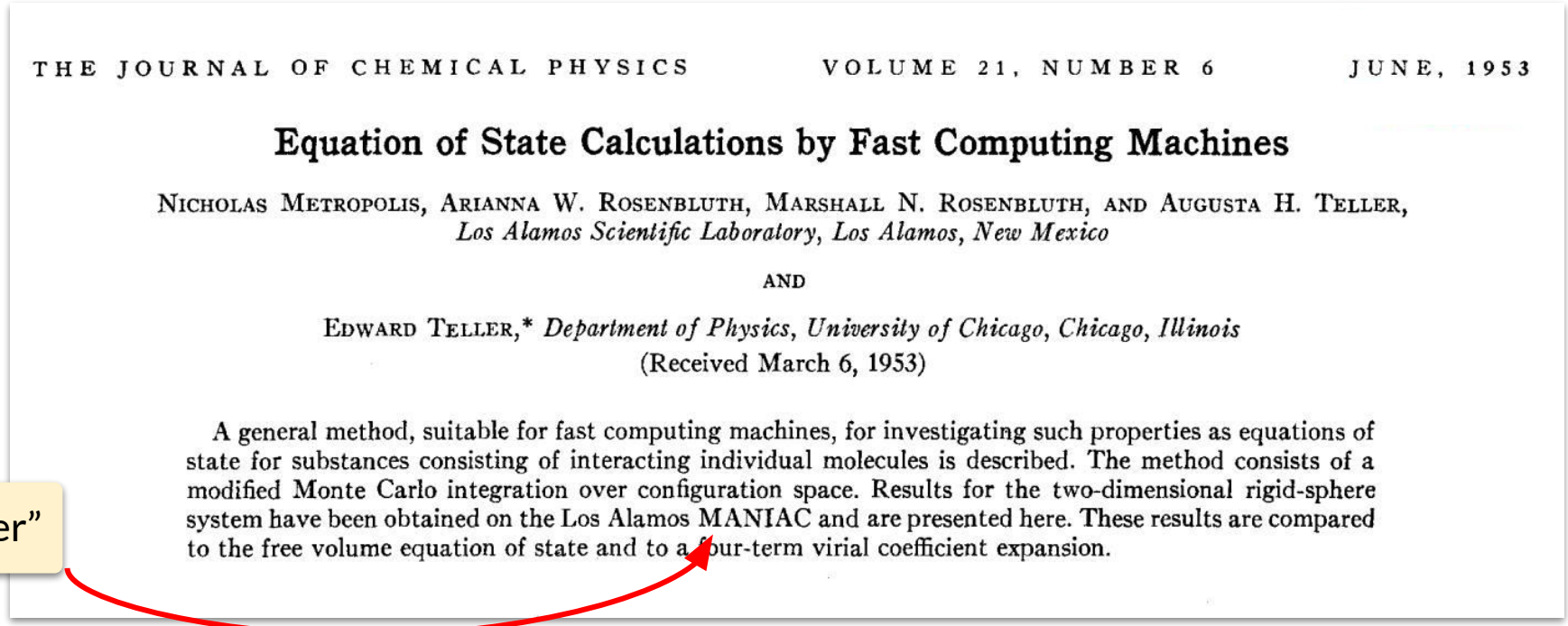

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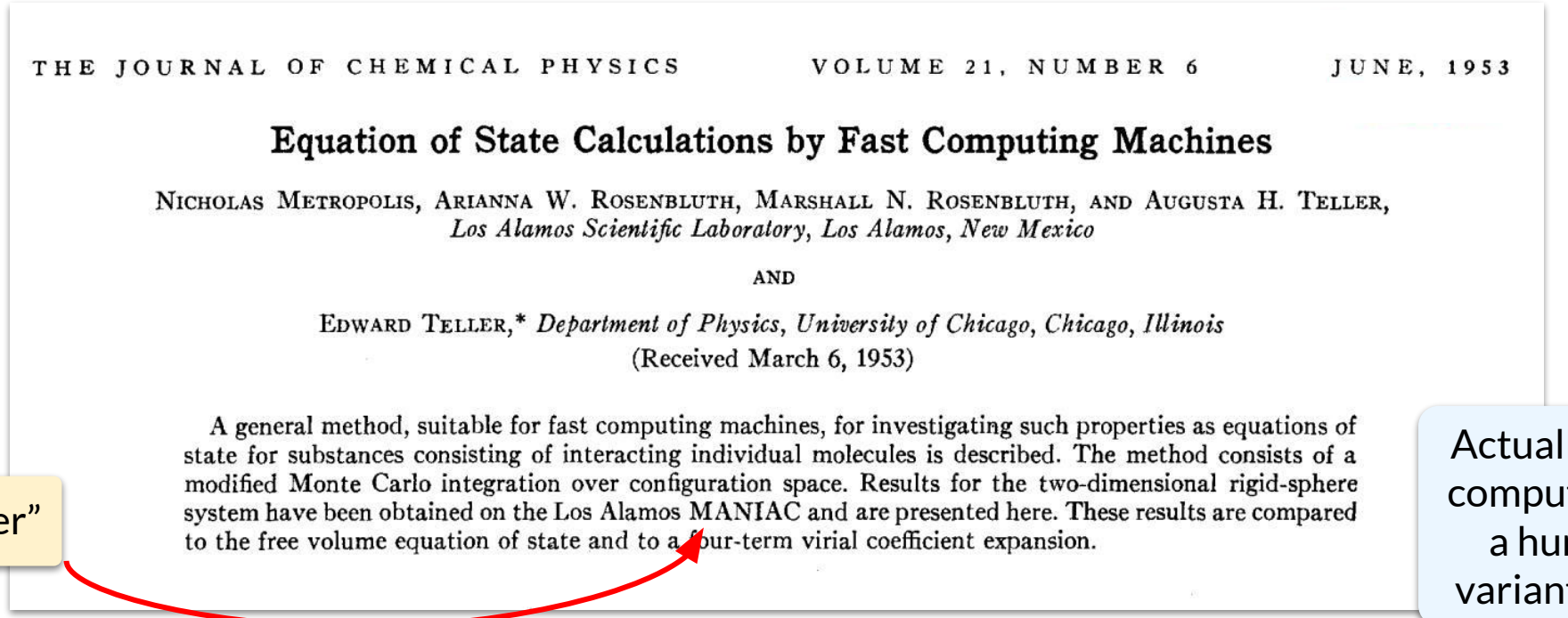

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"Fast computer"

Actually, the first computer to beat a human at a variant of chess!

Metropolis-Hastings (MH)

Animation of Metropolis Hastings Algorithm:

Source: Stata Blog

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Animation of Metropolis Hastings Algorithm:

Uses a Gaussian proposal distribution to sample from a more complex distribution!

(In this case, a Beta(5, 7) distribution).

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Animation of Metropolis Hastings Algorithm:

Uses a Gaussian proposal distribution to sample from a more complex distribution!

(In this case, a Beta(5, 7) distribution).

Notice that subsequent samples are (slightly) correlated.

