Machine Learning

Deterministic Approximative Inference

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Big Number

$$p(y) = \sum_{n=1}^{N} p(y, x_i)$$

- Number of atoms in the universe

$$10^{80} \approx (2^{\frac{10}{3}})^{80} \approx 2^{267}$$

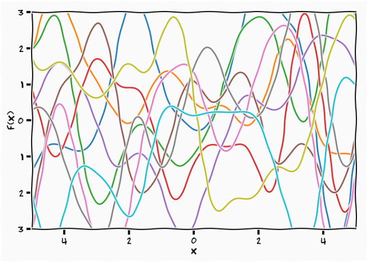
- Age of the universe in seconds

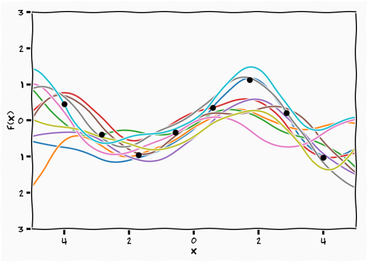
$$4.35 \cdot 10^{17} \approx 2^{59}$$

Big Number

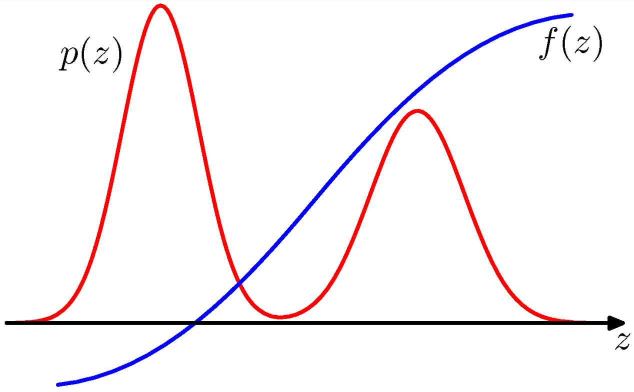
$$\infty$$

Big Number





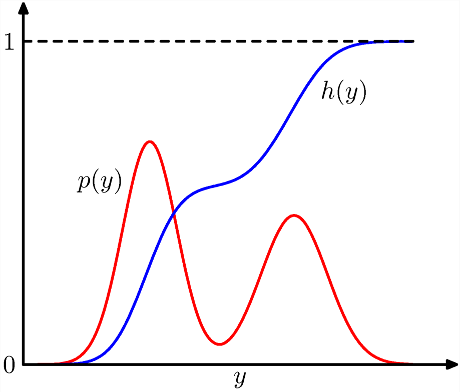
$$p(\mathbf{y}|\mathbf{x}) = \int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{x})\mathrm{d}\mathbf{f}$$



$$\mathbb{E}_{p(z)}[f] = \int f(z)p(z)\mathrm{d}z \approx \frac{1}{L}\sum_{l=1}^{L} f(z^{(l)})$$

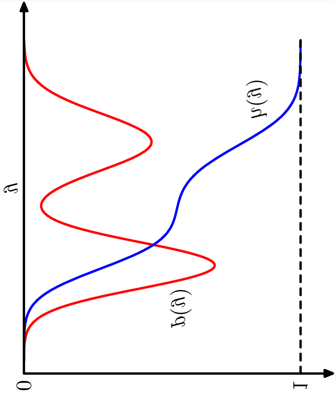
$$\mathbf{z}^{(l)} \sim p(\mathbf{z})$$

Basic Probabilities



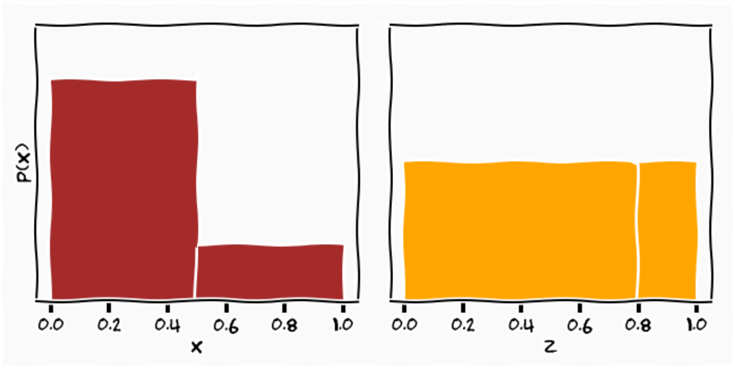
$$z = h(y) = \int_{-\infty}^{y} p(y)\mathrm{d}y$$

