CS423: Probabilistic Programming

Variational Inference

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Posterior inference

Given:

- Prior p(x) and likelihood p(y|x).
- Observation 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.

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Variational inference:

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

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Uber's pyro
Google's Edward
Anglican, Stan

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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)
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    (map f (list 0.8  1.2  7.8  2.4  8.2
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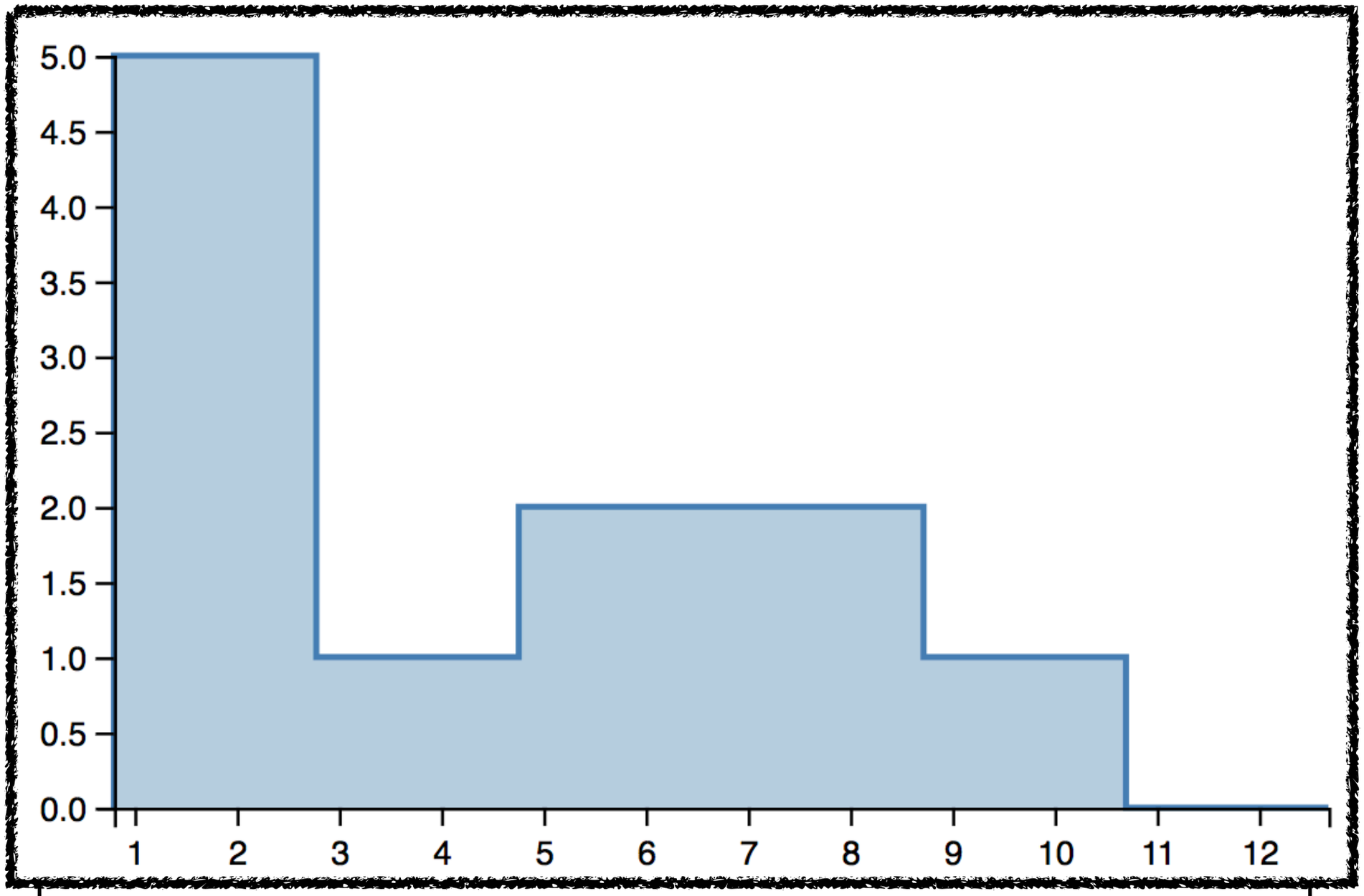