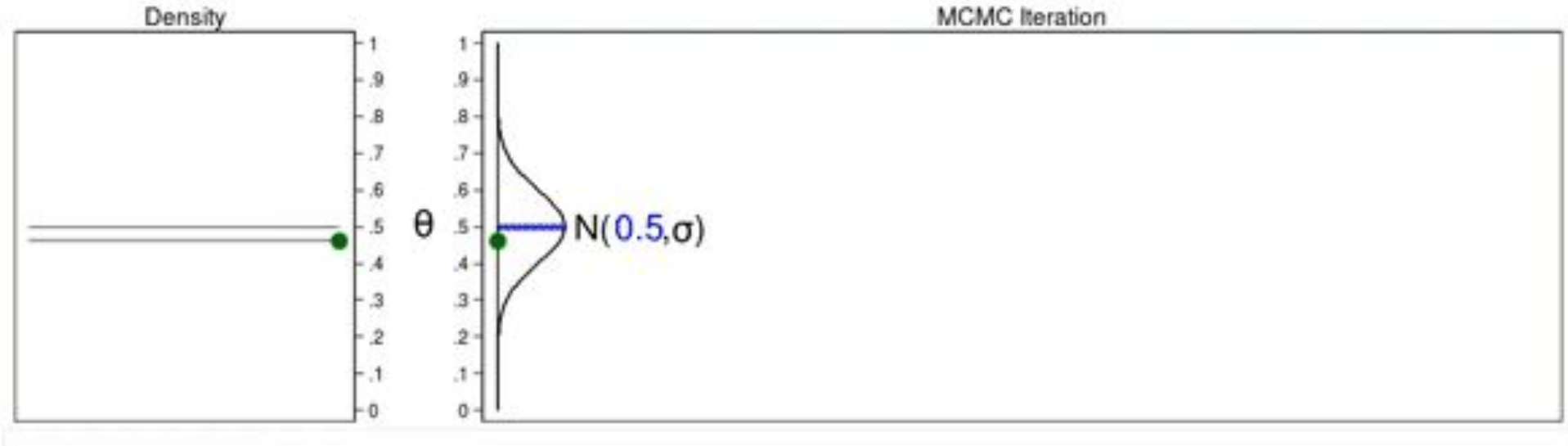
Source: Stata Blog

Metropolis-Hastings (MH)

Animation of ~~Metropolis Hastings Algorithm~~:
regular sampling from a simple distribution.

Compare that with exact sampling.

E.g., from a Gaussian distribution.



Here, all samples are independent.

Source: Stata Blog

Quick Note on “Posterior Sampling”

MCMC is often synonymous with “posterior sampling” (drawing samples from a posterior distribution).

However: methods so far have not really been posterior-distribution specific!

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MCMC is often synonymous with “posterior sampling” (drawing samples from a posterior distribution).

However: methods so far have not really been posterior-distribution specific!

⇒ They just require: access to (unnormalized) PDF from which we want to sample.

⇒ Which is well suited to posterior sampling (but also to other inference as well).

Gibbs Sampling

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Think of it as an *"axially aligned, carefully designed, transition function that always yields an acceptance ratio of 1"*.

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Think of it as an *"axially aligned, carefully designed, transition function that always yields an acceptance ratio of 1"*.

Why is it useful if the acceptance ratio is high?

- Less wasted samples!
- In high dimensional space, a bad (or even just simple) transition distribution can lead to very low acceptance ratio…

⇒ bad numerical properties!

Gibbs Sampling — Algorithm

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Suppose we have an ordered set of variables in our model: $x_1, \ldots, x_n$

And an initial configuration: $x^0 = (x_1^0, \ldots, x_n^0)$

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Repeat until convergence for $t = 1, 2, 3, \ldots$

- Set $x \leftarrow x^{t-1}$
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Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

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For each sample…

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Set buffer to previous sample

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For each variable (*dimension*)

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Sample from conditional of $p(x)$
($x_{i\text{-}1}$ denotes "*all other variables*")

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Replace variable (*dimension*) with sample

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Set next sample to buffer

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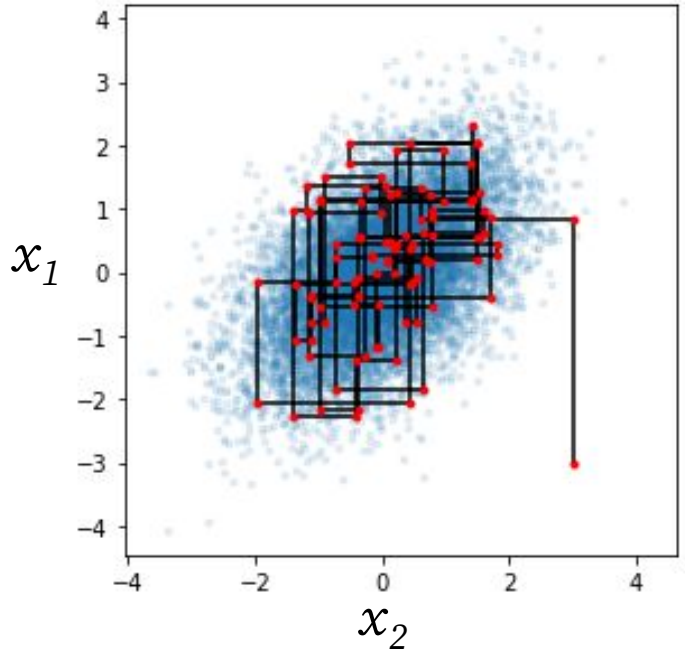
Looks like this:



Source: Jessica Stringham, Gibbs Sampling in Python

Gibbs Sampling

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⇒ *"It's up to you to figure out"* :D

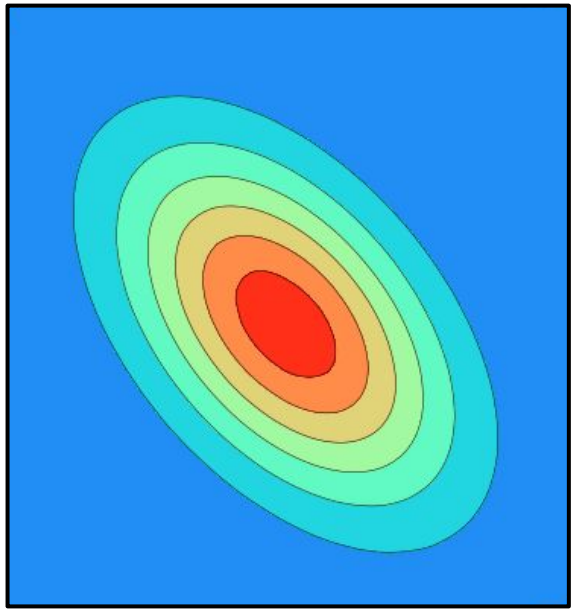
In some cases:

