Inference and Representation
Lecture 7

Joan Bruna
Courant Institute, NYU

Markov-Chain Monte-Carlo (MCMC)

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

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

Markov-Chain Monte-Carlo (MCMC)

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

- 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:

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

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

- 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 $n' \geq n$.

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

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 $n' \geq n$.

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

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

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

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

Metropolis-Hastings Algorithm

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

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

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

$$\int \pi(u)P(u,v)du = \int \pi(v)P(v,u)du = \pi(v)\ .$$

- 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).

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

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

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

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

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

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.

Assume wlog $\tilde{p}(x_j)K(x_j, x_i) \geq \tilde{p}(x_i)K(x_i, x_j)$.

Then $R(x_i, x_j) = 1$ and $R(x_j, x_i) = \frac{p(x_i)K(x_i,x_j)}{p(x_j)K(x_j,x_i)}$.

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

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

$$= p(x_j)P(x_j, x_i)$$

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.

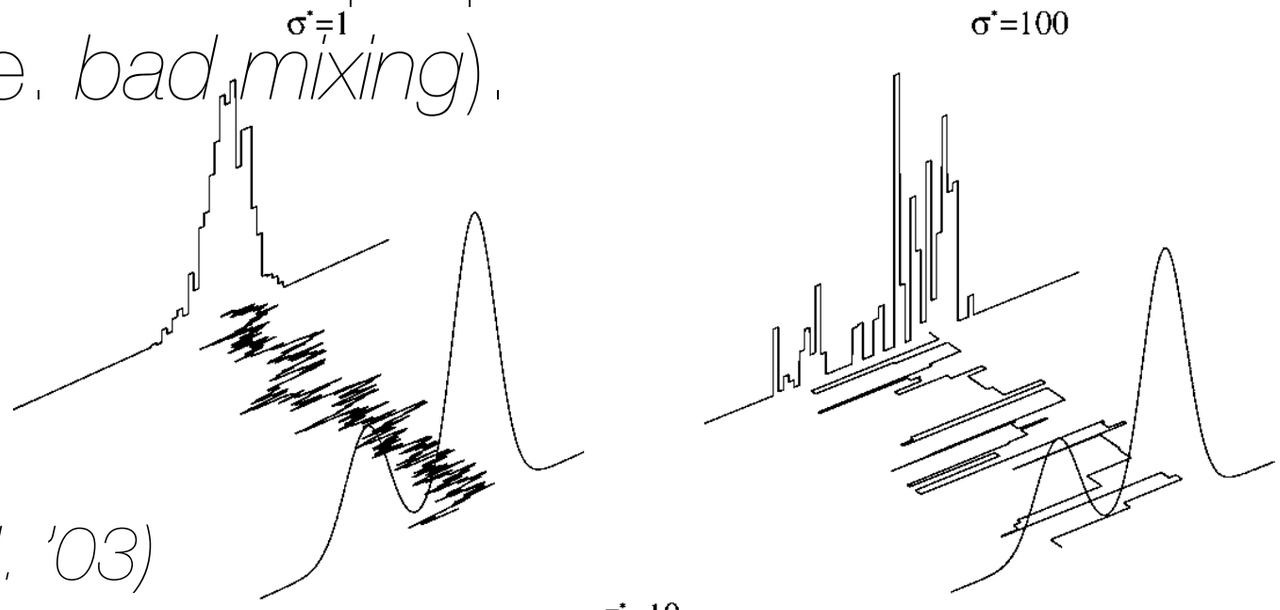
Metropolis-Hastings

- 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.

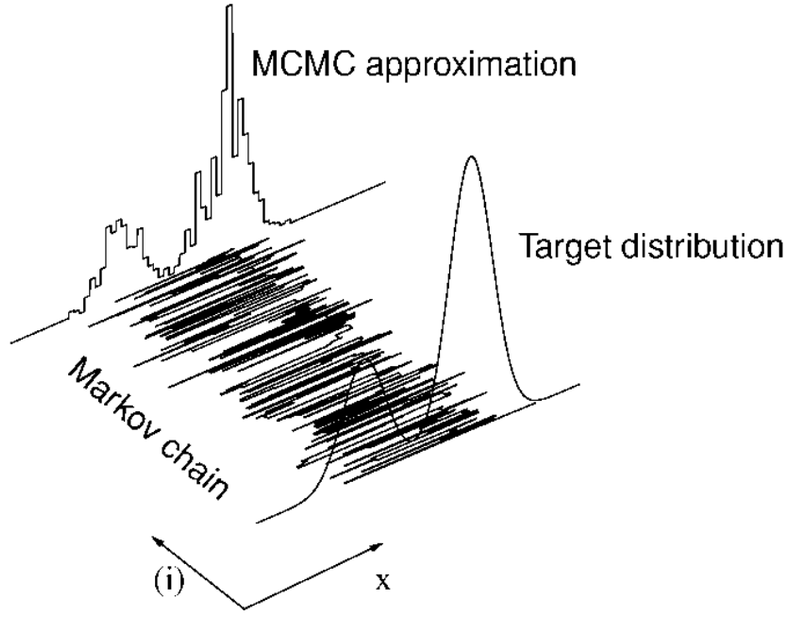
- Two important particular cases:
  - $K(x_j, x_i) = q(x_j)$ is independent of the current state.
    Acceptance probability becomes
    $$R(x_i, x_j) = \min\left(1, \frac{p(x_j)q(x_i)}{p(x_i)q(x_j)}\right) = \min\left(1, \frac{w(x_j)}{w(x_i)}\right) .$$
    - Similar to importance sampling, except that 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*).

