

CS492: Probabilistic Programming Variational Inference

Hongseok Yang
KAIST

Posterior inference

Given:

- Prior $p(x)$ and likelihood $p(y|x)$.
- Observations y .

Goal:

- Find a good approximation of $p(x|y)$.

Monte-Carlo approach:

- Approximates posterior $p(x|y)$ by samples.
- Exact in the limit, but scalability issue.
- MCMC, importance sampling, etc.

Monte-Carlo approach:

- Approximates posterior $p(x|y)$ by samples.
- Exact in the limit, but scalability issue.
- MCMC, importance sampling, etc.

Variational inference:

- Approximates $p(x|y)$ by a distribution $q_\theta(x)$.
- Scales, but not exact (biased).
- Stochastic variational inference, expectation propagation, etc.

Monte-Carlo approach:

- Approximates posterior $p(x|y)$ by samples.
- Exact in the limit, but scalability issue.
- MCMC, importance sampling, etc.

Variational inference:

- Approximates $p(x|y)$ by a distribution $q_\theta(x)$.
- Scales, but not exact (biased).
- Stochastic variational inference, expectation propagation, etc.

Monte-Carlo approach:

- Approximates posterior $p(x|y)$ by samples.
- Exact in the limit, but scalability issue.
- MCMC, importance sampling, etc.

Variational inference:

- Approximates $p(x|y)$ by a distribution $q_\theta(x)$.
- Scales, but not exact (biased).
- Stochastic variational inference, expectation propagation, etc.

Microsoft's infer.NET

Monte-Carlo approach:

- Approximates posterior $p(x|y)$ by samples.
- Exact in the limit, but scalability issue.

Uber's pyro

Google's Edward

Anglican, Stan

Variational inference:

- Approximates $p(x|y)$ by a distribution $q_\theta(x)$.
- Scales, but not exact (biased).
- Stochastic variational inference, expectation propagation, etc.

Microsoft's infer.NET

Learning outcome

- Should be able to use stochastic variational inference (SVI) algorithms for data analysis.
- Should be able to derive key equations for a basic SVI algorithm with score estimator.
- Should be able to implement this basic SVI algorithm for probabilistic PLs.

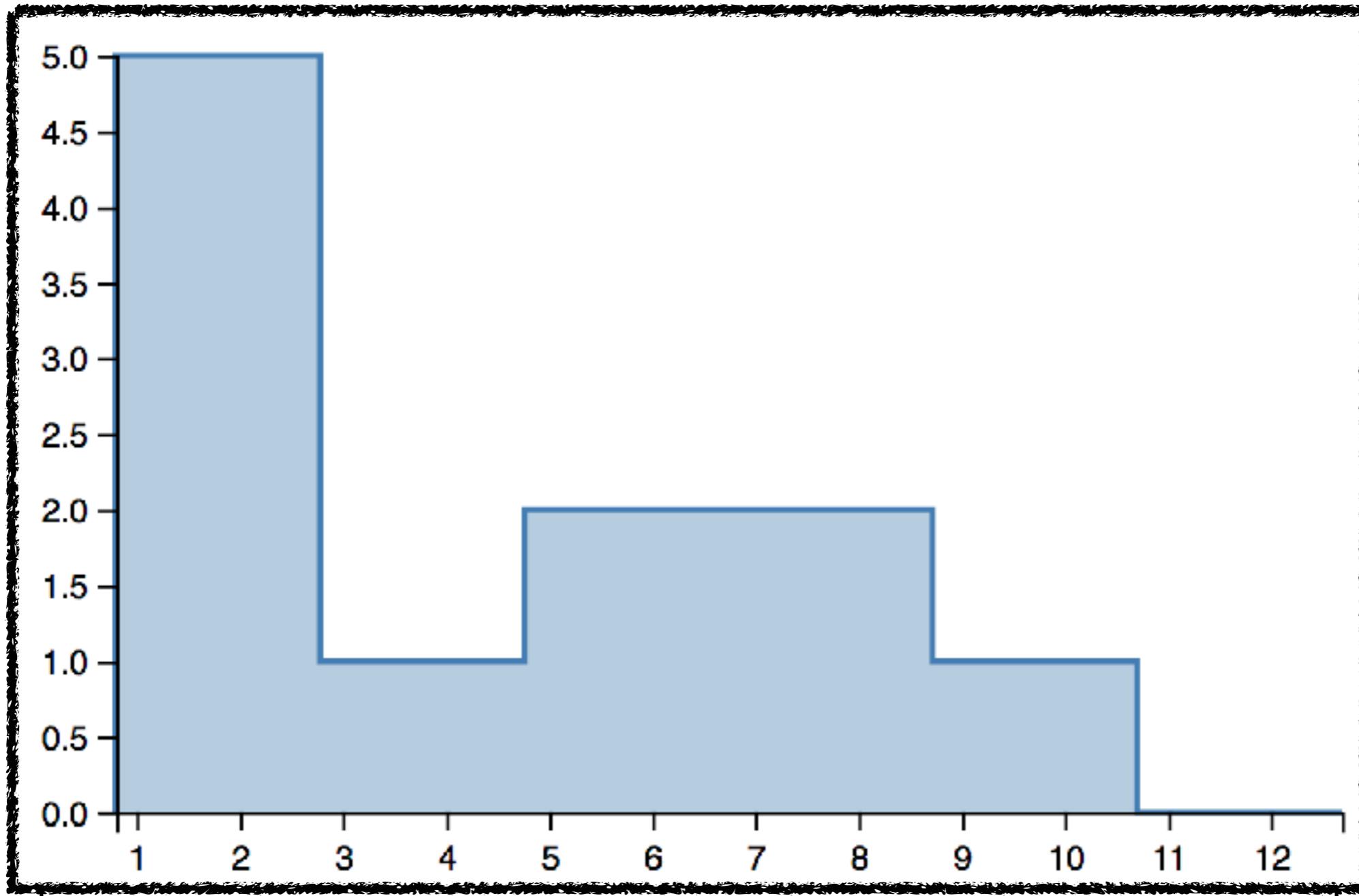
Using stochastic
variational inference
in Anglican