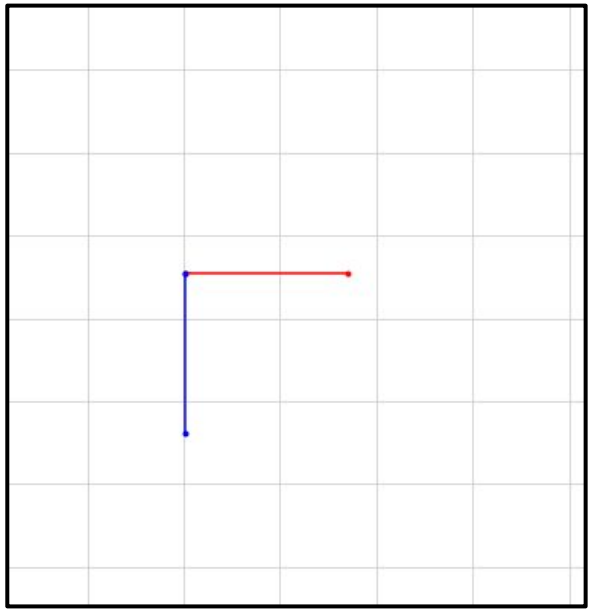
- You can sample from this conditional in closed form (*in certain models*, *e.g.*, *LDA*).
- You run a subroutine to sample from this conditional.
  - As an example: Metropolis-Hastings algorithm!
  - Sometimes this "fixes" low acceptance rate issues, since MH is now over only *one variable* (much lower dimensionality).

Gibbs Sampling

Animation:

Gibbs sampling in practice!





Source: Sandipan Dey, Bayesian Machine Learning

Gradient Based MCMC

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Gradient Based MCMC

One final strategy to avoid low acceptance rate in Metropolis-Hastings (particularly in high dimensions) — using gradients ✨.

Background — the issue with simple proposals in MH:

- You could achieve a higher acceptance rate by just taking small steps (*e.g.*, use a symmetric distribution with small variance centered at previous sample).
- *However*, small steps ⇒ bad mixing and very slow progress of the algorithm (*i.e.*, high correlation ⇒ need many more samples for same statistical properties).

Gradient Based MCMC

A few popular MCMC methods leverage the *gradient of the PDF* in order to propose a sample in a high mass region from potentially far away in space.

(These methods original came from the field of quantum chromodynamics)

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A few popular MCMC methods leverage the *gradient of the PDF* in order to propose a sample in a high mass region from potentially far away in space.

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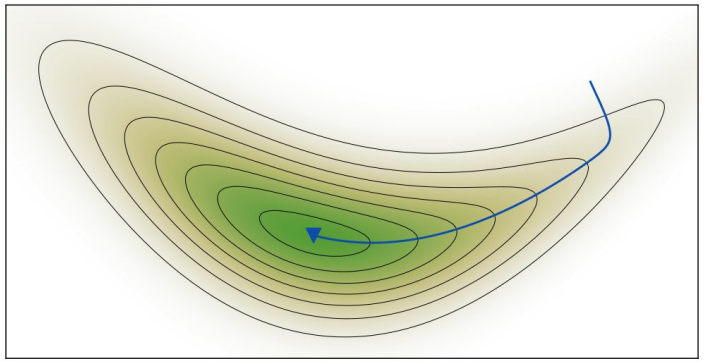
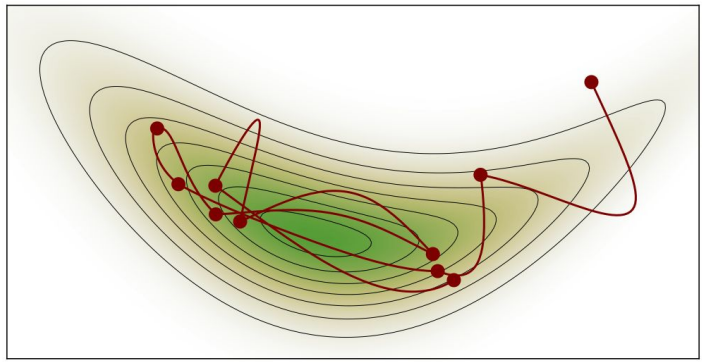
They are called: **Langevin Monte Carlo** (LMC) and **Hamiltonian Monte Carlo** (HMC).



Gradient Descent Path



Hamiltonian Monte Carlo Samples

Gradient Based MCMC

We could do a full lesson on these methods alone — for now will keep it brief!

(And provide more resources for those who are interested to learn more).

Gradient Based MCMC

Suppose we have a given PDF $p(x), \quad x \in \mathbb{R}^n$.

Consider an objective function: $f(x) = -\log p(x)\,.$

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Consider an objective function: $f(x) = -\log p(x)\,.$

The gradient of this objective is:

$$\nabla_x f(x) = \left[\frac{d}{dx_1} f(x), \ldots, \frac{d}{dx_n} f(x)\right]^\top$$

Gradient Based MCMC

If we wanted to perform *optimization* (*e.g.*, to find a minimum of the objective), we could perform gradient descent:

$$x_t = x_{t-1} - \eta_t \nabla_x f(x_{t-1})$$

where η_t is the learning rate/step size at iteration t.

Gradient Based MCMC — Langevin Monte Carlo (LMC)

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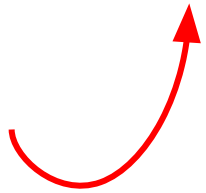
Compare with gradient descent



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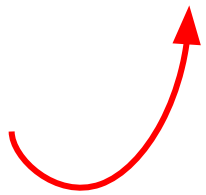

Main difference is an extra "stochastic term"

Can view this as "*gradient descent plus noise*"

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Gradient Based MCMC — Langevin Monte Carlo (LMC)

Intuitively:

You are moving toward higher-mass regions of the PDF (in expectation).

Source: Roy Friedman, “A Simplified Overview of Langevin Dynamics”

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Gradient Based MCMC — Langevin Monte Carlo (LMC)

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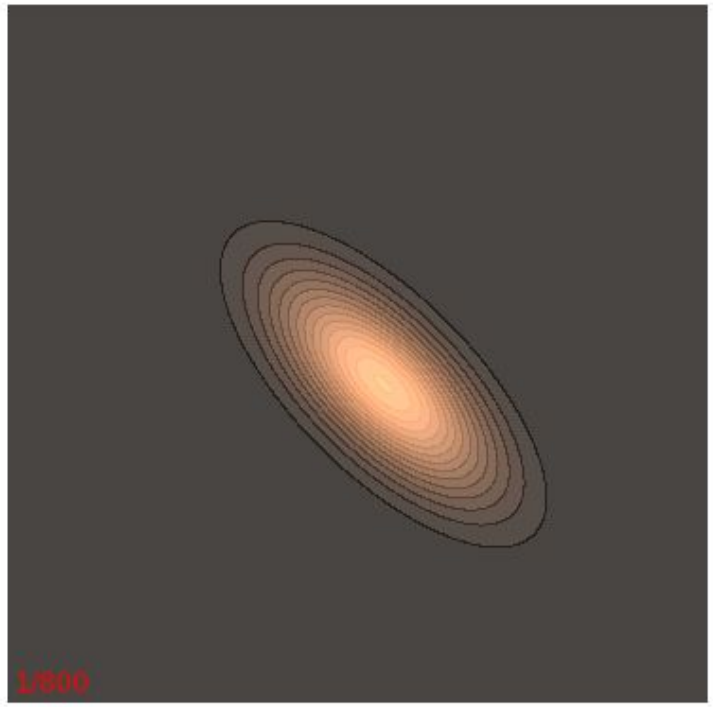
You are moving toward higher-mass regions of the PDF (in expectation).