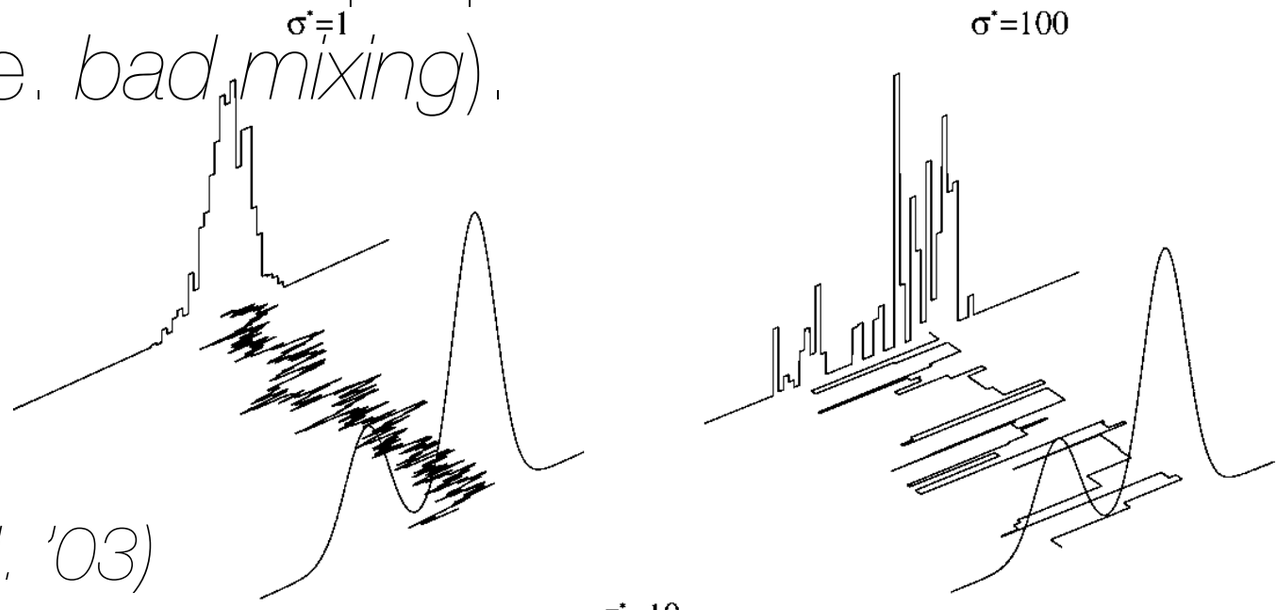


(figure from Andrieu et al. '03)



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*).



(figure from Andrieu et al. '03)

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

Revisiting Gibbs Sampling

- Recall the Gibbs sampling we saw in Lecture 4.

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

- 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

Lemma: The kernel K satisfies detailed balance wrt $p(x)$.

Revisiting Gibbs Sampling

Lemma: The kernel K satisfies detailed balance wrt $p(x)$.

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.

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

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

Mixing Time in MCMC

- We have seen that the correctness of MCMC relies on a Markov chain having the appropriate stationary distribution.

