Inference and Representation
Lecture 6

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Lecture 6 Objectives

- Gaussian Mixture Models
- The Expectation-Maximization Algorithm
- Markov-Chain Monte-Carlo (MCMC)

Gaussian Mixture Models (GMM)

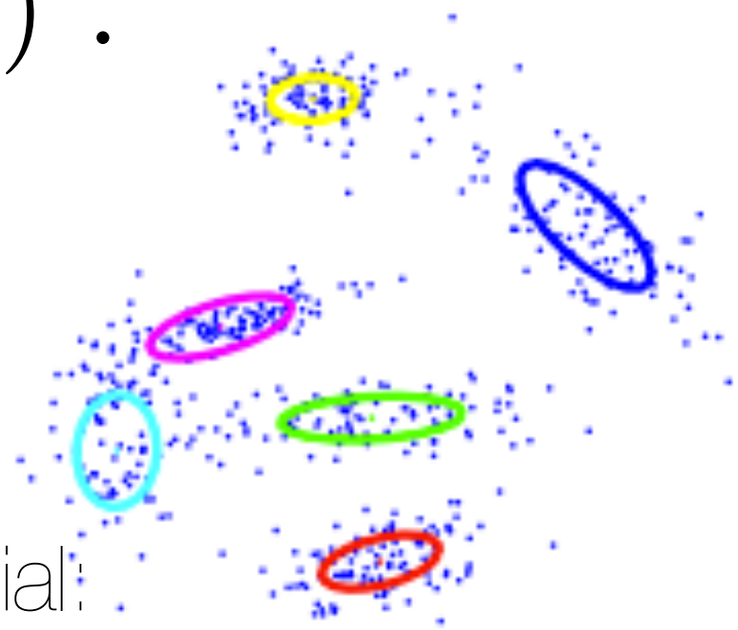
- A generalization of K-Means is given by a Gaussian Mixture:

$$k \sim \mathbf{Mult}(\pi) \ , \ x \sim \mathcal{N}(\mu_k, \Sigma_k) \ .$$

- This is also a discrete latent variable model:

$$z \in \{0,1\}^K \ , \ \sum_k z_k = 1 \ .$$

- The distribution of the latent variable is multinomial:



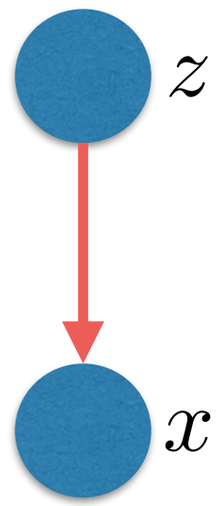
(figure from R.Salakhutdinov)

$$p(z_k = 1) = \pi_k \ , \ 0 \leq \pi_k \leq 1 \ , \ \sum_k \pi_k = 1 \ .$$

Gaussian Mixture Models (GMM)

- We can write

$$p(z) = \prod_{k=1}^{K} \pi_k^{z_k} \qquad p(x \mid z_k = 1) = \mathcal{N}(x; \mu_k, \Sigma_k)$$



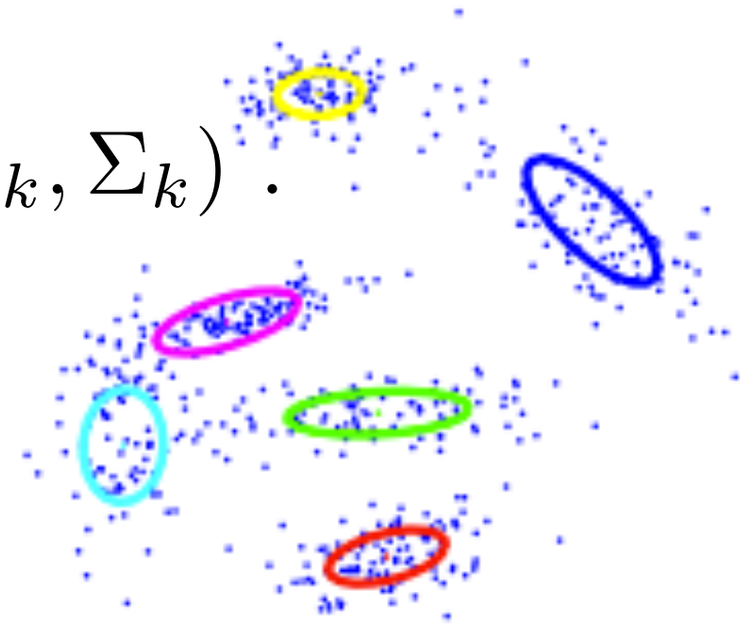
- Thus

$$p(x \mid z) = \prod_{k=1}^{K} \mathcal{N}(x; \mu_k, \Sigma_k)^{z_k}$$

- Joint and marginal distributions are given by

$$p(x, z) = p(x \mid z)p(z) \ ,$$

$$p(x) = \sum_z p(x, z) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x; \mu_k, \Sigma_k) \ .$$



GMM and Posterior Inference

- What about the conditional p(z | x) ? Ie, given data, which mixture components are "responsible" ?

$$p(z_k = 1 \mid x) = \frac{p(z_k = 1, x)}{\sum_{k' \leq K} p(z_{k'} = 1, x)} = \frac{p(z_k = 1)p(x \mid z_k = 1)}{\sum_{k' \leq K} p(z_{k'} = 1)p(x \mid z_{k'} = 1)}$$

$$= \frac{\pi_k \mathcal{N}(x; \mu_k, \Sigma_k)}{\sum_{k'} \pi_{k'} \mathcal{N}(x; \mu_{k'}, \Sigma_{k'})}$$

- The posterior probability that $z_k = 1$ is a weighted average of prior probabilities that depends upon the data.
- Q: How to estimate the parameters $\{\pi, \mu, \Sigma\}$?