But also: adding noise such you have some probability of visiting lower-mass regions.

⇒ balanced so that the probability of visiting any region is proportional to the density in that region.

(Unlike gradient descent, where you only move towards higher-mass regions.)



Source: Roy Friedman, "A Simplified Overview of Langevin Dynamics"

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Gradient Based MCMC — Langevin Monte Carlo (LMC)

So does it work?

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You can prove that the stationary distribution of this Markov chain is equal to $p(x)$, in the limit, as $T \to \infty$ and $\epsilon_t \to 0$.

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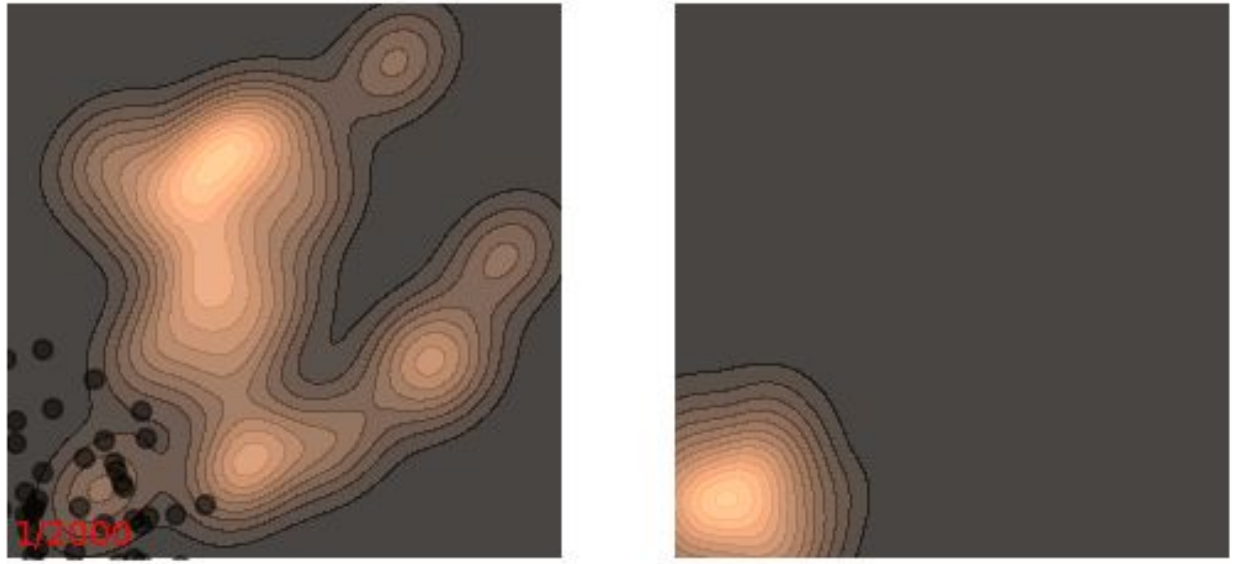
For an empirical illustration:

(using a small ϵ_t).



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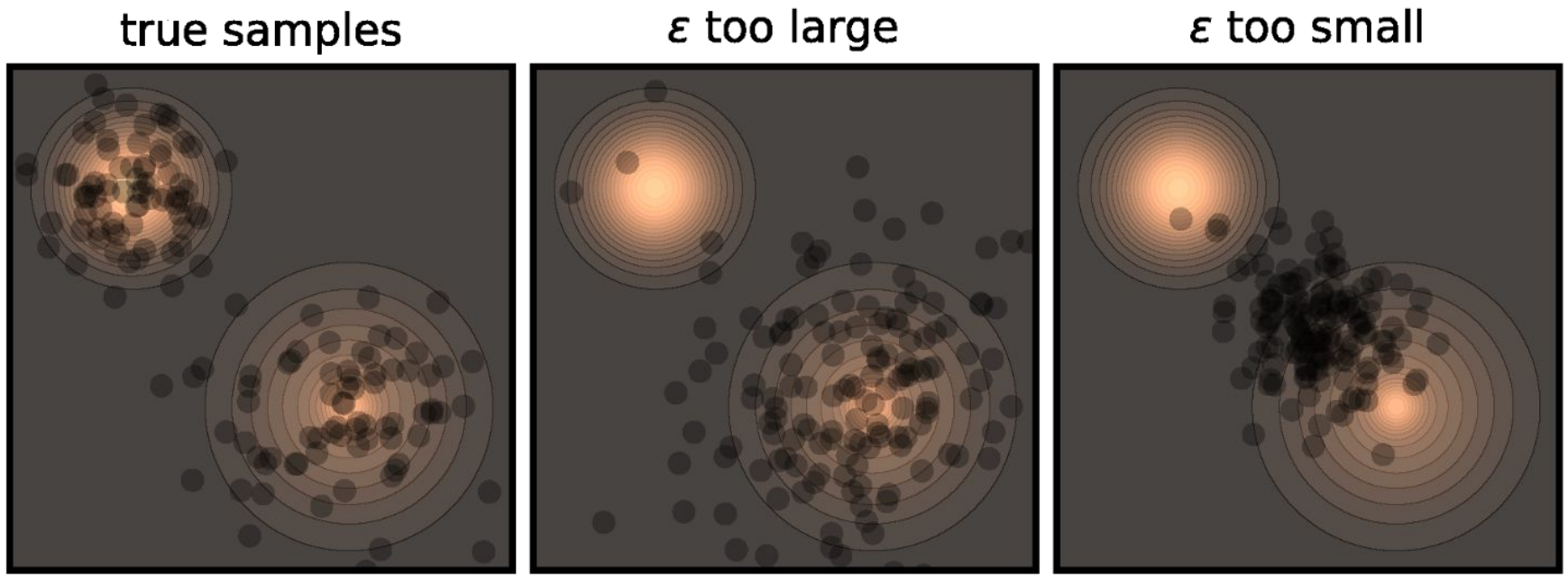
- If step size is too large ⇒ samples will be biased (incorrect stationary distribution).
- If step size is too small ⇒ takes much longer (bad *mixing* properties).