Mixing Time in MCMC

- We have seen that the correctness of MCMC relies on a Markov chain having the appropriate stationary distribution.
- We have also seen that this stationary distribution is associated with the leading eigenvector of its kernel.

$$\text{i.e, given initial guess } \mu,\ \mu P^t \to \pi \text{ as } t \to \infty.$$

Mixing Time in MCMC

- We have seen that the correctness of MCMC relies on a Markov chain having the appropriate stationary distribution.
- We have also seen that this stationary distribution is associated with the leading eigenvector of its kernel.

$$\textbf{i.e, given initial guess } \mu,\ \mu P^t \to \pi \text{ as } t \to \infty.$$

- How fast does the chain converge to its leading eigenvector?

$$\text{i.e. how small } \|\mu P^t - \pi\| \text{ is as } t \to \infty?$$

Mixing Time in MCMC

- We have seen that the correctness of MCMC relies on a Markov chain having the appropriate stationary distribution.
- We have also seen that this stationary distribution is associated with the leading eigenvector of its kernel.

$$\text{i.e, given initial guess } \mu,\ \mu P^t \to \pi \text{ as } t \to \infty.$$

- How fast does the chain converge to its leading eigenvector?

$$\text{i.e. how small } \|\mu P^t - \pi\| \text{ is as } t \to \infty?$$

- The convergence is dictated by the *second largest eigenvalue:*

$$\|\mu P^t - \pi\|_{TV} \leq \lambda_2^t \sqrt{\frac{1}{\min_j \pi_j}}\ .$$

Mixing Time in MCMC

- We have seen that the correctness of MCMC relies on a Markov chain having the appropriate stationary distribution.
- We have also seen that this stationary distribution is associated with the leading eigenvector of its kernel.

$$\textbf{i.e, given initial guess } \mu,\ \mu P^t \to \pi \text{ as } t \to \infty.$$

- How fast does the chain converge to its leading eigenvector?

$$\textbf{i.e. how small } \|\mu P^t - \pi\| \text{ is as } t \to \infty?$$

- The convergence is dictated by the *second largest eigenvalue:*

$$\|\mu P^t - \pi\|_{TV} \leq \lambda_2^t \sqrt{\frac{1}{\min_j \pi_j}}\ .$$

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

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

Φ **is the conductance of** P**:**

$$\min_{\Omega' \subset \Omega} \frac{\sum_{i \in \Omega', j \notin \Omega'} \pi_i P(i,j)}{\pi(\Omega')(1 - \pi(\Omega'))}\ .$$

Interlude: the Stein Method

- More generally, how can we evaluate whether a sample $\{x_1, \ldots, x_n\}$ is legitimate for a certain $p(x)$, possibly known up to normalization?

Interlude: the Stein Method

- More generally, how can we evaluate whether a sample $\{x_1, \ldots, x_n\}$ is legitimate for a certain $p(x)$, possibly known up to normalization?

- 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 $\mathcal{H} = \{h : \Omega \to \mathbb{R}\}$.

Interlude: the Stein Method

- More generally, how can we evaluate whether a sample $\{x_1, \ldots, x_n\}$ is legitimate for a certain $p(x)$, possibly known up to normalization?

- 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 $\mathcal{H} = \{h : \Omega \to \mathbb{R}\}$.

- 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

$$\mathbb{E}_Y\{(\mathcal{A}f)Y\} = 0 \text{ for all } f \in \mathcal{F} \Leftrightarrow \quad Y \text{ has distribution } Q.$$

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

$$\mathbb{E}_Y\{(\mathcal{A}f)Y\} = 0 \text{ for all } f \in \mathcal{F} \Leftrightarrow \quad Y \text{ has distribution } Q.$$

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

$$\mathbb{E}\{f'(Y) - Yf(Y)\} = 0 \text{ for all } f \in C^1 \;\Leftrightarrow\; Y \sim \mathcal{N}(0,1)\ .$$

(Stein's lemma)

So we can consider $(\mathcal{A}f)(x) = f'(x) - xf(x)$ in that case.

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

$$\mathbb{E}_Y\{(\mathcal{A}f)Y\} = 0 \text{ for all } f \in \mathcal{F} \Leftrightarrow \quad Y \text{ has distribution } Q.$$

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

$$\mathbb{E}\{f'(Y) - Yf(Y)\} = 0 \text{ for all } f \in C^1 \;\Leftrightarrow\; Y \sim \mathcal{N}(0,1)\ .$$

(Stein's lemma)

So we can consider $(\mathcal{A}f)(x) = f'(x) - xf(x)$ in that case.

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 $f \in C^1$.

Interlude: the Stein Method

Given a test function h, in some cases we can find $f = f_h$ such that

$$(\mathcal{A}f)(x) = h(x) - \mathbb{E}_{Y\sim Q}(h(Y)) \ .$$

Interlude: the Stein Method

Given a test function h, in some cases we can find $f = f_h$ such that

$$(\mathcal{A}f)(x) = h(x) - \mathbb{E}_{Y\sim Q}(h(Y)) \ .$$

It results that

$$\mathbb{E}_{W\sim P}\{(\mathcal{A}f)W\} = \mathbb{E}_{W\sim P}\{h(W)\} - \mathbb{E}_{Y\sim P}\{h(Y)\} \ .$$

So we can control $\text{dist}(P, Q)$ by bounding the functional form on the lhs.