Mixture of two Gaussians

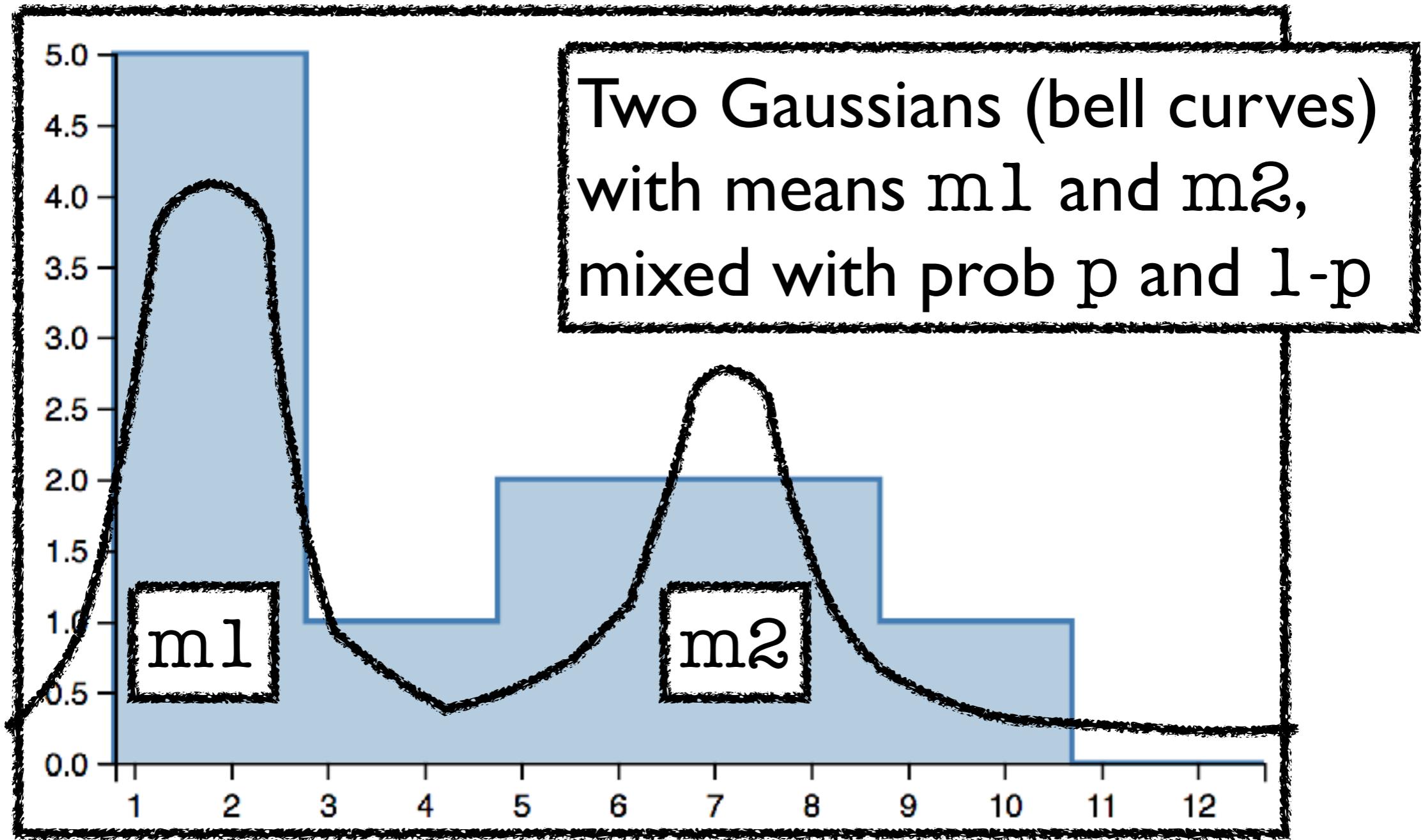
```
(defquery mixture []
  (let [p  (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f   (fn [y]
              (if (sample (flip p))
                  (observe (normal m1 1.) y)
                  (observe (normal m2 1.) y))))]
    (map f (list 0.8 1.2 7.8 2.4 8.2
                 10.7 5.3 2.6 1.2 3.4 5.6)))
  [p m1 m2]))
```

Mixture of two Gaussians

```
(defquery mixture []
  (let [p  (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f   (fn [y]
              (if (sample (flip p))
                  (observe (normal m1 1.) y)
                  (observe (normal m2 1.) y))))]
    (map f (list 0.8 1.2 7.8 2.4 8.2
                 10.7 5.3 2.6 1.2 3.4 5.6)))
  [p m1 m2]))
```