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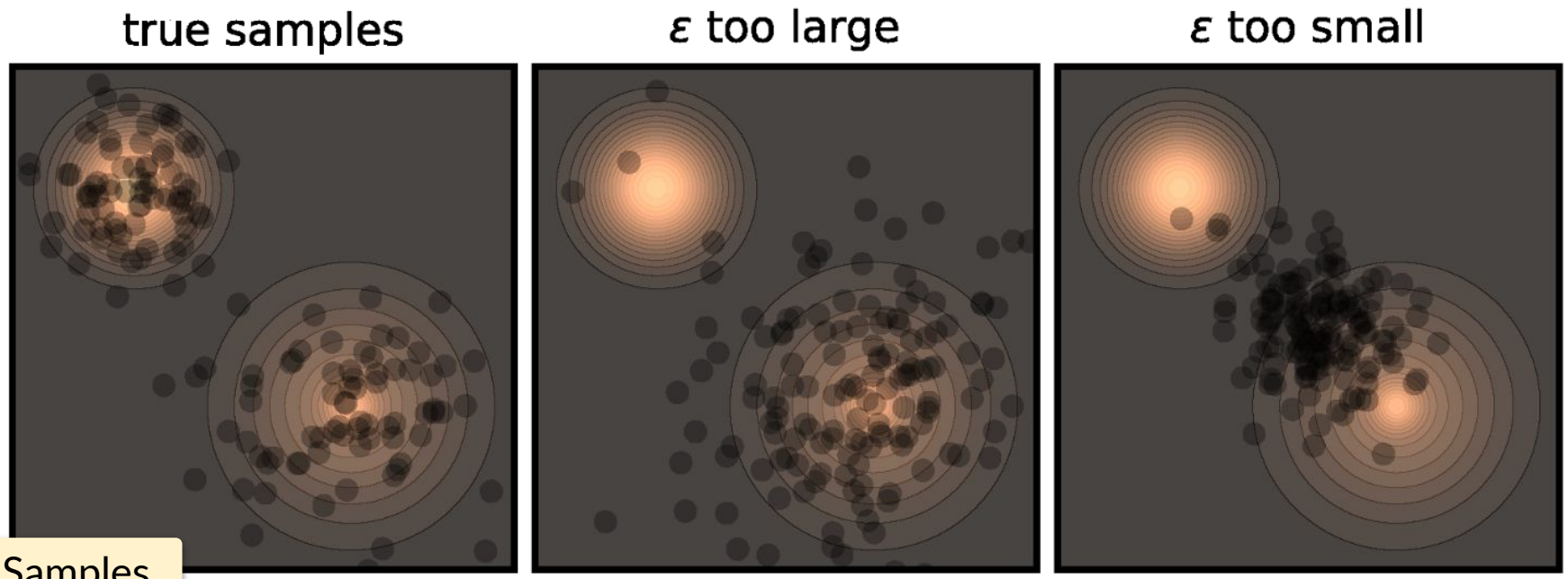

True Samples

Source: Roy Friedman, "A Simplified Overview of Langevin Dynamics"

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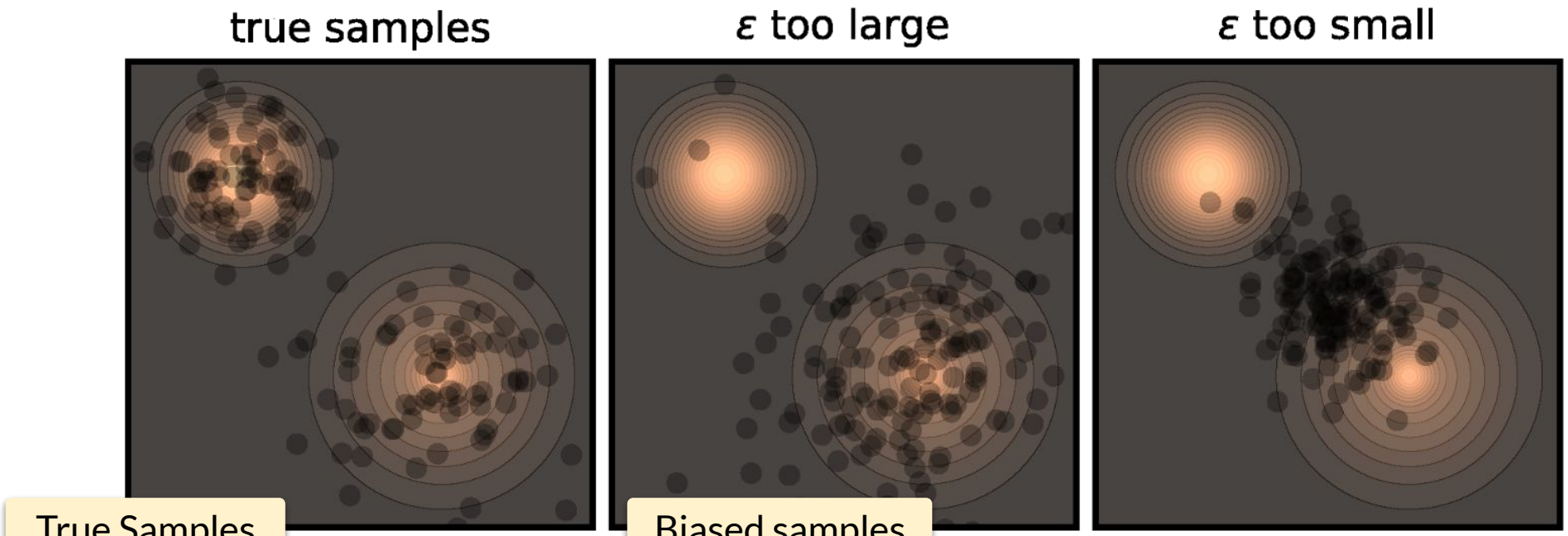

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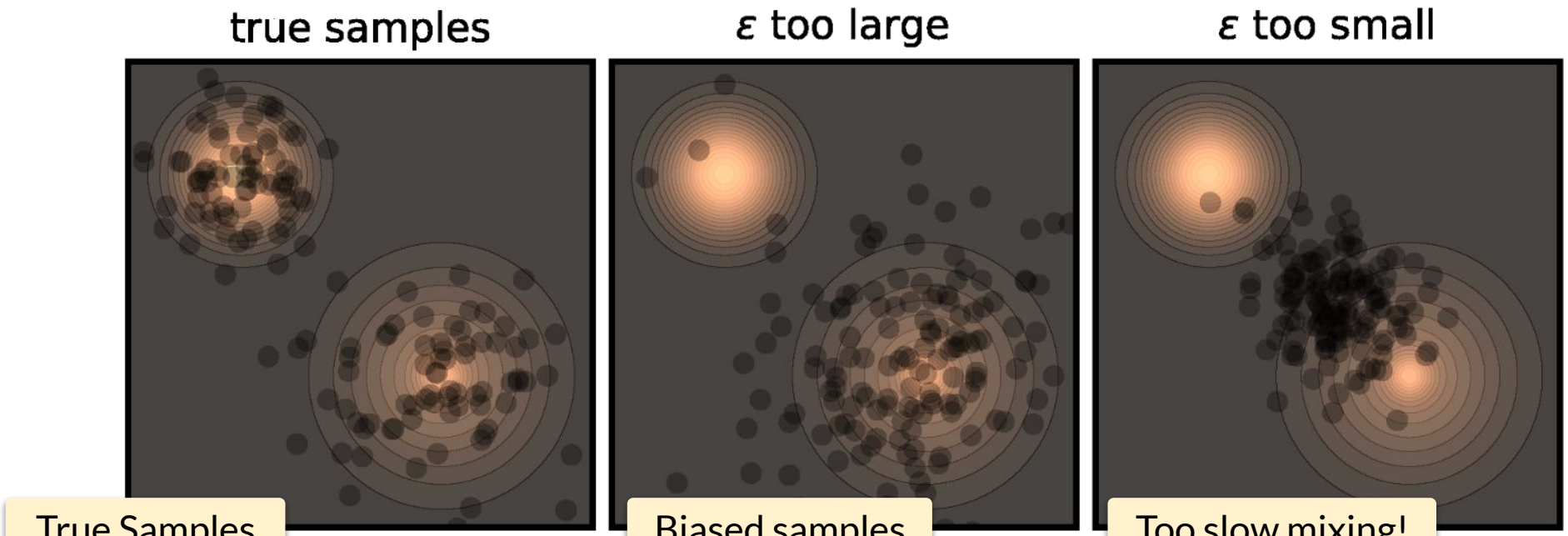

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In particular:

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- Then accept/reject as you would typically do in Metropolis-Hasting.
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Note: this is often called MALA - Metropolis adjusted Langevin algorithm.