Basic Probabilities



$$y = h^{-1}(z)$$

Change of Variables



Change of Variables

$$\int_{y \in \mathcal{Y}} p(y) \mathrm{d}y = \int_{x \in \mathcal{X}} p(x) \mathrm{d}x$$

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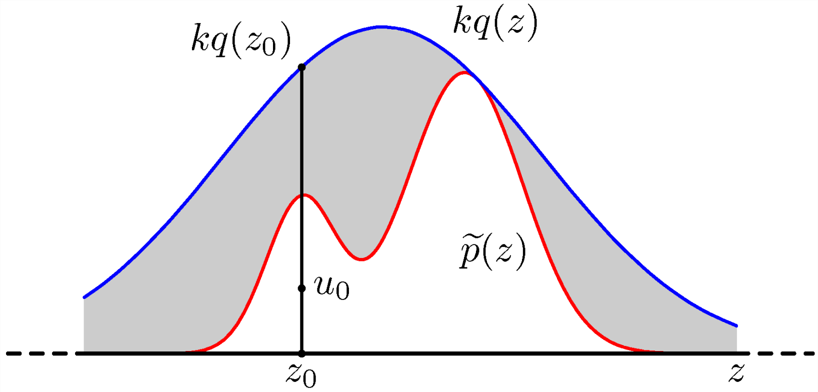
$$p(y) = p(x(y)) \frac{\mathrm{d}x}{\mathrm{d}y}$$

Starting point

- We can sample random numbers from the uniform distribution
- We can using the indefinite integral to transform the uniform to any distribution
- Want to use these distributions as proxies

Rejection Sampling



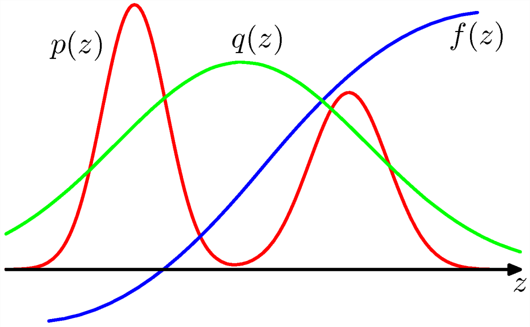
Importance Sampling Ch 11.1.4 [1]

$$\mathbb{E}_{p(\mathbf{z})}[f] = \int f(\mathbf{z}) p(\mathbf{z}) \mathrm{d}\mathbf{z} = \int f(\mathbf{z}) \frac{p(\mathbf{z})}{q(\mathbf{z})} q(\mathbf{z}) \mathrm{d}\mathbf{z} = \mathbb{E}_{q(\mathbf{z})}\left[f(\mathbf{z}) \frac{p(\mathbf{z})}{q(\mathbf{z})} \right]$$

$$\approx \frac{1}{L} \sum_{l=1}^{L} \frac{p(z^{(l)})}{q(z^{(l)})} \cdot f(\mathbf{z}^{(l)})$$

- Sample from proposal distribution and re-weight samples
- Accepts all samples

Importance Sampling



$$r_l = \frac{p(z^{(l)})}{q(z^{(l)})}$$

Metropolis Sampling

1. start with state $\mathbf{z}^{(0)}$

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   - if $A(\mathbf{z}^*, \mathbf{z}^{(0)}) > u \rightarrow \mathbf{z}^{(1)} = \mathbf{z}^*$
   - otherwise reject $\mathbf{z}^*$ and start over

Gibbs Sampling [1]

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5. cycle through variables

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- Create a random walk to encourage exploration
  - Gibbs sampling

Deterministic Approximations

Introduction

- Stochastic inference
  - approximate expectation with sum
  - works in the limit
  - hard to know how well we are doing
  - usually slow

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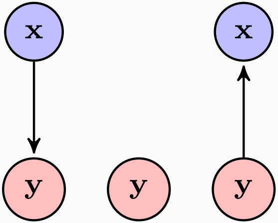
- Stochastic inference
  - approximate expectation with sum
  - works in the limit
  - hard to know how well we are doing
  - usually slow
- Idea
  - *can we reformulate inference as optimisation?*

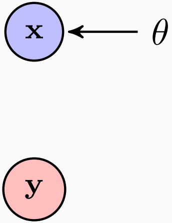
Machine Learning

$$p(\mathbf{Y})$$

- Given some observed data $\mathbf{Y}$
- Find a probabilistic model such that the probability of the data is maximised
- Idea: find an approximate model q that we can integrate