When is bounding lhs easier than bounding rhs?

Interlude: the Stein Method

Given a test function h, in some cases we can find $f = f_h$ such that

$$(\mathcal{A}f)(x) = h(x) - \mathbb{E}_{Y\sim Q}(h(Y)) \ .$$

It results that

$$\mathbb{E}_{W\sim P}\{(\mathcal{A}f)W\} = \mathbb{E}_{W\sim P}\{h(W)\} - \mathbb{E}_{Y\sim P}\{h(Y)\} \ .$$

So we can control $\mathrm{dist}(P, Q)$ by bounding the functional form on the lhs.

When is bounding lhs easier than bounding rhs?

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

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

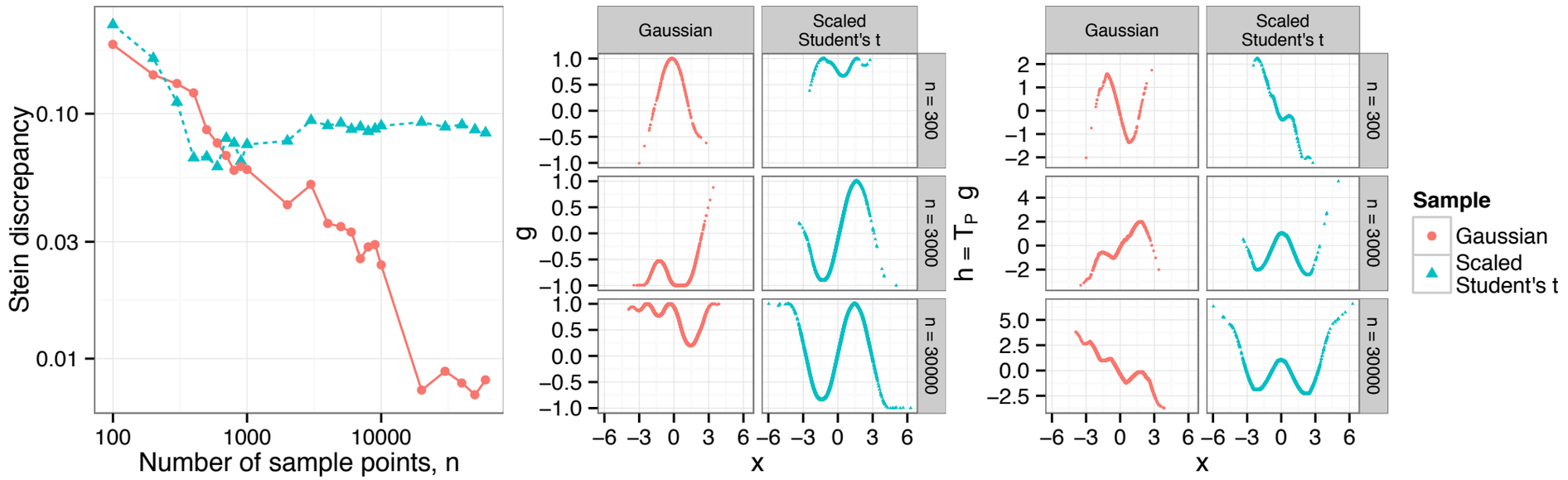


Figure 1: Left: Complete graph Stein discrepancy for a $\mathcal{N}(0, 1)$ target. Middle / right: Optimal Stein functions g and discriminating test functions $h = \mathcal{T}_P g$ recovered by the Stein program.