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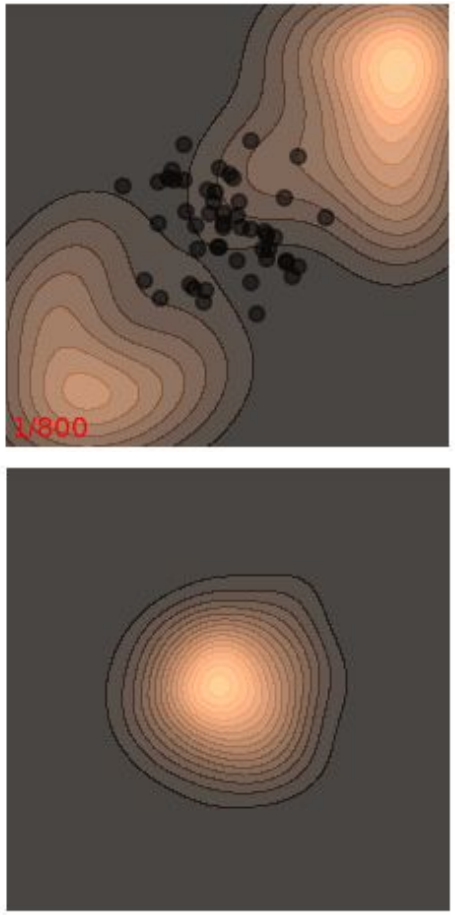

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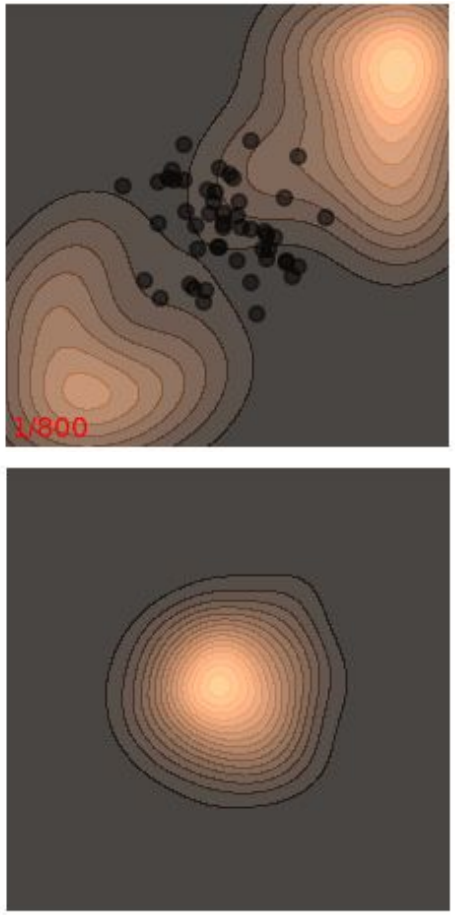
We will see that this strategy is used in variants of diffusion models, such as score-based generative models.



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- (And then still use Metropolis-Hastings to accept/or reject final proposal).
- ⇒ The potential for: even better mixing, and good acceptance rate, correct samples.

Gradient Based MCMC — Hamiltonian Monte Carlo (HMC)

HMC **Intuition** (high level):

Gradient Based MCMC — Hamiltonian Monte Carlo (HMC)

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The goal of MCMC is to yield samples for Monte Carlo expectations of the form:

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Monte Carlo estimate, given samples

Gradient Based MCMC — Hamiltonian Monte Carlo (HMC)

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Gradient Based MCMC — Hamiltonian Monte Carlo (HMC)

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$$\mathbb{E}_{p(x)}\left[g(x)\right] = \int p(x)g(x)dx = \int p(x,v)g(x)dx\,dv$$

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Monte Carlo estimate (only uses x samples!)

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In HMC, we define auxiliary variables such that (roughly speaking)...

You can write out the joint PDF in terms of a *Hamiltonian* (from physics/mechanics):

$$
\begin{aligned}
p(x, v) \propto p(x)p(v) &= e^{\log p(x)} e^{-\frac{1}{2}v^\top v} \\
&= e^{-E(x)} e^{-K(v)} \\
&= e^{-E(x)-K(v)} \\
&= e^{-H(x,v)}
\end{aligned}
$$

Auxiliary variable v is typically Gaussian, is independent from x, and is viewed as *momentum*.

We call H the *Hamiltonian*

Gradient Based MCMC — Hamiltonian Monte Carlo (HMC)

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⇒ Then you can simulate *Hamiltonian Dynamics*.

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⇒ Then you can simulate *Hamiltonian Dynamics*.

⇒ (*i.e.*, solve a differential equation to preserve the Hamiltonian energy…equivalent to keeping the same PDF value under the joint model $p(x, v)$.)

⇒ In practice: iteratively update x and v according to some update rules… *e.g.*:

Called the *leapfrog method*.

$$v \leftarrow v + \frac{\epsilon}{2}\nabla_x \log p(x)$$
$$x \leftarrow x + \epsilon v$$
$$v \leftarrow v + \frac{\epsilon}{2}\nabla_x \log p(x)$$

Not a perfect solution to Hamiltonian dynamics (a numerical approximation).

Gradient Based MCMC — Hamiltonian Monte Carlo (HMC)