Lower Bound

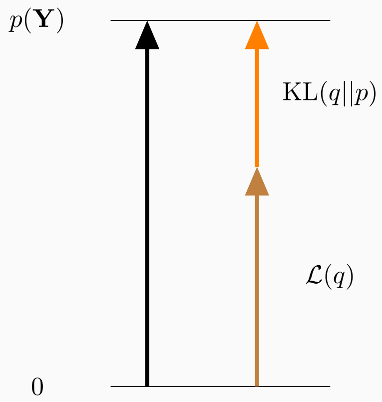


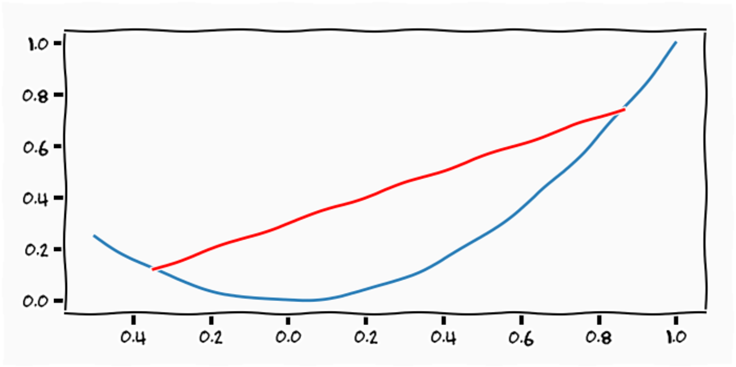


$$p(\mathbf{y}) = \int_{\mathbf{x}} p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{x}|\mathbf{y})}$$

$$q_\theta(\mathbf{x}) \approx p(\mathbf{x}|\mathbf{y})$$

Deterministic Approximation





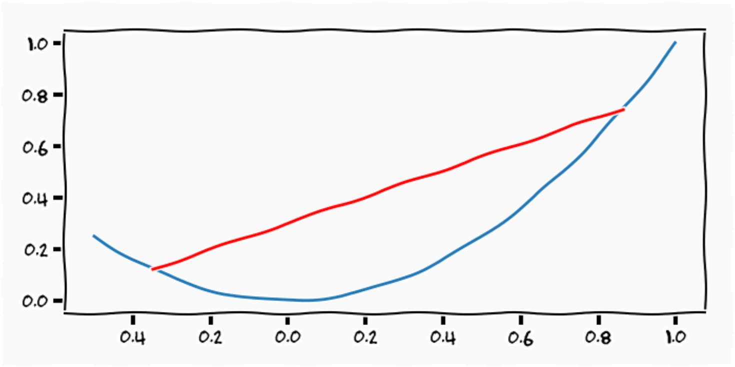
Convex Function

$$\lambda f(x_0) + (1-\lambda)f(x_1) \geq f(\lambda x_0 + (1-\lambda)x_1)$$

$$x \in [x_{min}, x_{max}]$$

$$\lambda \in [0,1]]$$

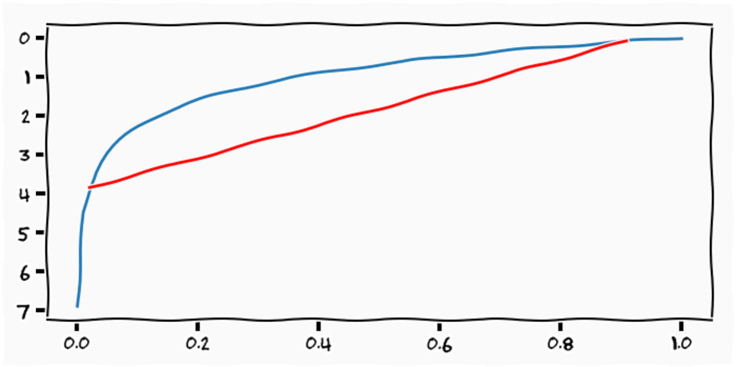
Jensen Inequality



$$\mathbb{E}[f(x)] \geq f(\mathbb{E}[x])$$

$$\int f(x)p(x)\mathrm{d}x \geq f\left(\int xp(x)\mathrm{d}x\right)$$

Jensen Inequality in Variational Bayes



$$\int \log(x)p(x)\mathrm{d}x \leq \log\left(\int xp(x)\mathrm{d}x\right)$$

moving the log inside the the integral is a lower-bound on the integral

Variational Bayes

$$p(y)$$

Variational Bayes

$$\log p(y)$$

Variational Bayes

$$\log\, p(y) = \log\, p(y) + \int \log\, \frac{p(x|y)}{p(x|y)} \mathrm{d}x$$

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$$\log\, p(y) = \log\, p(y) + \int \log\, \frac{p(x|y)}{p(x|y)} \mathrm{d}x$$
$$= \int q(x) \log\, p(y) \mathrm{d}x + \int q(x) \log\, \frac{p(x|y)}{p(x|y)} \mathrm{d}x$$