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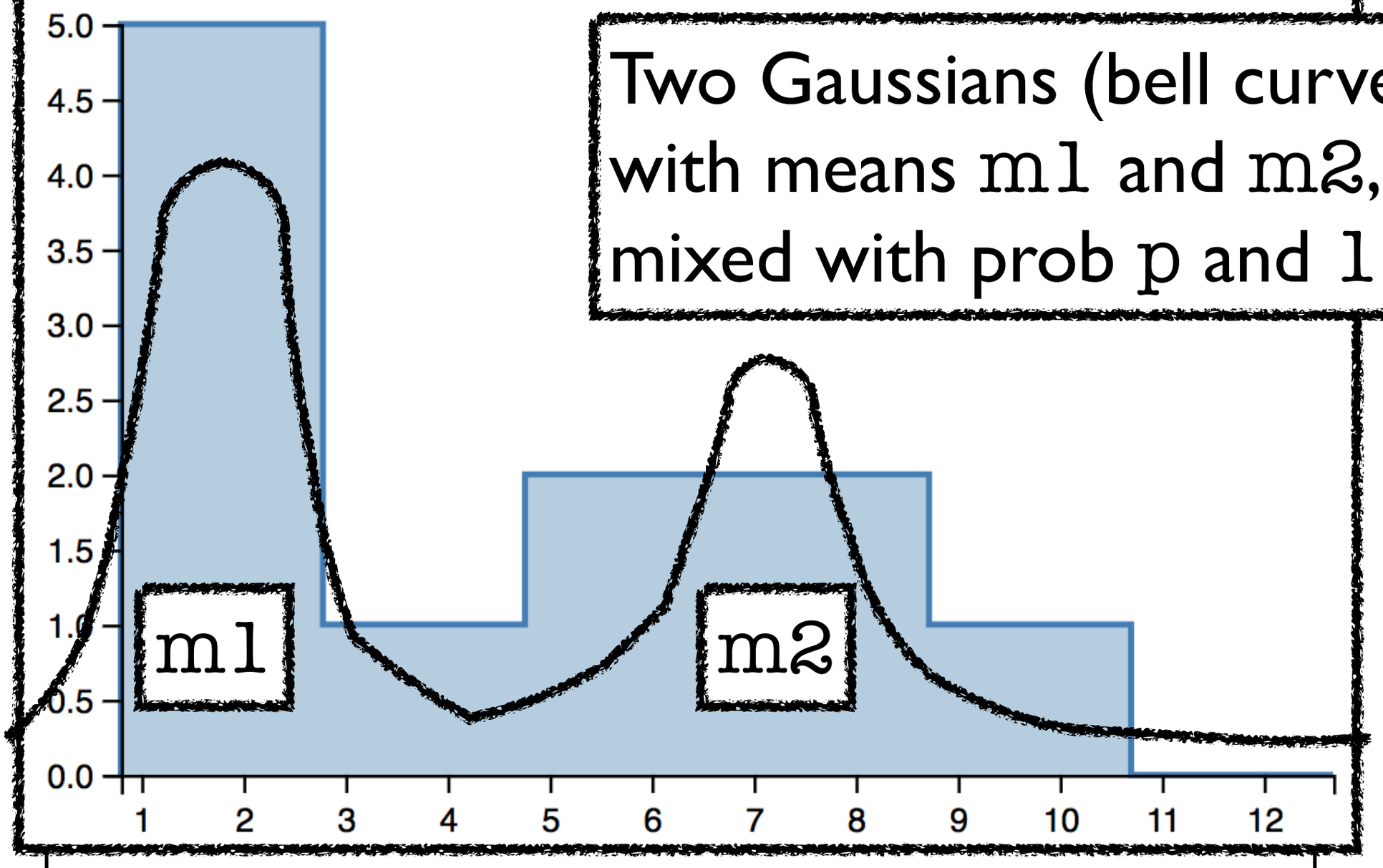
Two Gaussians (bell curves) with means `m1` and `m2`, mixed with prob `p` and `1-p`