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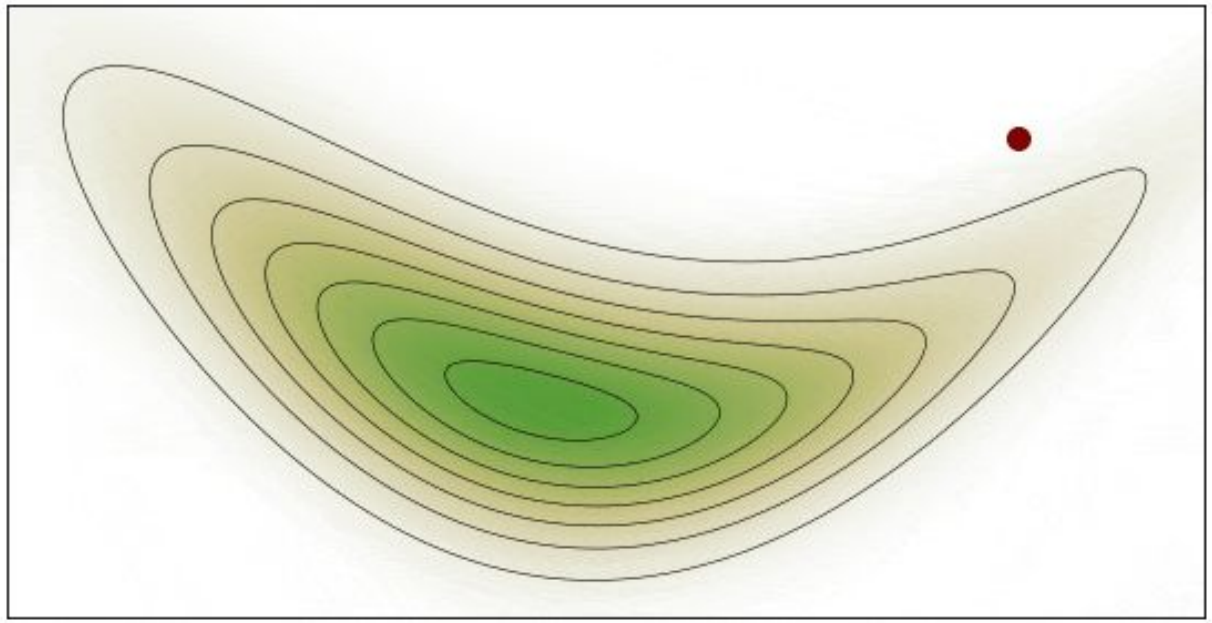
- Then you simulate Hamiltonian dynamics from this new point.
  - Following updates on previous slide → yields an updated (x, v) with similar PDF value.
- Then you do an accept/reject step (Metropolis-Hastings) to convert this into a valid MCMC algorithm (asymptotically exact samples).

Gradient Based MCMC

Animation:

HMC in practice!



MCMC Demo Website

Check out this MCMC Demo by Chi Feng

- https://chi-feng.github.io/mcmc-demo/app.html
- https://github.com/chi-feng/mcmc-demo

Variational Inference

Variational Inference — Overview

To begin, a few potential shortcomings of sampling-based approximate inference:

1. Although they are guaranteed to perform *correct inference* given enough time, it is difficult to tell the *approximation quality* after running for a finite amount of time.

2. MCMC methods may require choosing an appropriate proposal distribution (or various hyperparameters). This choice can be difficult.

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Variational Inference — Overview

Instead, we could take the strategy/philosophy of *inference as optimization*.

This method of approximate inference is known as **variational inference (VI)**.

The main idea:

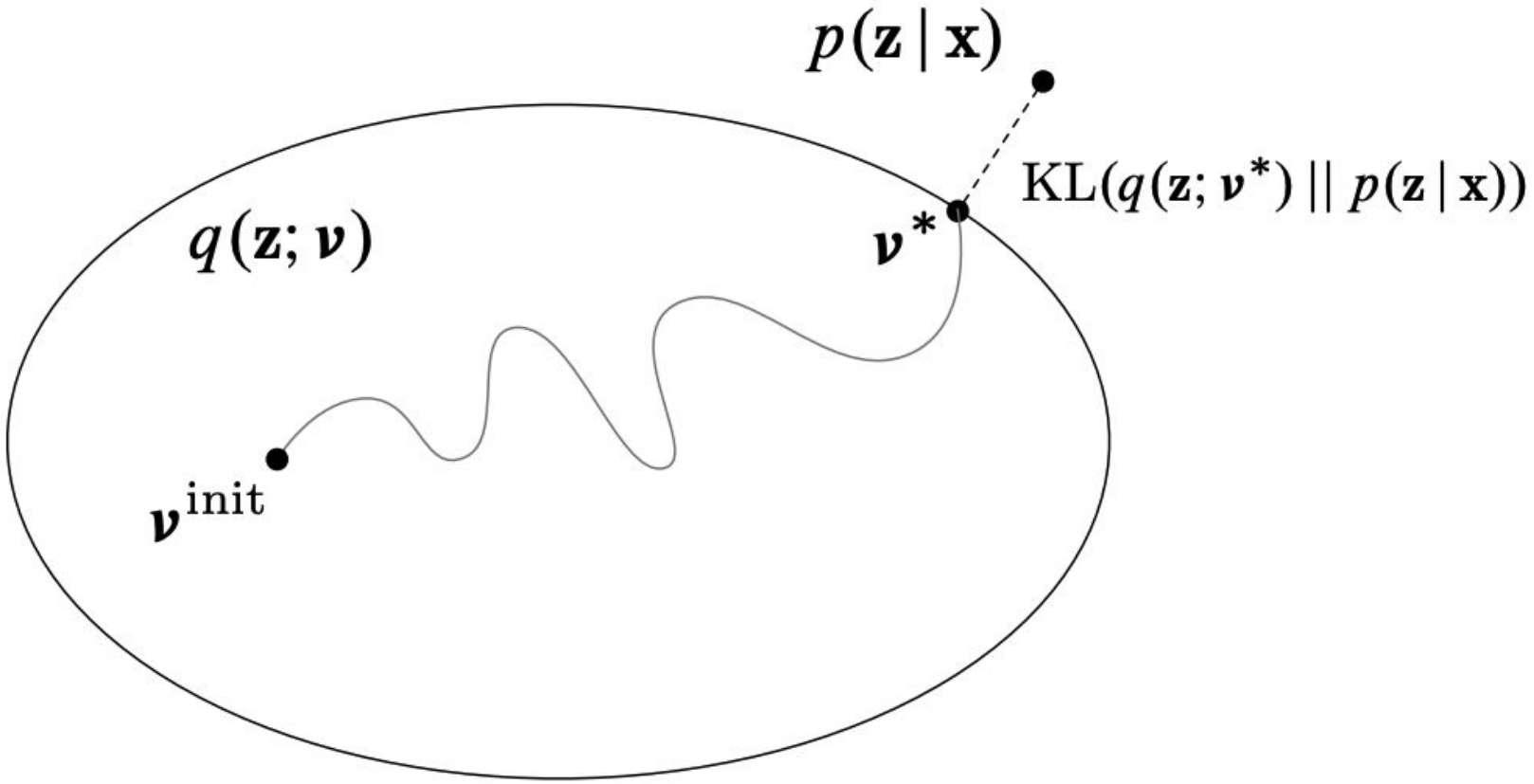
- Suppose we are given an intractable (*complex*) probability distribution $p(x)$.
- VI aims to solve an optimization problem over a set of tractable distributions Q.
- And, after optimization, return a $q(x) \in Q$ that is *most similar* to $p(x)$.
- We can then make an inference query on $q(x)$ instead of $p(x)$.c

Typically: in terms of KL divergence

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Variational Inference — Overview

From Dave Blei's Variational Inference Tutorial:



Source: Dave Blei, "Variational Inference"