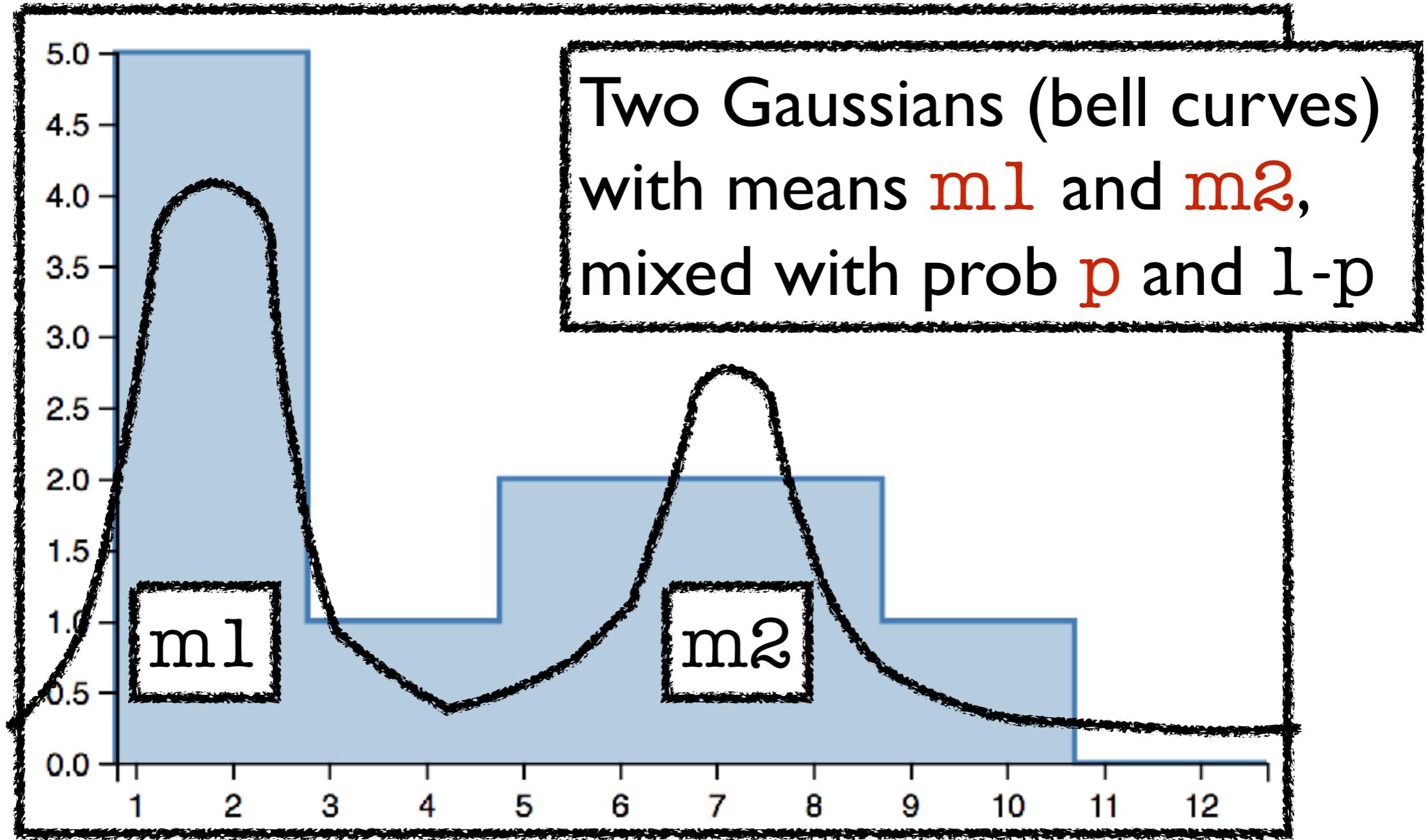


```
(map f (list 0.8 1.2 7.8 2.4 8.2  
           10.7 5.3 2.6 1.2 3.4 5.6))  
[p m1 m2]))
```



(map f (list 0.8 1.2 7.8 2.4 8.2
10.7 5.3 2.6 1.2 3.4 5.6))

[p m1 m2]))



```
(map f (list 0.8 1.2 7.8 2.4 8.2  
           10.7 5.3 2.6 1.2 3.4 5.6))
```

```
[p m1 m2]))
```

Mixture of two Gaussians

```
(defquery mixture []
  (let [p  (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f   (fn [y]
              (if (sample (flip p))
                  (observe (normal m1 1.) y)
                  (observe (normal m2 1.) y))))]
    (map f (list 0.8 1.2 7.8 2.4 8.2
                 10.7 5.3 2.6 1.2 3.4 5.6)))
  [p m1 m2]))
```

Mixture of two Gaussians

Labels for sample
expressions

```
(defquery mixture []
  (let [p  (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f   (fn [y]
              (if (sample (flip p))
                  (observe (normal m1 1.) y)
                  (observe (normal m2 1.) y))))]
    (map f (list 0.8 1.2 7.8 2.4 8.2
                 10.7 5.3 2.6 1.2 3.4 5.6)))
  [p m1 m2]))
```

Mixture of two Gaussians

Distribution on [0, 1]
Uniform in this case

```
(defquery mixture []
  (let [p (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f (fn [y]
            (if (sample (flip p))
                (observe (normal m1 1.) y)
                (observe (normal m2 1.) y))))]
    (map f (list 0.8 1.2 7.8 2.4 8.2
                  10.7 5.3 2.6 1.2 3.4 5.6)))
  [p m1 m2]))
```

Mixture of two Gaussians

```
(defquery mixture []
  (let [p  (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f   (fn [y]
              (if (sample (flip p))
                  (observe (normal m1 1.) y)
                  (observe (normal m2 1.) y)))]
    (map f (list 0.8 1.2 7.8 2.4 8.2
                 10.7 5.3 2.6 1.2 3.4 5.6)))
  [p m1 m2]))
```