Maximum Likelihood Estimation

- Given independent samples $X = \{x_1, \ldots, x_n\}$, the total log-likelihood is

$$E(\pi, \mu, \Sigma) = \log p(X \mid \pi, \mu, \Sigma) = \sum_{i \leq n} \log \left(\sum_k \pi_k \mathcal{N}(x_i; \mu_k, \Sigma_k) \right)$$

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- $$\frac{\partial E}{\partial \mu_k} = \sum_i \frac{\pi_k \mathcal{N}(x_i; \mu_k, \Sigma_k)}{\sum_{k'} \pi_{k'} \mathcal{N}(x_i; \mu_{k'}, \Sigma_{k'})} \Sigma_k^{-1}(x_i - \mu_k) \ .$$

- $$\mu_k = \frac{1}{N_k} \sum_i p(z_{i,k} = 1 \mid x_i) x_i \ , \ N_k = \sum_i p(z_{i,k} = 1 \mid x_i) \ .$$

Thus the mean μ_k is the weighted average of datapoints, with weights given by the posterior probabilities of belonging to component k.

Maximum Likelihood Estimation

- Similarly

$$\frac{\partial E}{\partial \Sigma_k} = 0 \;\Rightarrow\; \Sigma_k = \frac{1}{N_k} \sum_i p(z_{i,k} = 1 \mid x_i)(x_i - \mu_k)(x_i - \mu_k)^T \;.$$

$$\frac{\partial E}{\partial \pi_k} = 0 \;\Rightarrow\; \pi_k = \frac{N_k}{n} \;.$$

- MLE parameters do not have closed-form solution
  - Parameters depend upon posterior probabilities $p(z_k = 1 \mid x)$, which themselves depend upon parameters.
- Iterative algorithm: Expectation-Maximization (EM):
  - E-step: Update posterior probabilities with parameters fixed.
  - M-step: Update parameters with posterior probabilities fixed.

The EM algorithm

- It is designed to find MLE solutions of latent variable models.
- In general, we have log-likelihoods of the form

$$\log p(X \mid \theta) = \log \left(\sum_{Z} p(X, Z \mid \theta) \right) \quad , \quad \begin{array}{l} \theta = \text{model parameters} \ . \\ Z = \text{latent variables} \end{array}$$

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$$Z = \text{latent variables}$$

- Using current parameters θ_{old}, we compute the expected total likelihood of the model (E-step):

$$\mathcal{Q}(\theta, \theta_{old}) = \mathbb{E}_{Z \sim p(Z \mid X, \theta_{old})} \log p(X, Z \mid \theta)$$

- Then we update the parameters to maximize this likelihood:

$$\theta_{new} = \arg\max_{\theta} Q(\theta, \theta_{old}) \ .$$

EM and Variational Bound

- Q: Does this algorithm monotonically improve the likelihood?
- Assume for now that latent variables are discrete.

EM and Variational Bound

- Q: Does this algorithm monotonically improve the likelihood?
- Assume for now that latent variables are discrete.
- For any distribution $q(Z)$over latent variables, we have

$$\log p(X \mid \theta) = \log \left(\sum_Z p(X, Z \mid \theta) \right) = \log \left(\sum_Z q(Z) \frac{p(X, Z \mid \theta)}{q(Z)} \right)$$

$$\geq \sum_Z q(Z) \log \left(\frac{p(X, Z \mid \theta)}{q(Z)} \right) = \mathcal{L}(q, \theta) \ .$$

(Jensen's Inequality: $\mathbb{E}(f(X)) \geq f(\mathbb{E}(X))$ if f is convex)

Variational Bound

- We can express the variational lower bound as

$$\begin{aligned}\mathcal{L}(q, \theta) &= \mathbb{E}_{q(Z)} \left[\log p(X, Z \mid \theta)\right] - \mathbb{E}_{q(Z)} \log q(Z) \\ &= \mathbb{E}_{q(Z)} \left[\log p(X, Z \mid \theta)\right] + H(q) \ .\end{aligned}$$

$$H(q) \text{: Entropy of } q(Z).$$

- Also, we have

$$\log p(X \mid \theta) = \mathcal{L}(q, \theta) + KL(q(z)||p(z \mid x, \theta)) \ , \text{ where}$$

$$KL(q||p) = -\sum_z q(z) \log \left(\frac{p(z)}{q(z)}\right)$$

is the Kullback-Leibler divergence.

Variational Bound

- Thus, the divergence $KL(q||p)$ measures how far our variational approximation $q(z)$ is from the true posterior, and directly controls the bound on the log-likelihood.

- Using
$$\log p(X \mid \theta) = \mathcal{L}(q, \theta) + KL(q(z)||p(z \mid x, \theta))$$

- E-step: maximize lower bound $\mathcal{L}(q, \theta)$ with respect to *q*, holding parameters fixed.
- M-step: maximize lower bound $\mathcal{L}(q, \theta)$ with respect to parameters, holding *q* fixed.