Variational Inference — Overview

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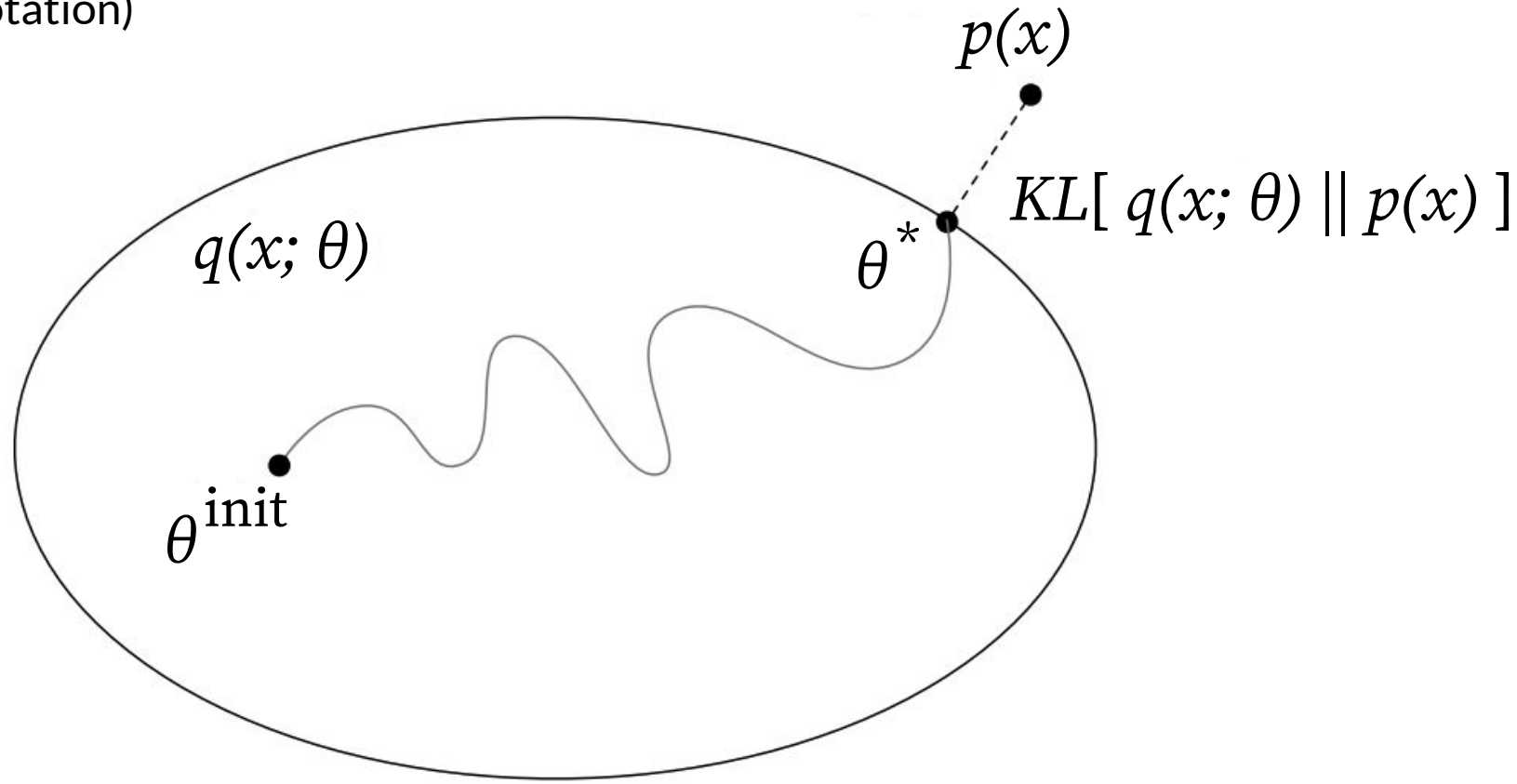
(replaced with our notation)



Source: Dave Blei, "Variational Inference"

Variational Inference — Overview

Main differences with sampling/MCMC methods:

- Unlike sampling, variational methods will almost never find the exact/globally optimal solution (even in the limit as $T \to \infty$).
- However, it is easy to determine if they have converged (at least to a local optima).
- In practice, variational inference methods often scale better.
- ⇒ Amenable to techniques like stochastic gradient optimization, parallelization over multiple processors, and acceleration using GPUs.
    - (While it's easier for VI, this is also a popular field of study for MCMC).

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Kullback-Leibler Divergence

Quick background on Kullback-Leibler (KL) Divergence.

To optimize for an optimal approximation $q(x)$, we must choose an approximating family Q, and an objective $J(q)$.

The objective should capture the similarity between $q(x)$ and $p(x)$.

The field of information theory provides a tool: **Kullback-Leibler (KL) divergence**.

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Kullback-Leibler Divergence

More formally:

The KL divergence between distributions q and p with *discrete support* is:

$$\mathrm{KL}\left[q \parallel p\right] = \sum_{x} q(x) \log\left(\frac{q(x)}{p(x)}\right)$$

And the KL divergence between distributions q and p with *continuous support* is:

$$\mathrm{KL}\left[q \parallel p\right] = \int_{x \in \mathcal{X}} q(x) \log\left(\frac{q(x)}{p(x)}\right) dx$$

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

Kullback-Leibler Divergence

The KL divergence has a couple of properties that make it useful in this setting:

- $\mathrm{KL}\left[q \parallel p\right] \geq 0$ for all q, p.
- $\mathrm{KL}\left[q \parallel p\right] = 0$ if and only if $q = p$.

Importantly, note that $\mathrm{KL}\left[q \parallel p\right] \neq \mathrm{KL}\left[p \parallel q\right]$.

⇒ *i.e.*, KL divergence is **not symmetric**.

⇒ (this is why we say that it is a “divergence” and not a “distance”).

Source: Stefano Ermon, Probabilistic Graphical Models (CS228) Class

To be continued…

In the next lecture!

Paper Presentations

Paper Presentations — Goal

- During the semester, each student gives **one 20-minute presentation** on a paper relevant to probabilistic and generative models.
- Ideally from a modern machine learning conference (e.g., NeurIPS, ICML, ICLR, AAAI, etc)
  - Could be a “classic” (older) paper relevant to modern models, as well.
- This will accomplish a few things:
  - Gives the class a chance to see a broad set of interesting probabilistic/generative modeling papers.
  - Gives each student (more) experience with distilling key content from a paper & presenting it.

Paper Presentations — Schedule

Starting at the **end of February** we will go through a few (~4) presentations per class (2nd half of class).

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In the spreadsheet, which I will share, students will sign up for a time slot during the semester.

To make it fair, students who sign up for presentations on the first two dates will get slightly more-lenient grading (a point of extra credit on this assignment).

A	B	C	D	E	F	G	H
Date	Presentation ID	Presenter Name **(sign up!)**	Paper Title	Link/url to paper	Discussion Lead 1 **(sign up!)**	Discussion Lead 2 **(sign up!)**	Scribe **(sign up!)**
February 28							
	1						
	2						
	3						
	4						
March 7							
	5						

In-Class Participation and Discussion

There is a grade for in-class participation/discussion (during student presentations).
Students will sign up for one of three roles (again in the spreadsheet).
Each student has to do each role once during semester.

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Roles 1 and 2 — Discussion Leads

- Read the paper before the class; Responsible for formulating a short list (~5 questions) for discussion; bring up a couple of these during class; submit all after class.

Role 3 — Scribe

- Read the paper before the class; take notes on paper during presentation; write up a ~1 page summary of the presentation.