Mixture of two Gaussians

```
(defquery mixture []
  (let [p  (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f   (fn [y]
              (if (sample (flip p))
                  (observe (normal m1 1.) y)
                  (observe (normal m2 1.) y))))]
    (map f (list 0.8 1.2 7.8 2.4 8.2
                 10.7 5.3 2.6 1.2 3.4 5.6)))
  [p m1 m2]))
```

```
(def r1 (nth (doquery :bbvb mixture []) 50000))
(def r2 (anglican.bbbv/get-variational r1))

(print (:p r2) "\n\n" (:m1 r2) "\n\n" (:m2 r2))
```

```
(defquery mixture []
  (let [p (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f (fn [y]
            (if (sample (flip p))
                (observe (normal m1 1.) y)
                (observe (normal m2 1.) y)))]
    (map f (list 0.8 1.2 7.8 2.4 8.2
                  10.7 5.3 2.6 1.2 3.4 5.6)))
  [p m1 m2]))
```

```
(def r1 (nth (doquery :bbvb mixture []) 50000))
(def r2 (anglican.bbbv/get-variational r1))

(print (:p r2) "\n\n" (:m1 r2) "\n\n" (:m2 r2))
```

```
(defquery mixture-posterior-approx []
  (let [p (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f (fn [y]
            (if (sample (flip p))
                (observe (normal m1 1.) y)
                (observe (normal m2 1.) y)))]
    (map f (list 0.8 1.2 7.8 2.4 8.2
                  10.7 5.3 2.6 1.2 3.4 5.6)))
  [p m1 m2]))
```

Approx. by Anglican query

```
(def r1 (nth (doquery :bbvb mixture []) 50000))
(def r2 (anglican.bbbv/get-variational r1))

(print (:p r2) "\n\n" (:m1 r2) "\n\n" (:m2 r2))
```

```
(defquery mixture-posterior-approx []
  (let [p (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f (fn [y]
            (if (sample (flip p))
                (observe (normal m1 1.) y)
                (observe (normal m2 1.) y)))]
    (map f (list 0.3 1.2 2.3 2.4 3.2
                  10.2 5.5 2.6 1.2 3.4 5.6)))
  [p m1 m2]))
```

Approx. by Anglican query
 (I) No obs.

```
(def r1 (nth (doquery :bbvb mixture []) 50000))
(def r2 (anglican.bbbv/get-variational r1))

(print (:p r2) "\n\n" (:m1 r2) "\n\n" (:m2 r2))
```

```
(defquery mixture-posterior-approx []
  (let [p (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f (fn [y]
            (if (sample (flip p))
                (observe (normal m1 1.) y)
                (observe (normal m2 1.) y)))]
    #mapf (list 0.3 1.2 2.8 2.4 3.2
               10.2 5.5 2.6 1.2 3.4 5.6))
  [p m1 m2]))
```

Approx. by Anglican query
 (1) No obs. (2) New params.

```
(def r1 (nth (doquery :bbvb mixture []) 50000))
(def r2 (anglican.bbbv/get-variational r1))

(print (:p r2) "\n\n" (:m1 r2) "\n\n" (:m2 r2))
```

```
(defquery mixture-posterior-approx []
  (let [p (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f (fn [y]
```

```
((0 anglican.runtime.beta-distribution)
(anglican.runtime/beta 6.765287422267994
5.346760324478156)}
```

```
((0 anglican.runtime.normal-distribution)
(anglican.runtime/normal 2.103819374566423
0.38317375867070796))
```

```
((0 anglican.runtime.normal-distribution)
(anglican.runtime/normal 7.242181702264095
0.4170153403540341))
```

l m1 l.) y)
l m2 l.) y))))]

~~8.2~~

~~2.34 5.6))~~

Anglican query
s. (2) New params.

```
(def r1 (nth (doquery :bbvb mixture []) 50000))
(def r2 (anglican.bbbv/get-variational r1))

(print (:p r2) "\n\n" (:m1 r2) "\n\n" (:m2 r2))
```

```
(defquery mixture-posterior-approx []
  (let [p (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f (fn [y]
```

```
((0 anglican.runtime.beta-distribution)
(anglican.runtime/beta 6.765287422267994
5.346760324478156))
```

```
((0 anglican.runtime.normal-distribution)
(anglican.runtime/normal 2.103819374566423
0.38317375867070796))
```

```
((0 anglican.runtime.normal-distribution)
(anglican.runtime/normal 7.242181702264095
0.4170153403540341))
```

l m1 l.) y)
l m2 l.) y))))]

~~8.2~~

~~2.34 5.6))~~

Anglican query
s. (2) New params.

```
(def r1 (nth (doquery :bbvb mixture []) 50000))
(def r2 (anglican.bbbv/get-variational r1))

(print (:p r2) "\n\n" (:m1 r2) "\n\n" (:m2 r2))
```

```
(defquery mixture-posterior-approx []
  (let [p (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f (fn [y]
```

```
((0 anglican.runtime.beta-distribution)
(anglican.runtime/beta 6.765287422267994
5.346760324478156)}
```

```
((0 anglican.runtime.normal-distribution)
(anglican.runtime/normal 2.103819374566423
0.38317375867070796))
```

```
((0 anglican.runtime.normal-distribution)
(anglican.runtime/normal 7.242181702264095
0.4170153403540341))
```

l m1 l.) y)
l m2 l.) y))))]
8.2
2.34 5.6))

y Anglican query
s. (2) New params.

```
(def r1 (nth (doquery :bbvb mixture []) 50000))
(def r2 (anglican.bbbv/get-variational r1))

(print (:p r2) "\n\n" (:m1 r2) "\n\n" (:m2 r2))
```

```
(defquery mixture-posterior-approx []
  (let [p (sample :p (beta 1 1))
        m1 (sample :m1 (normal 0 5))
        m2 (sample :m2 (normal 0 5))
        f (fn [y]
```

```
((0 anglican.runtime.beta-distribution)
(anglican.runtime/beta 6.765287422267994
5.346760324478156)}
```

```
((0 anglican.runtime.normal-distribution)
(anglican.runtime/normal 2.103819374566423
0.38317375867070796))
```

```
((0 anglican.runtime.normal-distribution)
(anglican.runtime/normal 7.242181702264095
0.4170153403540341))
```

l m1 l.) y)
l m2 l.) y))))]

~~8.2~~

~~2.34 5.6))~~

Anglican query
s. (2) New params.