Correctness of EM

- Suppose current parameter value is $\theta^{(n)}$.
- Consider the variational bound by picking $q(z) = p(z|x, \theta^{(n)})$:

$$\log p(X|\theta) - \log p(X|\theta^{(n)}) \geq \mathcal{L}(p(z|x, \theta^{(n)}), \theta) - \log p(X|\theta^{(n)})$$

$$= \sum_z p(z|x, \theta^{(n)}) \log \left(\frac{p(x|z, \theta)p(z|\theta)}{p(z|x, \theta^{(n)})p(x|\theta^{(n)}} \right)$$

$$= \Delta(\theta|\theta^{(n)}).$$

with $\Delta(\theta^{(n)}|\theta^{(n)}) = 0$.

Correctness of EM

- Thus $$\theta^{(n+1)} = \arg\max_{\theta} \Delta(\theta|\theta^{(n)})$$

$$\begin{aligned}
\theta^{(n+1)} &= \arg\max_{\theta} \Delta(\theta|\theta^{(n)}) \\
&= \arg\max_{\theta} \sum_{z} p(z|x,\theta^{(n)}) \log\{(p(x|z,\theta)p(z|\theta)\} \\
&= \arg\max_{\theta} \sum_{z} p(z|x,\theta^{(n)}) \log\{(p(x,z|\theta)\}\} \\
&= \arg\max_{\theta} \mathbb{E}_{z\sim p(z|x,\theta^{(n)})} \log p(X,Z|\theta) \ .
\end{aligned}$$

Approximate Inference

- We will see two major approximate inference paradigms:
  - Variational Inference (next lectures)
  - Markov-Chain Monte-Carlo (now)

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- MCMC
  - the Metropolis-Hastings algorithm
  - revisiting Gibbs sampling
  - extensions (Langevin, HMC)
  - *Interlude:* assessing sample quality in MCMC with Stein's Method.

Approximate Inference via Sampling

- Suppose $p(x) = \frac{\tilde{p}(x)}{Z}$ and we only know $\tilde{p}(x)$.

- Q: How to infer properties of $p(x)$ **without knowing** Z?
  - e.g, marginal distributions

$$\bar{p}(x_1) = \int p(x) dx_2 \dots dx_n \ .$$

  - or more generally moments of the form

$$\mathbb{E}(\phi(X)) = \int \phi(x) p(x) dx \ , \ X \sim p(x)$$

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- **Monte-Carlo** approximation replaces integrals with sums over iid samples:

$$\mathbb{E}(\phi(X)) \approx \frac{1}{N} \sum_{i \leq N} \phi(X_i) \ , \ X_i \sim p \ .$$

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  - **Key property:** This is also (mostly) true even when samples are not independent!

Importance Sampling

- Suppose first we know $p(x)$ for all x, but we don't know how to sample, nor how to integrate under $p(x)$.
- Q: Can we approximate $$\mathbb{E}(f(X)) = \int p(x)f(x)dx$$

with samples from *another* distribution with density $q(x)$?

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- Q: Can we approximate

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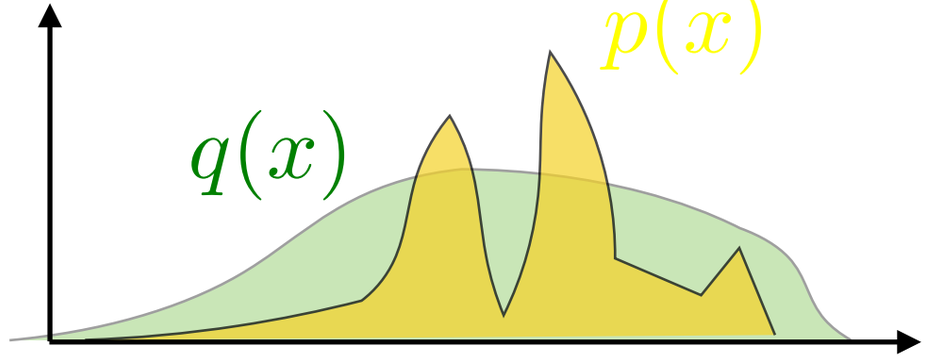
with samples from *another* distribution with density $q(x)$?

- Assume that $\text{Supp}(p) \subseteq \text{Supp}(q)$.



- Then

$$\int f(x)p(x)dx = \int f(x)\frac{p(x)}{q(x)}q(x)dx = \mathbb{E}_q(f(x)w(x)) \text{ , where}$$

$$w(x) = \frac{p(x)}{q(x)} \text{ .}$$

Importance Sampling

- So we can estimate the integral as

$$\widehat{\mathbb{E}(f(x))} = \frac{1}{N} \sum_{i \leq N} f(x^{(i)}) w(x^{(i)}) \ , \ x^{(i)} \sim q \ .$$

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- Q: How good is this estimator?

Unbiased: $\mathbb{E}_q \left\{ \widehat{\mathbb{E}_p(f(x))} \right\} = \mathbb{E}_p\{f(x)\}.$

$\mathbf{var}_q \{f(x)w(x)\} = \mathbb{E}_q\{f^2(x)w^2(x)\} - \mathbb{E}_p\{f(x)\}^2 \ .$

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- We can consider the proposal q(x) that minimizes the variance:

$$\mathbb{E}_q\{f^2(x)w^2(x)\} \geq (\mathbb{E}_q|f(x)|w(x)|)^2 = \left(\int |f(x)|p(x)dx \right)^2 \ ,$$

which is attained if $q(x) = \frac{|f(x)|p(x)}{\int |f(x)|p(x)dx}$

Importance Sampling

- Remarks:
  - In general, it is not possible to sample from optimal $q(x)$.
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$$\left(p(x) = \frac{\tilde{p}(x)}{Z} \right)$$

We have $$\mathbb{E}_p\{f(x)\} = \frac{\int f(x)w(x)q(x)dx}{\int w(x)q(x)dx} \ , \text{ with } w(x) = \frac{\tilde{p}(x)}{q(x)} \ .$$

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$$\left(p(x) = \frac{\tilde{p}(x)}{Z} \right)$$

We have $\mathbb{E}_p\{f(x)\} = \dfrac{\int f(x)w(x)q(x)dx}{\int w(x)q(x)dx}$, with $w(x) = \dfrac{\tilde{p}(x)}{q(x)}$.