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

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

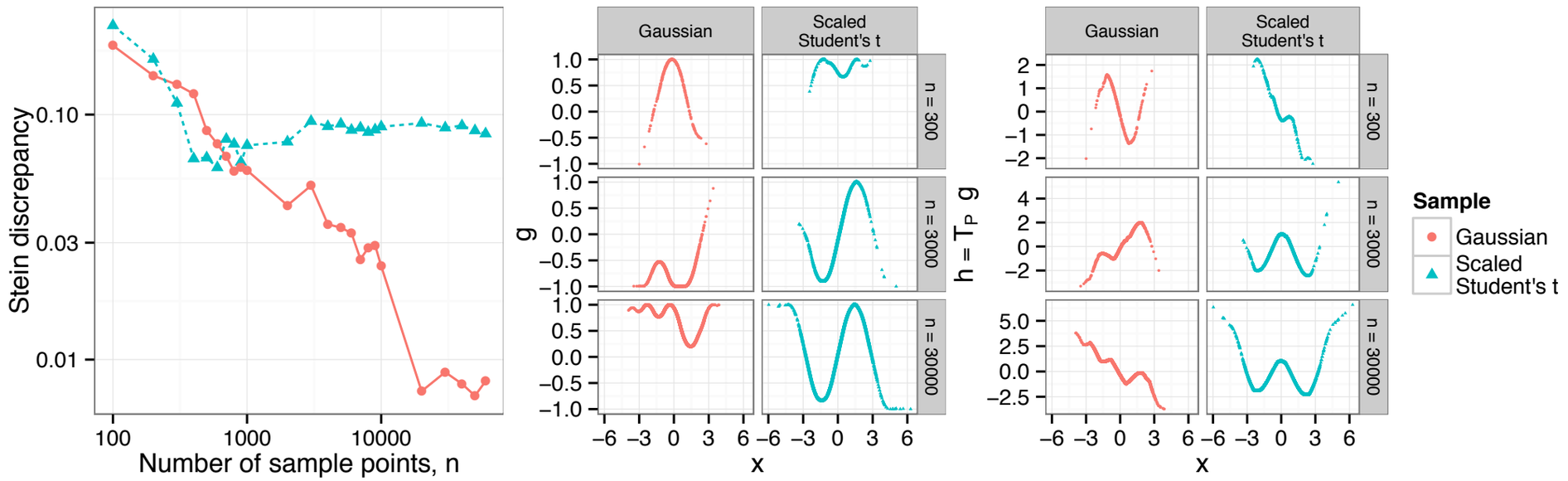


Figure 1: Left: Complete graph Stein discrepancy for a $\mathcal{N}(0, 1)$ target. Middle / right: Optimal Stein functions g and discriminating test functions $h = \mathcal{T}_P g$ recovered by the Stein program.

  - 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]

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

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

$U(x)$: potential energy $K(y)$: kinetic energy

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

MCMC Extensions

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

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

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

$U(x)$: potential energy $K(y)$: kinetic energy

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

- Langevin Dynamics. [see Neal'10]

Discretization of a stochastic differential equation whose equilibrium distribution is the posterior

$$\nabla\theta_t = \frac{\epsilon}{2}\left(\nabla \log p(\theta_t) + \sum_{i \le N} \nabla \log p(x_i \mid \theta_t)\right) + \eta_t \ , \ \eta_t \sim \mathcal{N}(0, \epsilon) \ .$$

Variational Inference

- Q: What does *variational* mean?

Variational Inference

- Q: What does *variational* mean?
- In general, it refers to the idea of expressing a quantity of interest θ^* (e.g. a posterior probability) as the solution of an optimization problem:

$$\theta^* = \inf_{\theta \in \mathcal{M}} f(\theta) \ .$$

Variational Inference

- Q: What does *variational* mean?
- In general, it refers to the idea of expressing a quantity of interest θ^* (e.g. a posterior probability) as the solution of an optimization problem:

$$\theta^* = \inf_{\theta \in \mathcal{M}} f(\theta) \ .$$

- Approximating the solution can now be accomplished by
  - Simplifying the domain $\mathcal{M}$.
  - Simplifying the function f .
- Such approximations are particularly powerful in presence of convex structures.
- Let us start with variational inference in the exponential family.

Exponential Families

- Suppose we have iid data $x_1, \ldots x_n$ and we consider a collection of *sufficient statistics* $\{\phi_k(X)\}_k$

- The empirical expectations of these statistics are

$$\hat{\mu}_k = \frac{1}{n} \sum_i \phi_k(x_i)$$

- Q: Can we build a distribution $p(x)$ consistent with these empirical moments? i.e.

Exponential Families

- Suppose we have iid data $x_1, \ldots x_n$ and we consider a collection of *sufficient statistics* $\{\phi_k(X)\}_k$

- The empirical expectations of these statistics are

$$\hat{\mu}_k = \frac{1}{n} \sum_i \phi_k(x_i)$$

- Q: Can we build a distribution $p(x)$ consistent with these empirical moments? i.e.

$$\mathbb{E}_{X \sim p(x)}\{\phi_k(X)\} = \hat{\mu}_k \quad \text{for all } k.$$

- In general, this is an underdetermined problem. How to choose wisely amongst all possible solutions?

Exponential Families and Maximum Entropy

- A reasonable choice is to consider the distribution with *maximum entropy* subject to the empirical moments:

$$p^* = \arg\max_p H(p) \ , \ s.t. \ \mathbb{E}_p\{\phi_k(X)\} = \hat{\mu}_k \text{ for all } k.$$

$$\text{Shannon Entropy: } H(p) = -\mathbb{E}\{\log(p)\} \ .$$

Exponential Families and Maximum Entropy

- A reasonable choice is to consider the distribution with *maximum entropy* subject to the empirical moments:

$$p^* = \arg\max_p H(p) \ , \ s.t. \ \mathbb{E}_p\{\phi_k(X)\} = \hat{\mu}_k \text{ for all } k.$$

$$\text{Shannon Entropy: } H(p) = -\mathbb{E}\{\log(p)\} \ .$$

- The general form of maximum entropy is

$$p(x) \propto \exp\left\{\sum_k \lambda_k \phi_k(x)\right\}$$

λ_k: Lagrange multipliers adjusted such that $\mathbb{E}_p \phi_k(X) = \hat{\mu}_k$ for all k.