Variational inference from the users' perspective

- Approximates a posterior by a distribution.
- In Anglican, the approximation has the form of the original query except that
 1. all observes are gone;
 2. dist. parameters at sample are constants, different from the original parameters.

What does stochastic
variational inference do?

Variational inference

1. Fix a family of approximating distr. $\{q_\theta(x)\}_\theta$.
2. Find θ s.t. $q_\theta(x)$ is closest to post. $p(x|y)$.

Variational inference

1. Fix a family of approximating distr. $\{q_\theta(x)\}_\theta$.
2. Find θ s.t. $q_\theta(x)$ is closest to post. $p(x|y)$.

Don't sum. Optimise.

Variational

Three choices:

1. Fix a family of approximating distr. $\{q_\theta(x)\}_\theta$.
2. Find θ s.t. $q_\theta(x)$ is closest to post. $p(x|y)$.

Don't sum. Optimise.

Variational

Three choices:

(I) Which family?

1. Fix a family of approximating distr. $\{q_\theta(x)\}_\theta$.
2. Find θ s.t. $q_\theta(x)$ is closest to post. $p(x|y)$.

Don't sum. Optimise.

Variational

Three choices:

(1) Which family?

(2) What does “closest” mean?

1. Fix a family of approximating distr. $\{q_\theta(x)\}_\theta$.
2. Find θ s.t. $q_\theta(x)$ is closest to post. $p(x|y)$.

Don't sum. Optimise.

Variational

Three choices:

- (1) Which family?
- (2) What does “closest” mean?
- (3) How to optimise?

1. Fix a family of approximating distr. $\{q_\theta(x)\}_\theta$.
2. Find θ s.t. $q_\theta(x)$ is closest to post. $p(x|y)$.

Don't sum. Optimise.

Variational

Three choices:

- (1) Which family?
- (2) What does “closest” mean?
- (3) How to optimise?

1. Fix a family of approximating distr. $\{q_\theta(x)\}_\theta$.
2. Find θ s.t. $q_\theta(x)$ is closest to post. $p(x|y)$.

Don't sum. Optimise.

Basic (but not uncommon) choices.

- I. Which family?**
- 2. What does “closest” mean?**
- 3. How to optimize?**

Basic (but not uncommon) choices.

I. Which family?

- Mean field — $q_\theta(x_1, \dots, x_n) = \prod_k q_\theta(x_k)$.
2. What does “closest” mean?
 3. How to optimize?

Basic (but not uncommon) choices.

I. Which family?

- Mean field — $q_\theta(x_1, \dots, x_n) = \prod_k q_\theta(x_k)$.

2. What does “closest” mean?

- KL divergence — $\text{KL}[q_\theta(x) \parallel p(x|y)]$.

3. How to optimize?

Basic (but not uncommon) choices.

I. Which family?

- Mean field — $q_\theta(x_1, \dots, x_n) = \prod_k q_\theta(x_k)$.

2. What does “closest” mean?

- KL divergence — $\text{KL}[q_\theta(x) \parallel p(x|y)]$.

3. How to optimize?

- Stochastic gradient descent.

Basic (but not uncommon) choices.

I. Which family?

- Mean field — $q_\theta(x_1, \dots, x_n) = \prod_k q_\theta(x_k)$.

2. What does “closest” mean?

- KL divergence — $\text{KL}[q_\theta(x) \parallel p(x|y)]$.

3. How to optimize?

- Stochastic gradient descent.

Mean-field approximation

Mean-field approximation

Approximating distribution q_θ formed by independent random variables:

$$q_\theta(x_1, \dots, x_n) = \prod_k q_\theta(x_k).$$

E.g. $q_\theta(x_1, x_2) = \text{normal}(x_1; \theta_1, 2) \times \text{normal}(x_2; \theta_2, 2)$.

Very crude. But popular, because it simplifies optimisation in variational inference.

Naive mean-field approx. for probabilistic programs

1. Remove all observe expressions.
2. Replace all $(\text{sample} (\text{dist } e_1 \dots e_n))$ by $(\text{sample} (\text{dist } \theta_1 \dots \theta_n))$.