So now we can estimate both numerator and denominator:

$$\widehat{\mathbb{E}_p\{f(x)\}} = \frac{\sum_{i \leq N} f(x^{(i)})w(x^{(i)})}{\sum_{i \leq N} w(x^{(i)})} = \sum_{i \leq N} f(x^{(i)})\tilde{w}(x^{(i)}) \ ,$$

$\tilde{w}(x^{(i)}) = \dfrac{w(x^{(i)})}{\sum_{j \leq N} w(x^{(j)})}$: normalized importance weights.

Limitations of Importance Sampling

- The efficiency of importance sampling relies on how well we can approximate the *typical set* of $p(x)$:

$$\Lambda(p) = \{x \in \Omega \; ; \log p(x) \approx \mathbb{E}\{\log p(X)\}\} \; .$$

- As the dimensionality of Ω increases, capturing the typical set becomes intractable.

- In some sense, importance sampling is too rigid: the proposal sampling distribution $q(x)$ cannot fit generic complicated densities efficiently.

- Therefore, we need a more powerful, adaptive tool to capture the typical samples of $p(x)$, that can extend to high-dimensional densities.

Markov-Chain Monte-Carlo (MCMC)

- Recall the challenge: produce nearly independent samples of $p(x)$ without knowing the partition function Z in $p(x) = \frac{\tilde{p}(x)}{Z}$

- Idea: instead of *explicitly* characterizing $p(x)$, we turn to a powerful *implicit* characterization: $p(x)$ as the limit of a Markov diffusion process.

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- As we will see, we can construct such Markov Chain without knowing Z!

Markov-Chain Monte-Carlo (MCMC)

- Recall the challenge: produce nearly independent samples of $p(x)$ without knowing the partition function Z in $p(x) = \frac{\tilde{p}(x)}{Z}$

- As it turns out, we can design a Markov Chain whose stationary distribution is $p(x)$ without knowing Z.

- Q: How does that solve our problem?
  1. Run the Markov chain from an arbitrary initial point x_0
  2. After enough iterations, the resulting point will be a sample of $p(x)$

- So:
  - How to design the chain?
  - How many steps are needed?

Markov Chains flash review

- We consider:

  A state-space Ω (discrete or continuous)

  A *stochastic* kernel P that updates the densities at each time step:

$$q^{(t+1)}(u) = \int_{\Omega} P(u,v) q^{(t)}(v) dv \ .$$

$$P(u,v) \geq 0 \ , \ \int P(u,v) dv = 1 \ , \ \forall \ u \in \Omega \ .$$

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called stochastic matrix

- In a discrete state space, the kernel can be viewed as a matrix, and

$$P(k,l) = \text{Probability to transition from state } k \text{ to state } l.$$

Markov-Chains Flash Review

Definition: A Markov Chain is irreducible if
$Pr($ visit state u from state $v) > 0$ for all u, $v \in \Omega$.

Definition: A Markov Chain is aperiodic if there exists $n > 0$ such that $Pr(X_{n'} = i \mid X_0 = i) > 0$ for all $n' \geq n$. $\forall\ i$

Definition: A stationary distribution π of a Markov Chain P is such that $\pi = P\pi$.

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Theorem: [**Perron-Frobenius**] An irreducible aperiodic Markov Chain P admits a unique stationary distribution.

Remark: The stationary distribution(s) correspond to eigenvectors of P of leading eigenvalue $(= 1)$.

Metropolis-Hastings Algorithm

Definition: A Markov Chain P is reversible with respect to π if

$$\forall\ u, v \in \Omega\ ,\ \pi(u)P(v,u) = \pi(v)P(u,v)\,.$$

Fact: If P is reversible wrt π then π is a stationary for P.

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$$(P\pi)(u) = \sum_v P(u,v)\pi(v) = \sum_v \pi(u)P(v,u) = \pi(u)$$

- How to build a Markov Chain such that it is reversible wrt $p(x)$? without involving the partition function?

Metropolis-Hastings

- We start with a *proposal* Markov chain K such that
  - $\forall\ i \in \Omega\ ,\ K_{i,i} > 0\ ,$ and
  - $G = (\Omega, E(K))$ is connected, where i and j are connected if $K_{i,j} K_{j,i} > 0$.

(we can travel from any state to any other state in finite time using K).

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(we can travel from any state to any other state in finite time using K).

- Then we adapt it to $p(x)$ as follows:

$$R(x_j, x_i) = \min\left\{1, \frac{\tilde{p}(x_j)K(x_j, x_i)}{\tilde{p}(x_i)K(x_i, x_j)}\right\}\ ,$$

$$P(x_j, x_i) = K(x_j, x_i)R(x_j, x_i) + \delta(x_j - x_i)r(x_i),\ \text{with}$$

$$r(x_i) = \int_\Omega K(y, x_i)(1 - R(y, x_i))dy\ .$$

$$= \text{Probability to reject the update.}$$

Metropolis-Hastings

Fact: The kernel P is irreducible, aperiodic and satisfies the detailed balance condition wrt p.
Therefore p is the unique stationary distribution of P.

diagonal part ($\delta(x_i - x_j)r(x_i)$) can be ommited (why?)