Exponential Families

- The exponential family associated with ϕ is defined as the parametric family:

$$p_\theta(x) = \exp\{\langle \theta, \phi(x) \rangle - A(\theta)\} \ , \ \text{with}$$

$$A(\theta) = \log \int \exp\{\langle \theta, \phi(x) \} dx \qquad \text{log-partition function}$$

Exponential Families

- The exponential family associated with ϕ is defined as the parametric family

$$p_\theta(x) = \exp\{\langle \theta, \phi(x) \rangle - A(\theta)\} \ , \ \text{with}$$

$$A(\theta) = \log \int \exp\{\langle \theta, \phi(x) \} dx \qquad \text{log-partition function}$$

- It is well defined for the family of parameters

$$\Omega = \{\theta \ ; \ A(\theta) < \infty\}$$

- Several well-known models belong to the exponential family:
  - Energy based models
  - Gaussian Mixtures
  - Latent Dirichlet Allocation

Exponential Families

- **Proposition:** The log-partition function $A(\theta)$ satisfies

  - $$\frac{\partial A}{\partial \theta_k}(\theta) = \mathbb{E}_\theta\{\phi_k(X)\} = \int \phi_k(x) p_\theta(x) dx \ .$$

  - $A(\theta)$ is convex in its domain Ω.

- Higher order derivatives always exist.

Legendre Transform

Let $f : \mathbb{R} \to \mathbb{R}$ be a convex function.

The Legendre Transform f^* of f is defined as

$$f^*(u) = \sup_x (xu - f(x))$$

- f* is the convex conjugate of f
- Equivalent definition in the differentiable case:

f and g are Legendre transforms of each other if their first derivatives are inverses of each other:

$$\forall\ x,\ g'(f'(x)) = x\ ,\ \forall\ u,\ f'(g'(u)) = u\ .$$

- It follows that $f^{**} = f$

Conjugate Duality

- Conjugate duality representation of convex functions:

$$A^*(\mu) = \sup_{\theta \in \Omega} \{\langle \mu, \theta \rangle - A(\theta)\}$$

$$\text{canonical parameters} \quad \longleftrightarrow \quad \text{moment parameters}$$

$$\theta_k \qquad\qquad\qquad \mu_k$$

- Q: How to interpret the dual conjugate?

Conjugate Duality

- Conjugate duality representation of convex functions:

$$A^*(\mu) = \sup_{\theta \in \Omega} \{\langle \mu, \theta \rangle - A(\theta)\}$$

$$\text{canonical parameters} \quad \longleftrightarrow \quad \text{moment parameters}$$

$$\theta_k \qquad\qquad\qquad\qquad \mu_k$$

- Q: How to interpret the dual conjugate?

  $A^*(\mu)$: Negative entropy of $p_{\theta(\mu)}$, where

  $p_{\theta(\mu)}$ is the exponential family distribution such that $\mathbb{E}_{\theta(\mu)}\phi(X) = \mu$.

Conjugate Duality

- Conjugate duality representation of convex functions:

$$A^*(\mu) = \sup_{\theta \in \Omega} \{\langle \mu, \theta \rangle - A(\theta)\}$$

$$\text{canonical parameters} \quad \longleftrightarrow \quad \text{moment parameters}$$

$$\theta_k \qquad\qquad\qquad\qquad \mu_k$$

- Q: How to interpret the dual conjugate?

  $A^*(\mu)$: Negative entropy of $p_{\theta(\mu)}$, where

  $p_{\theta(\mu)}$ is the exponential family distribution such that $\mathbb{E}_{\theta(\mu)} \phi(X) = \mu$.