Variational Bayes

$$
\begin{aligned}
\log\, p(y) &= \log\, p(y) + \int \log\, \frac{p(x|y)}{p(x|y)} \mathrm{d}x \\
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$$= \int q(x) \log\, \frac{p(x|y)p(y)}{p(x|y)} \mathrm{d}x$$

$$= \int q(x) \log\, \frac{q(x)}{q(x)} \mathrm{d}x + \int q(x) \log\, p(x, y) \mathrm{d}x + \int q(x)\, \log\, \frac{1}{p(x|y)} \mathrm{d}x$$

$$
\begin{aligned}
\log p(y) &= \log p(y) + \int \log \frac{p(x|y)}{p(x|y)} \mathrm{d}x \\
&= \int q(x) \log p(y) \mathrm{d}x + \int q(x) \log \frac{p(x|y)}{p(x|y)} \mathrm{d}x \\
&= \int q(x) \log \frac{p(x|y)p(y)}{p(x|y)} \mathrm{d}x \\
&= \int q(x) \log \frac{q(x)}{q(x)} \mathrm{d}x + \int q(x) \log p(x,y) \mathrm{d}x + \int q(x) \log \frac{1}{p(x|y)} \mathrm{d}x \\
&= {\color{blue}\int q(x) \log \frac{1}{q(x)} \mathrm{d}x + \int q(x) \log p(x,y) \mathrm{d}x} + {\color{red}\int q(x) \log \frac{q(x)}{p(x|y)} \mathrm{d}x}
\end{aligned}
$$

The "posterior" term

$$KL(q(x)||q(x|y)) = \int q(x) \log \frac{q(x)}{p(x|y)} \mathrm{d}x$$

The "posterior" term

$$
\begin{aligned}
\color{red}{KL(q(x)||q(x|y))} &= \int q(x) \log \frac{q(x)}{p(x|y)} \mathrm{d}x \\
&= -\int q(x) \log \frac{p(x|y)}{q(x)} \mathrm{d}x
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KL(q(x)||q(x|y)) &= \int q(x)\,\log\frac{q(x)}{p(x|y)}\mathrm{d}x \\
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&\geq -\log\int p(x|y)\mathrm{d}x = -\log 1 = 0
\end{aligned}
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&= \int p(x|y)\, \log \underbrace{\frac{p(x|y)}{p(x|y)}}_{=1} \mathrm{d}x \\
&= 0
\end{aligned}
$$

Kullback-Leibler Divergence

$$KL(q(x)||p(x|y)) = \int q(x) \log \frac{q(x)}{p(x|y)} \mathrm{d}x$$

- Measure of divergence between distributions
- Not a metric (not symmetric)
- $KL(q(x)||p(x|y)) = 0 \Leftrightarrow q(x) = p(x|y)$
- $KL(q(x)||p(x|y)) \geq 0$

The "other terms"

$$\int q(x) \log \frac{1}{q(x)} \mathrm{d}x + \int q(x) \log p(x, y) \mathrm{d}x =$$

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$$= \underbrace{\int p(x|y)\mathrm{d}x}_{=1} \log p(y) = \log p(y)$$

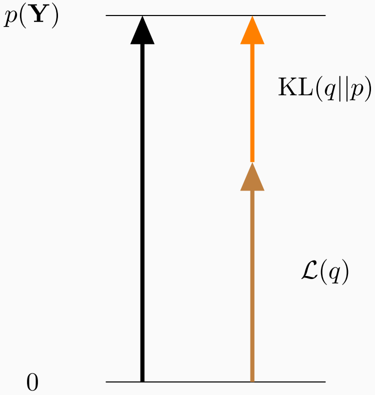
Variational Bayes

$$\log\, p(y) = \int q(x)\log\,\frac{1}{q(x)}\mathrm{d}x + \int q(x)\log\, p(x,y)\mathrm{d}x + \int q(x)\ \log\,\frac{q(x)}{p(x|y)}\mathrm{d}x$$