Assume wlog $\tilde{p}(x_j)K(x_j, x_i) \geq \tilde{p}(x_i)K(x_i, x_j)$.
Then $R(x_j, x_i) = 1$ and

$$R(x_i, x_j) = \frac{\tilde{p}(x_i)K(x_i,x_j)}{\tilde{p}(x_j)K(x_j,x_i)} = \frac{p(x_i)K(x_i,x_j)}{p(x_j)K(x_j,x_i)}.$$

$$p(x_i)P(x_j, x_i) = p(x_i)K(x_j, x_i) = p(x_i)K(x_j, x_i)\frac{p(x_j)K(x_i, x_j)}{p(x_j)K(x_i, x_j)}$$

$$= \frac{p(x_i)K(x_j, x_i)}{p(x_j)K(x_i, x_j)}p(x_j)K(x_i, x_j)$$

$$= R(x_i, x_j)K(x_i, x_j)p(x_j) = p(x_j)P(x_i, x_j).$$

Irreducible by assumption on K.

(ex: Why is it aperiodic?)

Metropolis-Hastings

- Practical Implementation:
  1. Given current state x_i, propose next step by sampling $x_s \sim K(\cdot, x_i)$
  2. Compute $$R = \min\left(1, \frac{p(x_s)K(x_s, x_i)}{p(x_i)K(x_i, x_s)}\right) .$$
  3. Accept new state x_s with probability R and go to step 1.

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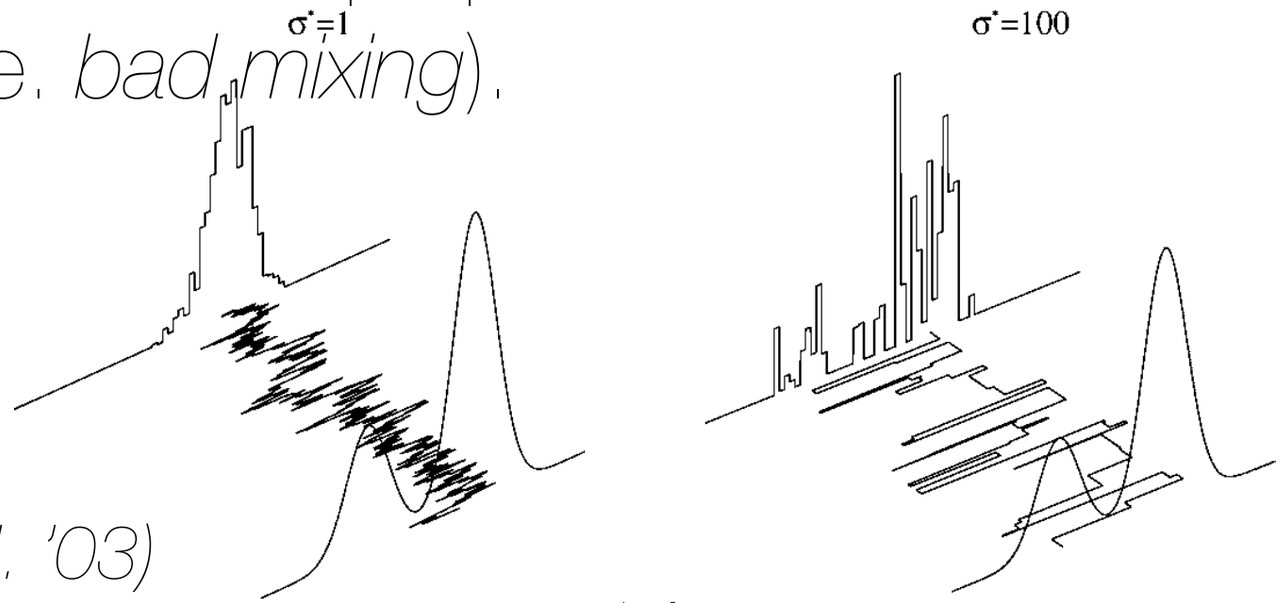
- Two important particular cases:
  - $K(x_j, x_i) = q(x_j)$ is independent of the current state.
    Acceptance probability becomes
    $$R(x_i, x_j) = \min\left(1, \frac{p(x_j)q(x_i)}{p(x_i)q(x_j)}\right) = \min\left(1, \frac{w(x_j)}{w(x_i)}\right) .$$
    - Similar to importance sampling, except that here samples are correlated (why?)
  - $K(x_j, x_i) = K(x_i, x_j)$ is symmetric.
    Acceptance probability becomes $R(x_i, x_j) = \min\left(1, \frac{p(x_j)}{p(x_i)}\right) .$
    - We always accept the sample as long as it "climbs" wrt the true density.

Metropolis-Hastings

- This algorithm *seems to be magic:* it only asks us to cover the target density with our proposal distribution!
- There is no "free lunch": a poor choice of proposal distribution results in bad approximations (i.e. *bad mixing*).