Model

```
(let [x (sample (beta 3 2))
      y (if (sample (flip x))
              (sample (normal (* x x) 1))
              (sample (normal (* 5 x) 1)))]
  (observe (normal y 1) 3)
  x)
```

Model

```
(let [x (sample (beta 3 2))
      y (if (sample (flip x))
              (sample (normal (* x x) 1))
              (sample (normal (* 5 x) 1)))]
  (observe (normal y 1) 3)
  x)
```

Approx. family

```
(let [x (sample (beta 3 2))
      y (if (sample (flip x))
              (sample (normal (* x x) 1))
              (sample (normal (* 5 x) 1)))]
  (observe (normal y 1) 3)
  x)
```

Model

```
(let [x (sample (beta 3 2))
      y (if (sample (flip x))
              (sample (normal (* x x) 1))
              (sample (normal (* 5 x) 1)))]
  (observe (normal y 1) 3)
  x)
```

Approx. family

```
(let [x (sample (beta 3 2))
      y (if (sample (flip x))
              (sample (normal (* x x) 1))
              (sample (normal (* 5 x) 1)))]
  (observe (normal y 1) 3)
  x)
```

Model

```
(let [x (sample (beta 3 2))
      y (if (sample (flip x))
              (sample (normal (* x x) 1))
              (sample (normal (* 5 x) 1)))]
  (observe (normal y 1) 3)
  x)
```

Approx. family

```
(let [x (sample (beta 3 2))
      y (if (sample (flip x))
              (sample (normal (* x x) 1))
              (sample (normal (* 5 x) 1)))]
  x)
```

Model

```
(let [x (sample (beta 3 2))
      y (if (sample (flip x))
              (sample (normal (* x x) 1))
              (sample (normal (* 5 x) 1)))]
  (observe (normal y 1) 3)
  x)
```

Approx. family

```
(let [x (sample (beta 3 2))
      y (if (sample (flip x))
              (sample (normal (* x x) 1))
              (sample (normal (* 5 x) 1)))]
  x)
```

Model

```
(let [x (sample (beta 3 2))
      y (if (sample (flip x))
              (sample (normal (* x x) 1))
              (sample (normal (* 5 x) 1)))]
  (observe (normal y 1) 3)
  x)
```

Approx. family

```
(let [x (sample (beta  $\theta_1 \theta_2$ ))
      y (if (sample (flip  $\theta_3$ ))
              (sample (normal  $\theta_4 \theta_5$ ))
              (sample (normal  $\theta_6 \theta_7$ )))]
  x)
```

Model

```
(let [x (sample (beta 3 2))
      y (if (sample (flip x)
                     (sample (normal (* x x) 1))
                     (sample (normal (* 5 x) 1)))]
      (observe (normal y 1) 3)
      x)
```

Approx. family

```
(let [x (sample (beta  $\theta_1 \theta_2$ ))
      y (if (sample (flip  $\theta_3$ ))
                     (sample (normal  $\theta_4 \theta_5$ ))
                     (sample (normal  $\theta_6 \theta_7$ )))]
      x)
```

All data-dependencies disappear.
But finding good θ_i 's gets easier.

Basic (but not uncommon) choices.

I. Which family?

- Mean field — $q_\theta(x_1, \dots, x_n) = \prod_k q_\theta(x_k)$.

2. What does “closest” mean?

- KL divergence — $\text{KL}[q_\theta(x) \parallel p(x|y)]$.

3. How to optimize?

- Stochastic gradient descent.

Kullback-Leibler (KL) divergence

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q] What is $\text{KL}[q(x) \parallel q(x)]$?

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q] What is $\text{KL}[q(x) \parallel q(x)]$?

[A] 0

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q2] Prove $\text{KL}[q(x) \parallel p(x)] \geq 0$. And .. = 0 iff $q=p$.

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q2] Prove $\text{KL}[q(x) \parallel p(x)] \geq 0$. And .. = 0 iff $q=p$.

[Hint] $\mathbb{E}_{q(x)}[\log(f(x))] \leq \log(\mathbb{E}_{q(x)}[f(x)])$.

KL divergence

Function $d : \text{Pr}(X) \times \text{Pr}(X) \rightarrow \text{partial } \mathbb{R}$ s.t.

- (1) $d(p, q) = 0$ iff $p = q$
- (2) $d(p, q) \geq 0$

Measures the similarity between p and q .

- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q2] Prove $\text{KL}[q(x) \parallel p(x)] \geq 0$. And .. $= 0$ iff $q = p$.

[Hint] $\mathbb{E}_{q(x)}[\log(f(x))] \leq \log(\mathbb{E}_{q(x)}[f(x)])$.

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q2] Prove $\text{KL}[q(x) \parallel p(x)] \geq 0$. And .. = 0 iff $q=p$.

[Hint] $\mathbb{E}_{q(x)}[\log(f(x))] \leq \log(\mathbb{E}_{q(x)}[f(x)])$.

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q3] $\text{KL}[[0 \mapsto .1; 1 \mapsto .8; 2 \mapsto .1] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q3] $\text{KL}[[0 \mapsto .1; 1 \mapsto .8; 2 \mapsto .1] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$

[A] 1.36

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q4] $\text{KL}[[0 \mapsto .1; 1 \mapsto .1; 2 \mapsto .8] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$

[A] 1.36

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q4] $\text{KL}[[0 \mapsto .1; 1 \mapsto .1; 2 \mapsto .8] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$

[A] 0.39

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q5] $\text{KL}[[0 \mapsto .8; 1 \mapsto .1; 2 \mapsto .1] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$

[A] 0.39

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q5] $\text{KL}[[0 \mapsto .8; 1 \mapsto .1; 2 \mapsto .1] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$

[A] 0.24

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q6] $\text{KL}[[0 \mapsto .3; 1 \mapsto .4; 2 \mapsto .3] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$

[A] 0.24

KL divergence from $q(x)$ to $p(x)$

- Denoted by $\text{KL}[q(x) \parallel p(x)]$.
- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Average log ratio of two probabilities.
- Measures how $q(x)$ is close to $p(x)$.

[Q6] $\text{KL}[[0 \mapsto .3; 1 \mapsto .4; 2 \mapsto .3] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$

[A] 0.31

KL divergence from $q(x)$ to $p(x)$

- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))].$

[Q6] $\text{KL}[[0 \mapsto .3; 1 \mapsto .4; 2 \mapsto .3] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$

[A] 0.31

KL divergence from $q(x)$ to $p(x)$

- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Asymmetric.