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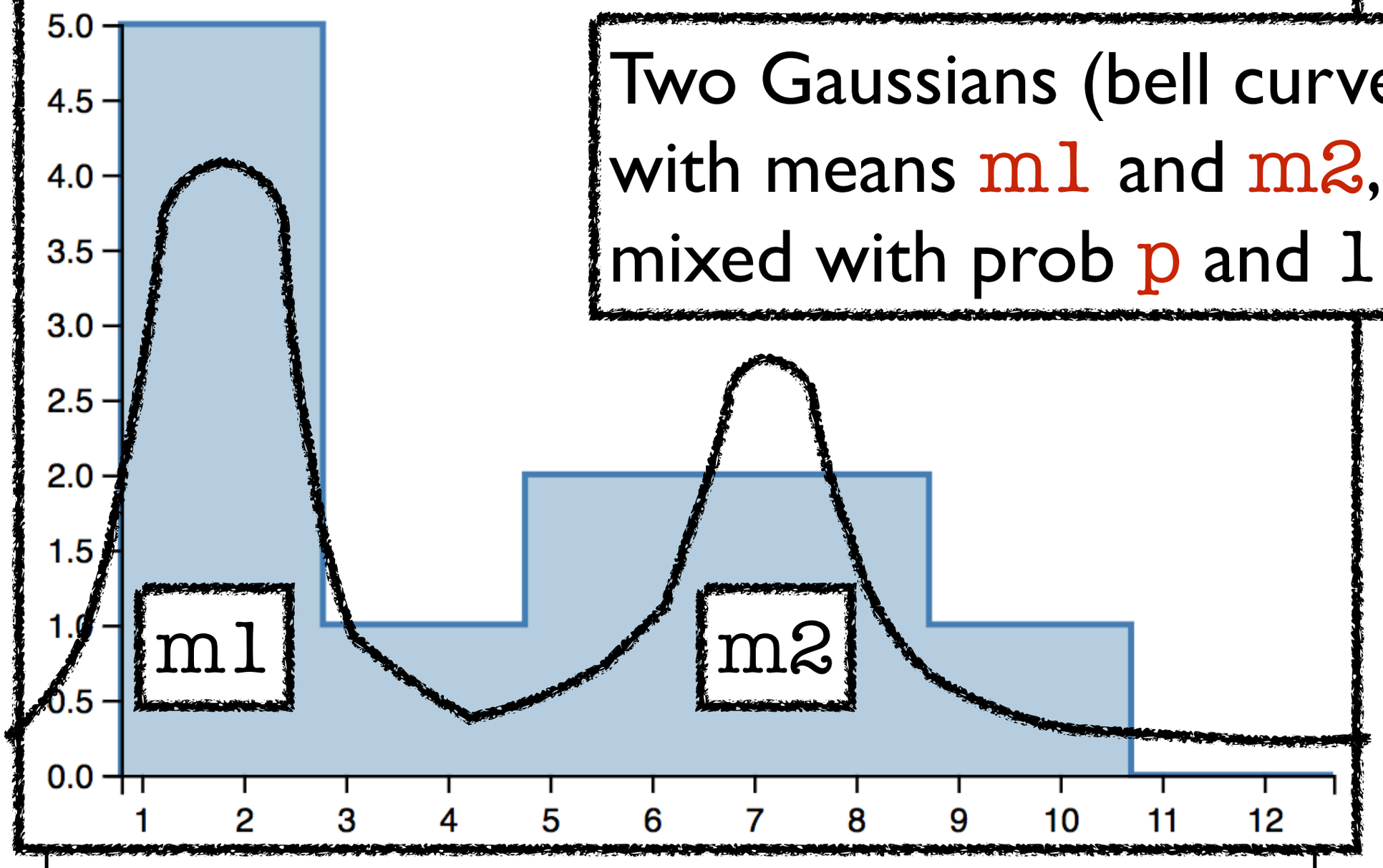