- Variational representation:

$$A(\theta) = \sup_{\mu} \{\langle \theta, \mu \rangle - A^*(\mu)\}$$

Variational Inference and Duality

- We derive the exact EM algorithm for exponential families with latent variables. Given observed variables Z and latent variables X, we consider

$$p_\theta(x,z) = \exp\left\{\langle\theta, \phi(x,z)\rangle - A(\theta)\right\} \ , \ \text{with}$$

$$A(\theta) = \log \int_{x,z} \exp\{\langle\theta, \phi(x,z)\rangle\} dx dz$$

Variational Inference and Duality

- We derive the exact EM algorithm for exponential families with latent variables. Given observed variables Z and latent variables X, we consider

$$p_\theta(x,z) = \exp\left\{\langle\theta, \phi(x,z)\rangle - A(\theta)\right\} \ , \ \text{with}$$

$$A(\theta) = \log \int_{x,z} \exp\{\langle\theta, \phi(x,z)\rangle\} dx dz$$

- Given observation $X = x$, the posterior distribution is

$$p(z \mid x) = \frac{\exp\{\langle\theta, \phi(x,z)\rangle\}}{\int \exp\{\langle\theta, \phi(x,z')\rangle\} dz'} = \exp\{\langle\theta\phi(x,z)\rangle - A_x(\theta)\}$$

$$A_x(\theta) = \log \int_z \exp\{\langle\theta, \phi(x,z)\rangle\} dz$$

Variational Inference and Conjugate Duality

- The MLE for our parameters $\boldsymbol{\theta}$ is obtained by maximizing the incomplete log-likelihood of the data:

$$\mathcal{L}(\theta, x) = \log \int_z \exp\{\langle \theta, \phi(x, z) \rangle - A(\theta)\} dz = A_x(\theta) - A(\theta) \ .$$

Variational Inference and Conjugate Duality

- The MLE for our parameters θ is obtained by maximizing the incomplete log-likelihood of the data:

$$\mathcal{L}(\theta, x) = \log \int_z \exp\{\langle \theta, \phi(x, z) \rangle - A(\theta)\} dz = A_x(\theta) - A(\theta) \ .$$

- The variational representation gives

$$A_x(\theta) = \sup_{\mu_x} \{\langle \theta, \mu_x \rangle - A_x^*(\mu_x)\}$$

$$A_x^*(\mu_x) = \sup_{\theta} \{\langle \theta, \mu_x \rangle - A_x(\theta)\}$$

Variational Inference and Conjugate Duality

- The MLE for our parameters θ is obtained by maximizing the incomplete log-likelihood of the data:

$$\mathcal{L}(\theta, x) = \log \int_z \exp\{\langle \theta, \phi(x, z) \rangle - A(\theta)\} dz = A_x(\theta) - A(\theta) \ .$$

- The variational representation gives

$$A_x(\theta) = \sup_{\mu_x} \{\langle \theta, \mu_x \rangle - A_x^*(\mu_x)\}$$

$$A_x^*(\mu_x) = \sup_{\theta} \{\langle \theta, \mu_x \rangle - A_x(\theta)\}$$

- It results in the lower-bound for the incomplete log-likelihood:

$$\mathcal{L}(\theta, x) \geq \langle \mu_x, \theta \rangle - A_x^*(\mu_x) - A(\theta) = \widetilde{\mathcal{L}}(\mu_x, \theta)$$

Variational Inference and Conjugate Duality

- EM is thus a coordinate ascent on the lower bound:

$$\mu_x^{(t+1)} = \arg\max_{\mu_x} \widetilde{\mathcal{L}}(\mu_x, \theta^{(t)}) \qquad \text{(E step)}$$

$$\theta^{(t+1)} = \arg\max_{\theta} \widetilde{\mathcal{L}}(\mu_x^{(t+1)}, \theta) \qquad \text{(M step)}$$

Variational Inference and Conjugate Duality

- EM is thus a coordinate ascent on the lower bound:

$$\mu_x^{(t+1)} = \arg\max_{\mu_x} \widetilde{\mathcal{L}}(\mu_x, \theta^{(t)}) \qquad \text{(E step)}$$

$$\theta^{(t+1)} = \arg\max_{\theta} \widetilde{\mathcal{L}}(\mu_x^{(t+1)}, \theta) \qquad \text{(M step)}$$

- E step is called expectation because the maximizer of $\widetilde{\mathcal{L}}(\mu_x, \theta)$ is, by duality, the expectation $\mu_x^{(t+1)} = \mathbb{E}_{\theta^{(t)}} \phi(x, Z)$

Variational Inference and Conjugate Duality

- EM is thus a coordinate ascent on the lower bound:

$$\mu_x^{(t+1)} = \arg\max_{\mu_x} \widetilde{\mathcal{L}}(\mu_x, \theta^{(t)}) \qquad \text{(E step)}$$

$$\theta^{(t+1)} = \arg\max_{\theta} \widetilde{\mathcal{L}}(\mu_x^{(t+1)}, \theta) \qquad \text{(M step)}$$

- E step is called expectation because the maximizer of $\widetilde{\mathcal{L}}(\mu_x, \theta)$ is, by duality, the expectation $\mu_x^{(t+1)} = \mathbb{E}_{\theta^{(t)}} \phi(x, Z)$

- Also, because $\max_{\mu} \{\langle \mu_x, \theta^{(t)} \rangle - A_x^*(\mu_x)\} = A_x(\theta^{(t)})$, after each E step the inequality becomes an equality, thus M step increases log-likelihood.