$$\geq -\int q(x)\log\, q(x)\mathrm{d}x + \int q(x)\log\, p(x,y)\mathrm{d}x$$

- The Evidence Lower BOnd
- Tight if $q(x) = p(x|y)$

Deterministic Approximation

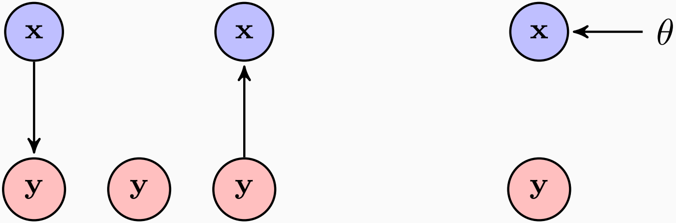


ELBO

$$\log p(y) \geq -\int q(x)\log q(x)\mathrm{d}x + \int q(x)\log p(x,y)\mathrm{d}x$$
$$= \mathbb{E}_{q(x)}\left[\log p(x,y)\right] - H(q(x)) = \mathcal{L}(q(x))$$

- if we maximise the ELBO we,
    - find an approximate posterior
    - lower bound the marginal likelihood
- *maximising* $p(y)$ is learning
- finding $q(x) \approx p(x|y)$ is prediction

Lower Bound



$$p(\mathbf{y}) = \int_{\mathbf{x}} p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{x}|\mathbf{y})}$$

$$q_\theta(\mathbf{x}) \approx p(\mathbf{x}|\mathbf{y})$$

Why is this useful?

Why is this a sensible thing to do?

– Ryan Adams[1]

[1] Talking Machines Season 2, Episode 5

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- If we can't formulate the joint distribution there isn't much we can do
- Taking the expectation of a log is usually easier than the expectation
- We are allowed to choose the distribution to take the expectation over

– Ryan Adams[1]

[1] Talking Machines Season 2, Episode 5

How to choose Q?

$$\mathcal{L}(q(x)) = \mathbb{E}_{q(x)}\left[\log p(x,y)\right] - H(q(x))$$

- We have to be able to compute an expectation over the joint distribution
- The second term should be trivial

Mean Field Approximation

$$q(\mathbf{X}) = \prod_i q_i(\mathbf{x}_i)$$
$$\mathcal{L}(q_j) = \mathcal{L}_j(q_j) + \mathcal{L}_{\neg j}(q_{\neg j}),$$

- Model originating if Physics
- We model marginals rather than the full distribution
- We can update each distribution in turn and cycle

Mean Field Variational Bayes

1. Formulate joint distribution over data and latent parameters

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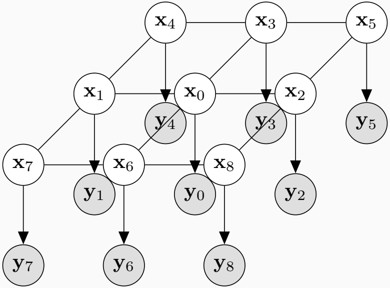
3. Fit marginal approximation by making bound tight
4. Iterate through variables

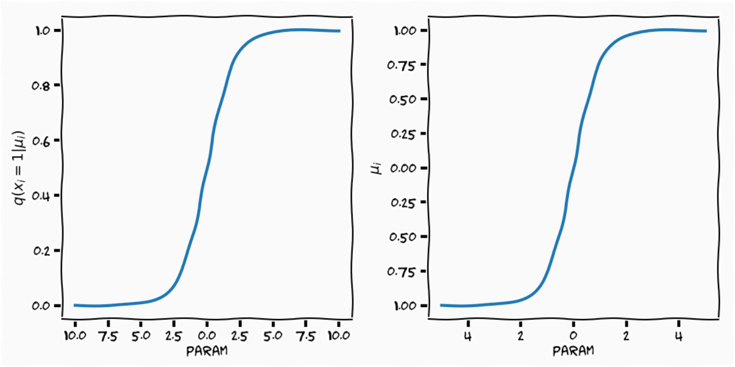
Lab



$$q(\mathbf{x}, \boldsymbol{\mu}) = \prod_{i}^{N} q(x_i, \mu_i)$$

$$\mu_i = \mathbb{E}[x_i]$$

Lab



$q(x_i = 1|\mu_i)$
1.0
0.8
0.6
0.4
0.2
0.0
10.0
7.5
5.0
2.5
0.0
2.5
5.0
7.5
10.0
PARAM
μ_i
1.00
0.75
0.50
0.25
0.00
0.25
0.50
0.75
1.00
4
2
0
2
4
PARAM

Summary

Summary

- Variational methods can be very efficient
  - really fun to work with
- Can be made black-box [2]
- Will never be correct
- Provides us with approximative posterior for predictions

eof

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