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Mixture of two Gaussians

Labels for sample expressions

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Mixture of two Gaussians

Distribution on [0,1]
Uniform in this case

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Means “black-box variational Bayes”
Stochastic variational-inference algorithm

```
        m2 (sample :m2 (normal 0 5))
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             (if (sample (flip p))
               (observe (normal m1 1.) y)
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(defquery mixture-posterior-approx []
  (let [p  (sample :p (beta 1 1))
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Approx. by Anglican query

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Approx. by Anglican query

(1) No obs.

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```
(defquery mixture-posterior-approx []
  (let [p   (sample :p (beta θ1 θ2))
        m1 (sample :m1 (normal θ3 θ4))
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        f    (fn [y]
               (if (sample (flip θ7))
                 (observe (normal m1 1.) y)
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    (map f (list 0.8 1.2 7.8 8.4 8.2
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Approx. by Anglican query
(1) No obs. (2) New params.

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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. $p(x|y)$.

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Don't sum. Optimise.

Variatic

Three choices:

1. Fix a family of approximating distr. $\{q_\theta(x)\}_\theta$.
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Three choices:
(1) Which family?

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Three choices:
(1) Which family?
(2) What does "closest" mean?

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Basic (but not uncommon) choices.

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

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Mean-field approximation

Mean-field approximation

Approximating distribution q_θ formed by independent random variables:

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

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 (sample (dist e_1 … e_n)) by (sample (dist θ_1 … θ_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)
```

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Approx. family

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Approx. family

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(let [x  (sample (beta θ1 θ2))
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             (sample (normal θ4 θ5))
             (sample (normal θ6 θ7)))]