[Q6] $\text{KL}[[0 \mapsto .3; 1 \mapsto .4; 2 \mapsto .3] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]$?

[A] 0.31

KL divergence from $q(x)$ to $p(x)$

- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Asymmetric.

[Q7] $\text{KL}[[0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4] \parallel [0 \mapsto .3; 1 \mapsto .4; 2 \mapsto .3]]?$

~~[Q6] $\text{KL}[[0 \mapsto .3; 1 \mapsto .4; 2 \mapsto .3] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$~~

[A] 0.31

KL divergence from $q(x)$ to $p(x)$

- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Asymmetric.

[Q7] $\text{KL}[[0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4] \parallel [0 \mapsto .3; 1 \mapsto .4; 2 \mapsto .3]]?$

~~[Q6] $\text{KL}[[0 \mapsto .3; 1 \mapsto .4; 2 \mapsto .3] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$~~

[A] 0.23

KL divergence from $q(x)$ to $p(x)$

- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Asymmetric.

[Q8] $\text{KL}[[0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4] \parallel [0 \mapsto .8; 1 \mapsto .1; 2 \mapsto .1]]?$

[Q6] ~~$\text{KL}[[0 \mapsto .3; 1 \mapsto .4; 2 \mapsto .3] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$~~

[A] 0.23

KL divergence from $q(x)$ to $p(x)$

- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Asymmetric.

[Q8] $\text{KL}[[0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4] \parallel [0 \mapsto .8; 1 \mapsto .1; 2 \mapsto .1]]?$

~~[Q6] $\text{KL}[[0 \mapsto .3; 1 \mapsto .4; 2 \mapsto .3] \parallel [0 \mapsto .5; 1 \mapsto .1; 2 \mapsto .4]]?$~~

[A] 0.32

KL divergence from $q(x)$ to $p(x)$

- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))]$.
- Asymmetric.

$\text{KL}[\text{approx} \parallel \text{true}]$ - mode seeking rewarded.
 $\text{KL}[\text{true} \parallel \text{approx}]$ - mode covering rewarded.

KL divergence from $q(x)$ to $p(x)$

$p = [0: 0.5, 1: 0.1, 2: 0.4]$
 $q_1 = [0: 0.7, 1: 0.2, 2: 0.1]$
 $q_2 = [0: 0.3, 1: 0.4, 2: 0.3]$
q1 and q2.
 $KL[p||q_1] = 0.32$ $KL[p||q_2] = 0.23$
 $KL[q_1||p] = 0.24$ $KL[q_2||p] = 0.31$

- $KL[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))].$
- Asymmetric.

$KL[approx \parallel true]$ - mode seeking rewarded.

$KL[true \parallel approx]$ - mode covering rewarded.

[Q9] Find best q_i s.t $KL[q_i||p]$ is minimum.

Do the same for $KL[p||q_i]$.

KL divergence from $q(x)$ to $p(x)$

- $\text{KL}[q(x) \parallel p(x)] := \mathbb{E}_{q(x)}[\log(q(x)/p(x))].$
- Asymmetric.
- Support requirement: $p(x)=0 \implies q(x)=0$.
- The closer to violation, the larger $\text{KL}[q||p]$.

Popular objective for variational inference

$$\operatorname{argmin}_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)].$$

Encourage mode seeking. Leads to q_{θ} that approximates one mode of $p(x|y)$ well.

Easier to optimise than $\text{KL}[p(x|y)||q_{\theta}(x)]$, since easier to draw samples from $q_{\theta}(x)$ than $p(x|y)$.

Basic (but not uncommon) choices.

I. Which family?

- Mean field — $q_\theta(x_1, \dots, x_n) = \prod_k q_\theta(x_k)$.

2. What does “closest” mean?

- KL divergence — $\text{KL}[q_\theta(x) \parallel p(x|y)]$.

3. How to optimize?

- Stochastic gradient descent.

**Gradient descent with
estimated gradient**

Gradient descent

Goal: $\operatorname{argmin}_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)]$.

- Hill-descending. Iteratively move θ towards the downward direction of the hill.
- “downward” means $\nabla_{\theta} \text{KL}[q_{\theta}(x)||p(x|y)]$.

Gradient descent

Pick θ_0

Gradient descent

Pick θ_1

$$\theta_2 \leftarrow \theta_1 - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_1}$$

Gradient descent

Pick θ_1

$$\theta_2 \leftarrow \theta_1 - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_1}$$



Gradient.

Direction towards minimising KL at θ_1 .

Gradient descent

Pick θ_1



Learning rate.

Some small positive number.

$$\theta_2 \leftarrow \theta_1 - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_1}$$



Gradient.

Direction towards minimising KL at θ_1 .

Gradient descent

Pick θ_1

$$\theta_2 \leftarrow \theta_1 - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_1}$$

$$\theta_3 \leftarrow \theta_2 - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_2}$$

Gradient descent

Pick θ_1

$$\theta_2 \leftarrow \theta_1 - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_1}$$

$$\theta_3 \leftarrow \theta_2 - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_2}$$

$$\theta_4 \leftarrow \theta_3 - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_3}$$

...

$$\theta_{n+1} \leftarrow \theta_n - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_n}$$

Gradient descent

Pick θ_1

Difficult to compute
gradient analytically.

$$\theta_2 \leftarrow \theta_1 - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_1}$$

$$\theta_3 \leftarrow \theta_2 - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_2}$$

$$\theta_4 \leftarrow \theta_3 - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_3}$$

...

$$\theta_{n+1} \leftarrow \theta_n - \eta \times (\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)])_{\theta=\theta_n}$$

Stochastic gradient descent

Estimate the gradient using samples.