Approximate Posterior Inference

- For most models, the posterior is analytically intractable:

$$p(z \mid x) = \frac{p(x \mid z)p(z)}{\int p(x \mid z')p(z')dz'}$$

- ***Variational Bayesian Inference:*** consider a parametric family of approximations $q(z \mid \beta)$ and optimize variational lower bound with respect to the variational parameters β .

Mean Field Variational Bayes

- Joint likelihood of observed and latent variables:

$$p(X, Z \mid \theta) \qquad \theta\text{: generative model parameters}$$

- Let us consider a posterior approximation $q(z|\beta)$of the form

$$q(z \mid \beta) = \prod_i q_i(z_i \mid \beta_i) \qquad \beta\text{: Variational parameters}$$

  - Mean-field approximation: we model hidden variables as being independent.

Mean Field Variational Bayes

- Joint likelihood of observed and latent variables:

$$p(X, Z \mid \theta) \qquad \theta\text{: generative model parameters}$$

- Let us consider a posterior approximation $q(z|\beta)$of the form

$$q(z \mid \beta) = \prod_i q_i(z_i \mid \beta_i) \qquad \beta\text{: Variational parameters}$$

  - Mean-field approximation: we model hidden variables as being independent.

- Corresponding lower-bound is given by

$$\log p(X \mid \theta) \geq \int q(z \mid \beta) \log \frac{p(x, z \mid \theta)}{q(z \mid \beta)} dz = \mathbb{E}_{q(z|\beta)}\{\log(p(X, Z \mid \theta)\} + H(q(z \mid \beta))$$

Mean Field Variational Bayes

- **Goal**: optimize lower-bound with respect to variational parameters.

Mean Field Variational Bayes

- **Goal**: optimize lower-bound with respect to variational parameters.
- As we have seen, this is equivalent to minimizing the divergence between true and approximate posterior:

$$\log p(X \mid \theta) = \widetilde{\mathcal{L}}(\theta, \beta) + D_{KL}(q_\beta(z)||p(z|x, \theta))$$

Mean Field Variational Bayes

- **Goal**: optimize lower-bound with respect to variational parameters.
- As we have seen, this is equivalent to minimizing the divergence between true and approximate posterior:

$$\log p(X \mid \theta) = \widetilde{\mathcal{L}}(\theta, \beta) + D_{KL}(q_\beta(z)||p(z|x, \theta))$$

- If $q(z \mid \beta)$ is a factorial distribution, the entropy term is tractable:

$$H(q(z|\beta)) = \sum_i H(q_i(z_i|\beta_i))$$

- Problematic term: $\nabla_\beta \mathbb{E}_{q(z|\beta)} \log p(X, Z|\theta)$

Mean Field Variational Bayes

[Paiskey, Blei, Jordan,'12]

- Denote $f(Z) = \log p(X, Z|\theta)$
- Then

$$\nabla_\beta \mathbb{E}_{q(z|\beta)} f(Z) = \nabla_\beta \int f(z) q(z|\beta) dz$$

$$= \int f(z) \nabla_\beta q(z|\beta) dz$$

$$= \int f(z) q(z|\beta) \nabla_\beta \log q(z|\beta) dz$$

$$= \mathbb{E}_q \{ f(Z) \nabla_\beta \log q(z|\beta) \}$$

Mean Field Variational Bayes

[Paiskey, Blei, Jordan,'12]

- Denote $f(Z) = \log p(X, Z|\theta)$
- Then

$$\nabla_\beta \mathbb{E}_{q(z|\beta)} f(Z) = \nabla_\beta \int f(z) q(z|\beta) dz$$

$$= \int f(z) \nabla_\beta q(z|\beta) dz$$

$$= \int f(z) q(z|\beta) \nabla_\beta \log q(z|\beta) dz$$

$$= \mathbb{E}_q \{ f(Z) \nabla_\beta \log q(z|\beta) \}$$

- Stochastic approximation of $\nabla_\beta \mathbb{E}_{q(z|\beta)} f(Z)$:

$$\nabla_\beta \mathbb{E}_{q(z|\beta)} f(Z) \approx \frac{1}{S} \sum_{s \leq S, z^{(s)} \sim q(z|\beta)} f(z^{(s)}) \nabla_\beta \log q(z^{(s)}|\beta)$$

Mean Field Variational Bayes

- The estimator of the gradient is unbiased, but it may suffer from large variance.
  - We may need a large number S of samples to stabilize the descent.
  - This estimator is also the basis of policy gradients in RL.

- Faster alternative?