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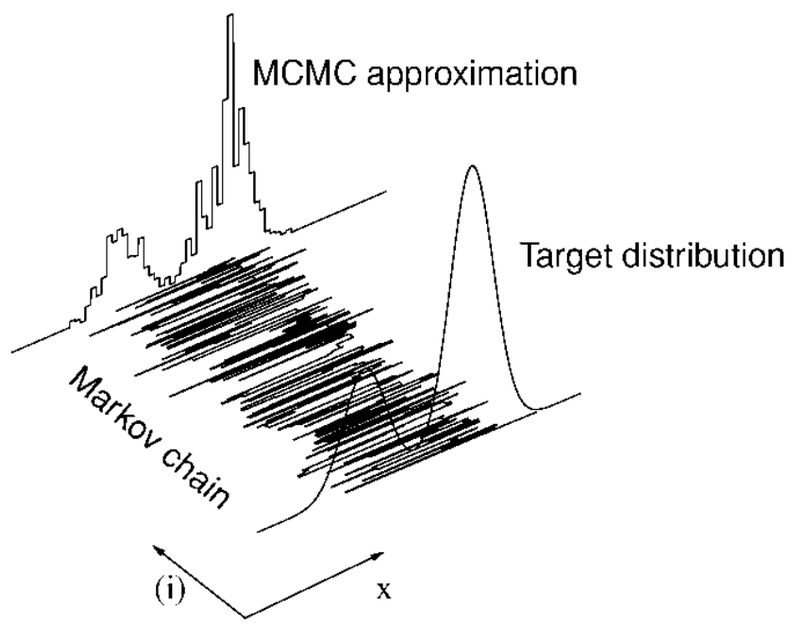

Metropolis-Hastings

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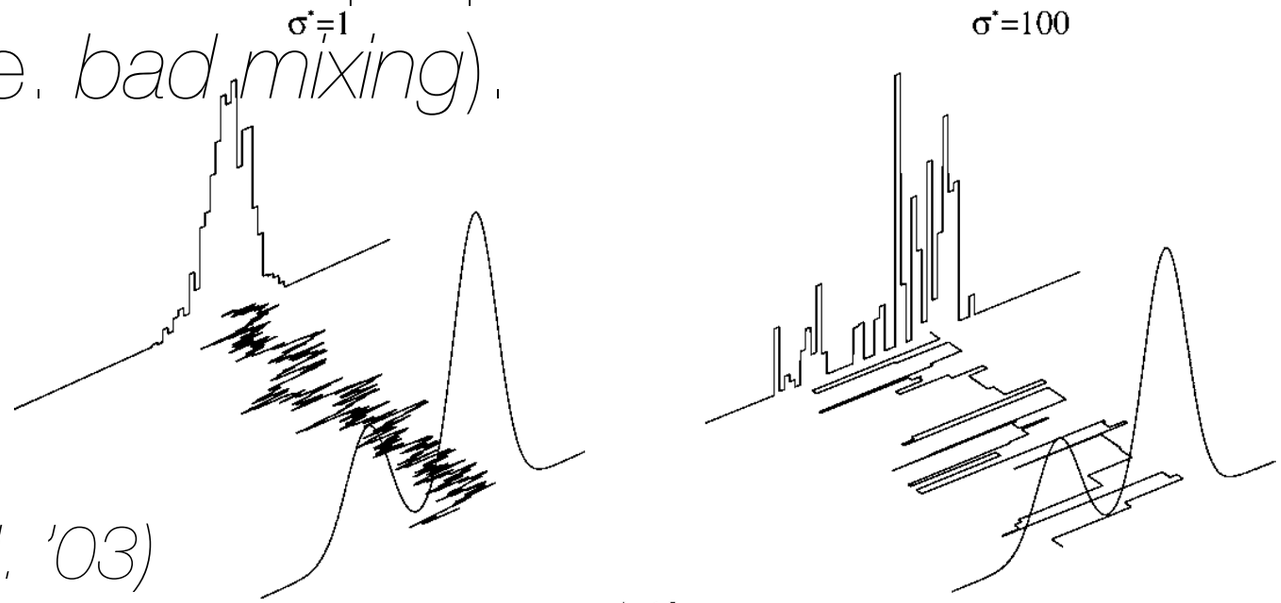

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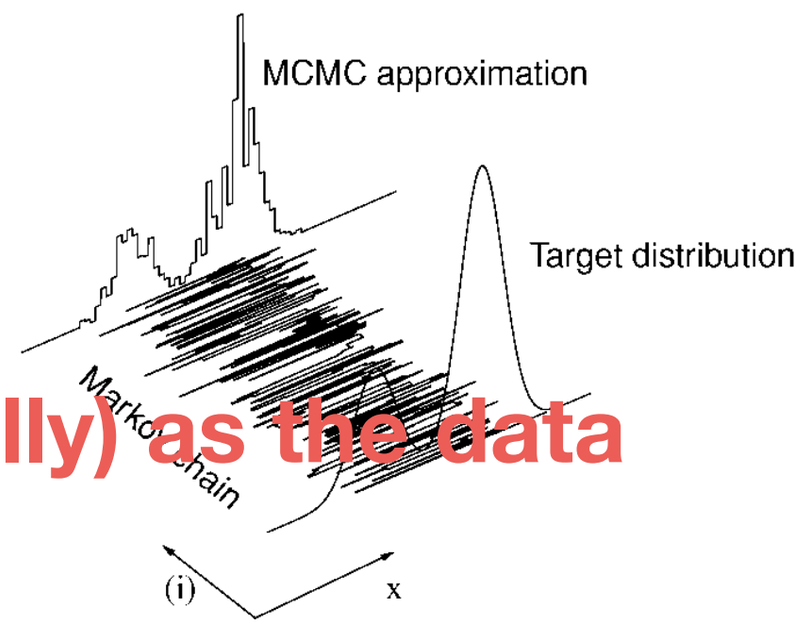

- **This danger increases (exponentially) as the data dimensionality increases.**

Revisiting Gibbs Sampling

- Recall the Gibbs sampling we saw in Lecture 3.