Stochastic gradient descent

Estimate the gradient using samples.

That is,

$$\nabla_{\theta} \text{KL}[q_{\theta}(x) || p(x|y)] \approx 1/N \times \sum_{i=1..N} f(x_i, \theta)$$

where

1. samples x_1, \dots, x_N are drawn from q_{θ} ;
2. function f is chosen by an estimator.

Stochastic gradient descent

Estimate the gradient using samples.

That is,

$$\nabla_{\theta} \text{KL}[q_{\theta}(x) || p(x|y)] \approx 1/N \times \sum_{i=1..N} f(\mathbf{x}_i, \theta)$$

where

1. samples $\mathbf{x}_1, \dots, \mathbf{x}_N$ are drawn from q_{θ} ;
2. function f is chosen by an estimator.

Stochastic gradient descent

Estimate the gradient using samples.

That is,

$$\nabla_{\theta} \text{KL}[q_{\theta}(x) || p(x|y)] \approx 1/N \times \sum_{i=1..N} f(x_i, \theta)$$

where

1. samples x_1, \dots, x_N are drawn from q_{θ} ;
2. function f is chosen by an estimator.

$$\nabla_{\theta} \text{KL}[q_{\theta}(x) || p(x|y)] \approx 1/N \times \sum_{i=1..N} f(x_i, \theta)$$

for x_1, \dots, x_N drawn from q_{θ} .

$$\nabla_{\theta} \text{KL}[q_{\theta}(x) || p(x|y)] \approx 1/N \times \sum_{i=1..N} f(x_i, \theta)$$

for x_1, \dots, x_N drawn from q_{θ} .

Score estimator (aka REINFORCE):

$$f(x, \theta) = (\nabla_{\theta} \log(q_{\theta}(x))) \times \log(q_{\theta}(x)/p(x,y))$$

$$\nabla_{\theta} \text{KL}[q_{\theta}(x) || p(x|y)] \approx 1/N \times \sum_{i=1..N} f(x_i, \theta)$$

for x_1, \dots, x_N drawn from q_{θ} .

Score estimator (aka REINFORCE):

$$f(x, \theta) = (\nabla_{\theta} \log(q_{\theta}(x))) \times \log(q_{\theta}(x)/p(x,y))$$

I. Direction to increase probability of x

$$\nabla_{\theta} \text{KL}[q_{\theta}(x) || p(x|y)] \approx 1/N \times \sum_{i=1..N} f(x_i, \theta)$$

for x_1, \dots, x_N drawn from q_{θ} .

Score estimator (aka REINFORCE):

$$f(x, \theta) = (\nabla_{\theta} \log(q_{\theta}(x))) \times \log(q_{\theta}(x)/p(x,y))$$

- I. Direction to increase probability of x
weighted by its log ratio.

$$\nabla_{\theta} \text{KL}[q_{\theta}(x) || p(x|y)] \approx 1/N \times \sum_{i=1..N} f(x_i, \theta)$$

for x_1, \dots, x_N drawn from q_{θ} .

Score estimator (aka REINFORCE):

$$f(x, \theta) = (\nabla_{\theta} \log(q_{\theta}(x))) \times \log(q_{\theta}(x)/p(x,y))$$

1. Direction to increase probability of x weighted by its log ratio.
2. No need to know $p(y)$.

$$\nabla_{\theta} \text{KL}[q_{\theta}(x) || p(x|y)] \approx 1/N \times \sum_{i=1..N} f(x_i, \theta)$$

for x_1, \dots, x_N drawn from q_{θ} .

Score estimator (aka REINFORCE):

$$f(x, \theta) = (\nabla_{\theta} \log(q_{\theta}(x))) \times \log(q_{\theta}(x)/p(x,y))$$

1. Direction to increase probability of x weighted by its log ratio.
2. No need to know $p(y)$.
3. $p(x,y)$ don't have to be differentiable wrt. x .

Score estimator

Goal: Estimate $\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)]$

I. Sample x_1, \dots, x_N from $q_{\theta}(x)$.

2. Return:

$$\frac{1}{N} \times \sum_{i=1..N} (\nabla_{\theta} \log(q_{\theta}(x_i)) \times \log(q_{\theta}(x_i)/p(x,y)))$$

Score estimator

Do the most of the derivation, but leave some part to the students.

Goal: Estimate $\nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)]$

- I. Sample x_1, \dots, x_N from $q_{\theta}(x)$.
2. Return:

$$1/N \times \sum_{i=1..N} (\nabla_{\theta} \log(q_{\theta}(x_i)) \times \log(q_{\theta}(x_i)/p(x,y)))$$

[Q] Prove that this estimator is unbiased. That is,

$$\mathbb{E}[1/N \times \sum_{i=1..N} (\nabla_{\theta} \log(q_{\theta}(x_i)) \times \log(q_{\theta}(x_i)/p(x,y)))]$$

$$= \nabla_{\theta} \text{KL}[q_{\theta}(x) \parallel p(x|y)]$$

Implementing this for
probabilistic programs

- Blackboard lecture.
- Look at the last part of Note6.pdf (for operational semantics) in the webpage.

Reference

1. Ranganath et al.'s AISTATS'14 paper "Black-Box Variational Inference" (<https://arxiv.org/abs/1401.0118>).
2. Section 7 of Tolpin et al.'s IFL'16 paper "Design and implementation of probabilistic programming language Anglican" (<https://arxiv.org/abs/1608.05263>)