 x)
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Model

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(let [x (sample (beta θ1 θ2))
      y (if (sample (flip θ3))
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  x)
```

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

Basic (but not uncommon) choices.

1. Which family?

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

2. What does “closest” mean?

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

3. How to optimize?

   - Stochastic gradient descent.

Kullback-Leibler (KL) divergence

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

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

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[Q1] What is KL[q(x) || q(x)]?

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[Q1] What is KL[q(x) || q(x)]?

[A] 0

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

- Denoted by KL[q(x) || p(x)].
- KL[q(x) || p(x)] := $\mathbb{E}_{q(x)}$[log(q(x)/p(x))].
  - Average log ratio of two probabilities.
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[Q2] Prove KL[q(x) || p(x)]≥0. And .. =0 iff q=p.

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

KL divergence

Function d : Pr(X) × Pr(X) →partial $\mathbb{R}$ s.t.
(1) d(p,q) = 0 iff p=q
(2) d(p,q) ≥ 0
Measures the similarity between p and q.

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

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[Q3] KL[[0↦.1;1↦.8;2↦.1] || [0↦.5;1↦.1;2↦.4]]?

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[Q3] KL[[0↦.1;1↦.8;2↦.1] || [0↦.5;1↦.1;2↦.4]]?

[A] 1.36

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[Q4] KL[[0↦.1;1↦.1;2↦.8] || [0↦.5;1↦.1;2↦.4]]?

[A] 1.36

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

[Q4] KL[[0↦.1;1↦.1;2↦.8] || [0↦.5;1↦.1;2↦.4]]?

[A] 0.39

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

- Denoted by KL[q(x) || p(x)].
- KL[q(x) || p(x)] := $\mathbb{E}_{q(x)}$[log(q(x)/p(x))].
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  - Measures how much q(x) is close to p(x).

[Q5] KL[[0↦.8;1↦.1;2↦.1] || [0↦.5;1↦.1;2↦.4]]?

[A] 0.39

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

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

[Q5] KL[[0↦.8;1↦.1;2↦.1] || [0↦.5;1↦.1;2↦.4]]?

[A] 0.24

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

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

[Q6] KL[[0↦.3;1↦.4;2↦.3] || [0↦.5;1↦.1;2↦.4]]?

[A] 0.24

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

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

[Q6] KL[[0↦.3;1↦.4;2↦.3] || [0↦.5;1↦.1;2↦.4]]?

[A] 0.31

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

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

[Q6] KL[[0↦.3;1↦.4;2↦.3] || [0↦.5;1↦.1;2↦.4]]?

[A] 0.31

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

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

[Q6] KL[[0↦.3;1↦.4;2↦.3] || [0↦.5;1↦.1;2↦.4]]?

[A] 0.31

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

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

[Q7] KL[[0↦.5;1↦.1;2↦.4] || [0↦.3;1↦.4;2↦.3]]?

~~[Q6] KL[[0↦.3;1↦.4;2↦.3] || [0↦.5;1↦.1;2↦.4]]?~~

[A] 0.31

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

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

[Q7] KL[[0↦.5;1↦.1;2↦.4] || [0↦.3;1↦.4;2↦.3]]?

~~[Q6] KL[[0↦.3;1↦.4;2↦.3] || [0↦.5;1↦.1;2↦.4]]?~~

[A] 0.23

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

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

[Q8] KL[[0↦.5;1↦.1;2↦.4] || [0↦.8;1↦.1;2↦.1]]?

~~[Q6] KL[[0↦.3;1↦.4;2↦.3] || [0↦.5;1↦.1;2↦.4]]?~~

[A] 0.23

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

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

[Q8] KL[[0↦.5;1↦.1;2↦.4] || [0↦.8;1↦.1;2↦.1]]?

~~[Q6] KL[[0↦.3;1↦.4;2↦.3] || [0↦.5;1↦.1;2↦.4]]?~~

[A] 0.32

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

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

KL[approx || true] - mode seeking rewarded.
KL[true || approx] - mode covering rewarded.

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

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- Asymmetric.

KL[approx || true] - mode seeking rewarded.
KL[true || 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)

- KL[q(x) || 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 KL[q||p].

Popular objective for variational inference

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

Encourage mode seeking. Leads to q_θ that approximates one mode of $p(x|y)$ well.

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

Basic (but not uncommon) choices.

1. Which family?

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

2. What does “closest” mean?

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

3. How to optimize?

   - Stochastic gradient descent.

Gradient descent with estimated gradient

Gradient descent

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

- 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_1

Gradient descent

Pick θ_1

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

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Gradient.
Direction towards minimising KL at θ_1.

Gradient descent

Learning rate.
Some small positive number.

Pick θ_1

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

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…

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

Gradient descent

Difficult to compute gradient analytically.

Pick θ_1

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

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Estimate the gradient using samples.

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That is,

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

where

1. samples $x_1, \ldots, x_N$ are drawn from q_θ;

2. function f is chosen by an estimator.

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

for $x_1, \ldots, x_N$ drawn from q_θ.

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

for $x_1, \ldots, x_N$ drawn from q_θ.

Score estimator (aka REINFORCE):

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

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1. Direction to increase probability of x

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

for $x_1, \ldots, x_N$ 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.

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

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

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Score estimator (aka REINFORCE):

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1. Direction to increase probability of x weighted by its log ratio.
2. No need to know p(y).
3. p(x,y) needs not be differentiable wrt. x.

Score estimator

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

1. Sample $x_1, \ldots, x_N$ from $q_\theta(x)$.
2. Return:

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

Score estimator

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

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

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

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

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

Implementing algo. for probabilistic programs

- Blackboard lecture.

- Look at the handwritten note and its correction in the web page.

- Also, have a look at the last part of Note6.pdf (for operational semantics).

Reference

1. Ranganath et al.'s AISTATS14 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)