1. Select $k \in \{1, \ldots n\}$ from a uniform distribution.
2. Set $x_j^{(n+1)} = x_j^{(n)}$ for $j \neq k$.
3. Sample $x_k^{(n+1)}$ from $p(x_k \mid x_{-k}^{(n)})$.

- Q: Is this a "correct" algorithm? i.e, can we guarantee that samples from this algorithm come from *p(x)*?

- Consider $K(y, x) = \begin{cases} p(y_k \mid x_{-k}) & \text{if } y_{-k} = x_{-k} \\ 0 & \text{otherwise.} \end{cases}$

If $p(\cdot \mid x_{-k}) > 0$ then the resulting graph for K is connected

$\Rightarrow$ its resulting Markov Chain is irreducible and aperiodic.

- Does it satisfy detailed balance wrt *p(x)* ?

Revisiting Gibbs Sampling

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We need to show that $p(x)K(x', x) = p(x')K(x, x')$.
Suppose that $x \neq x'$ and they differ in exactly one position k.

$$\begin{aligned} p(x)K(x', x) &= n^{-1}p(x)p(x'_k|x_{-k}) \\ &= n^{-1}p(x_k|x_{-k})p(x_{-k})p(x'_k|x_{-k}) \\ &= n^{-1}p(x_k|x'_{-k})p(x'_{-k})p(x'_k|x'_{-k}) \\ &= p(x')K(x, x')\,. \end{aligned}$$

Therefore, here $K = P$ (we accept the sample with probability 1).

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  - Second largest eigenvalues can be bounded using the Cheeger bound:

$$\lambda_2 \leq 1 - \frac{\Phi^2}{2} \ , \text{where}$$

$$\Phi \text{ is the conductance of } P\text{:} \quad \min_{\Omega' \subset \Omega} \frac{\sum_{i \in \Omega', j \notin \Omega'} \pi_i P(i,j)}{\pi(\Omega')(1 - \pi(\Omega'))} \ .$$

Interlude: the Stein Method

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- The *Stein method* (70') is a powerful tool to control the distance between two probability distributions using a metric of the form

$$d(P, Q) = \sup_{h \in \mathcal{H}} \left| \mathbb{E}_{X \sim P} h(X) - \mathbb{E}_{Y \sim Q} h(Y) \right| ,$$

for a given family of functions $\mathcal{H} = \{h : \Omega \to \mathbb{R}\}$.

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for a given family of functions $\mathcal{H} = \{h : \Omega \to \mathbb{R}\}$.

- If we know Q, we know how its moments $E_{Y \sim} f(Q)$ behave for different f.

Stein's method reverses this: can we characterize
the distribution by finding functional relationships between moments?

Interlude: the Stein Method

Suppose that Q is fixed, known distribution.

We look for an operator $\mathcal{A}$ acting on functions $f : \Omega \to \mathbb{R}$ such that

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Ex: If Q is a standard normal $\mathcal{N}(0,1)$, we have

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Thus, if $P = Q$, then $\mathbb{E}_{X\sim P}\{(\mathcal{A}f)(X)\} = 0$ for all $f \in C^1$.

Hope: if $P \approx Q$, then $\mathbb{E}_{X\sim P}\{(\mathcal{A}f)(X)\} \approx 0$ for all $f \in C^1$.

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Two very important special cases:

- Gaussian Case: $(\mathcal{A}f)(x) = f'(x) - xf(x)$, with
$$f(x) = e^{x^2/2}\int_{-\infty}^{x}[h(s) - \mathbb{E}(h(Y))]e^{-s^2/2}ds.$$
- Markov case: $(\mathcal{A}f)(x) = \langle f(x), \nabla \log p(x)\rangle + (\mathrm{div} f)(x)$.

Crucial point: The Stein operator does not depend upon normalizing constant Z!

Evaluating sample quality

- Gorham and Mackey (NIPS'15) exploit the Stein operator to evaluate samples out of any MCMC algorithm.
  - Algorithm solves a linear program that bounds

$$\sup_{f \in \mathcal{H}} \sum_{i \leq n} (\langle f(x_i), \nabla \log p(x_i) \rangle + \operatorname{div} f(x_i)) \ .$$

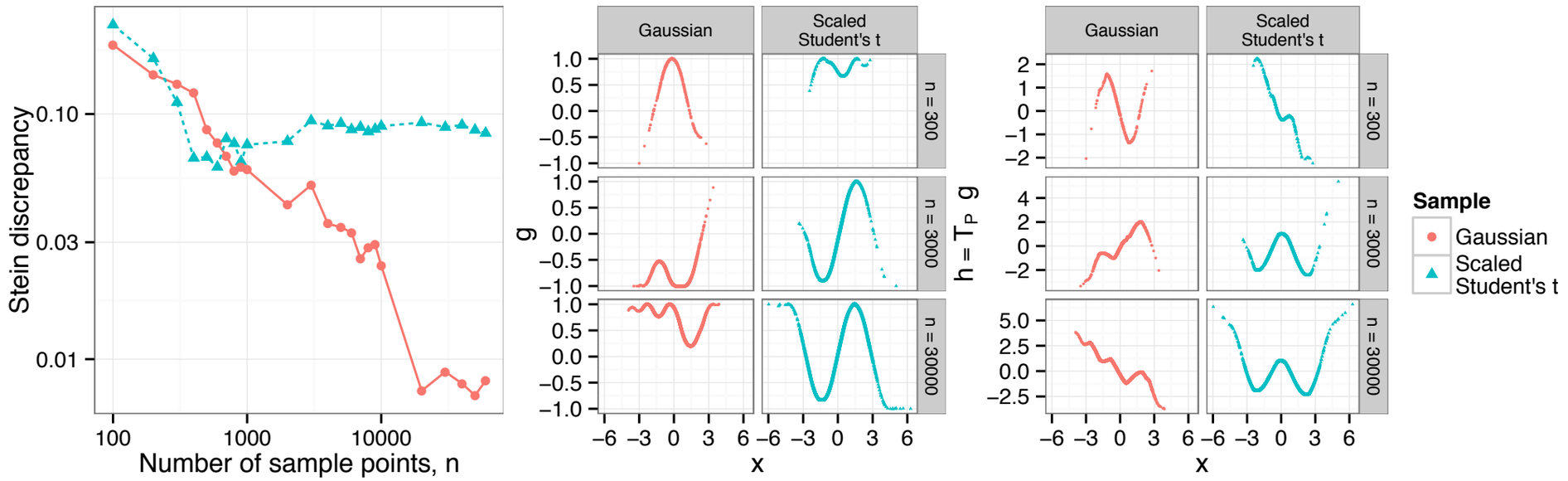

Figure 1: Left: Complete graph Stein discrepancy for a $\mathcal{N}(0, 1)$ target. Middle / right: Optimal Stein functions g and discriminating test functions $h = \mathcal{T}_P g$ recovered by the Stein program.

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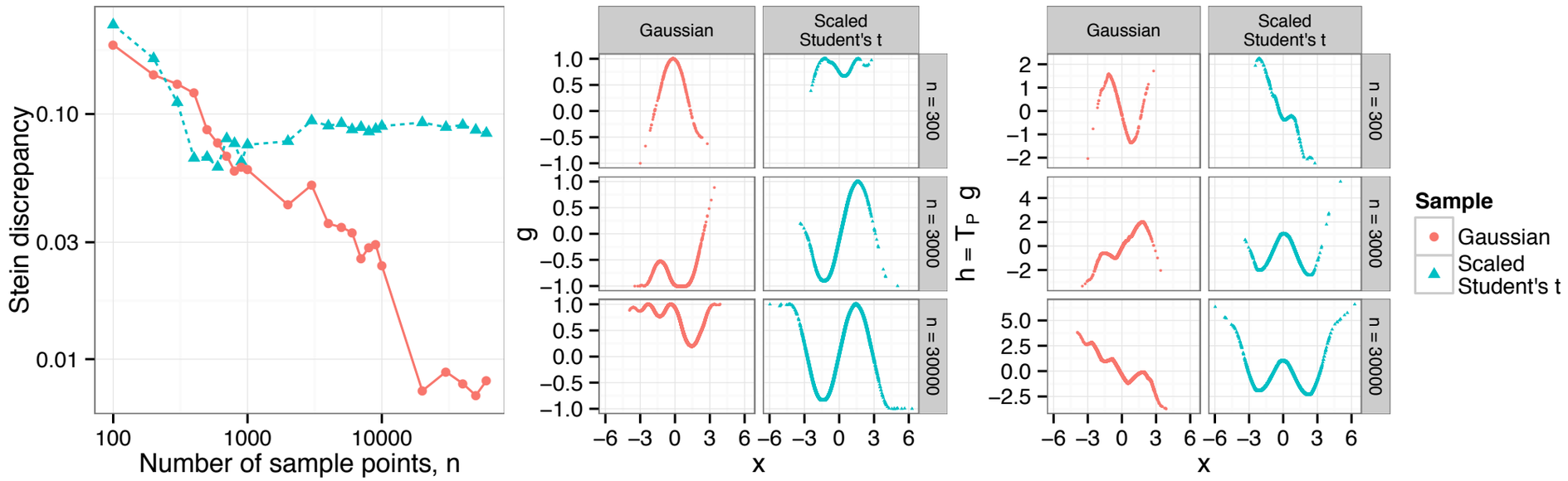

Figure 1: Left: Complete graph Stein discrepancy for a $\mathcal{N}(0, 1)$ target. Middle / right: Optimal Stein functions g and discriminating test functions $h = \mathcal{T}_P g$ recovered by the Stein program.

  - No assumption on the origin of the samples.
  - Similar to Maximum-Mean Discrepancy (MMD) but Stein's method operates under weaker assumptions and is more efficient.

MCMC Extensions

- Hamiltonian Monte-Carlo (HMC) [Duane et al.'87][Neal'11]

$$\text{Embeds a Gibbs distribution of the form } p(x) = \frac{e^{-T^{-1}U(x)}}{Z}$$

$$\text{into } p(x,y) = \frac{e^{-T^{-1}(U(x)+K(y))}}{Z} \;, \quad \begin{array}{l} x\text{: position} \\ y\text{: momentum} \end{array}$$

$$U(x)\text{: potential energy} \quad K(y)\text{: kinetic energy}$$

$$K(y) \propto \|y\|^2 \Rightarrow p(y|x) \text{ is Gaussian .}$$

- Langevin Dynamics.