Approximate Inference for Neural Networks

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Outline

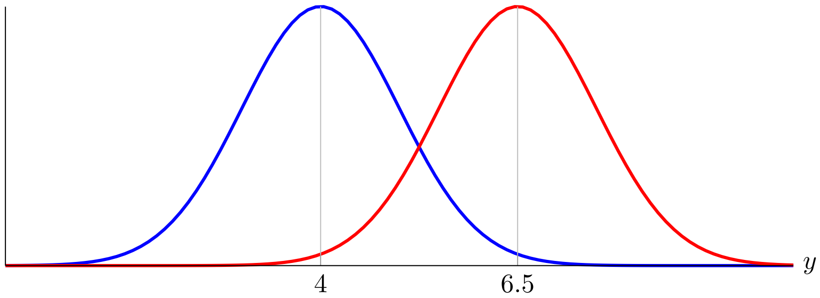
Outline

1. **EM algorithm**

2. **Variational EM**

3. **Approximate inference for Neural Networks**
   - Bayesian Deep Neural Networks
   - Laplace Approximation

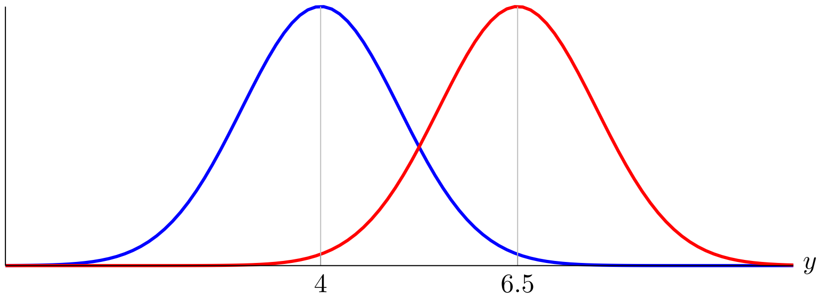
Problem definition - Example



z_n

y_n

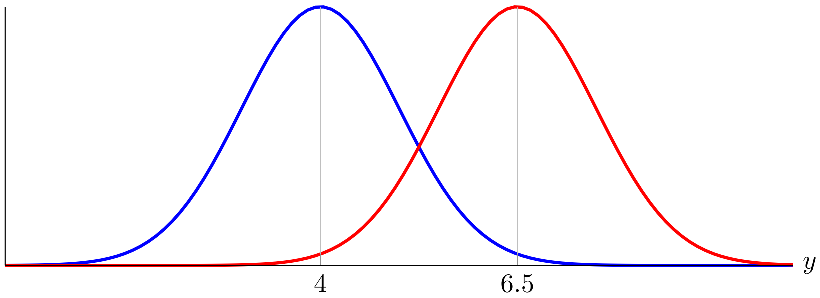
Problem definition - Example



z_n $\quad$ 0

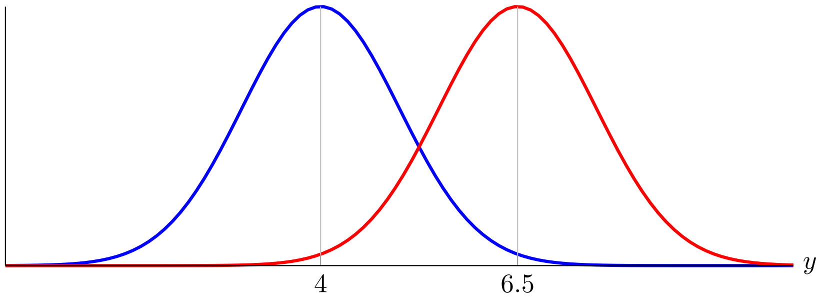
y_n

Problem definition - Example



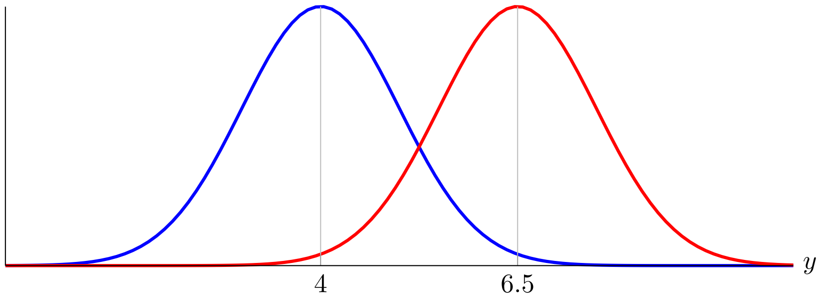
z_n	0
y_n	4.3

Problem definition - Example



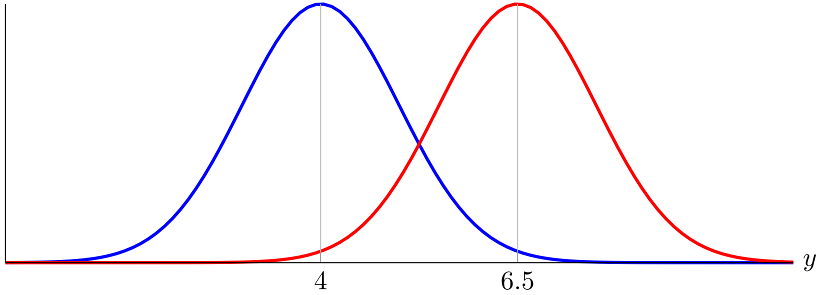
z_n	0	1
y_n	4.3	

Problem definition - Example



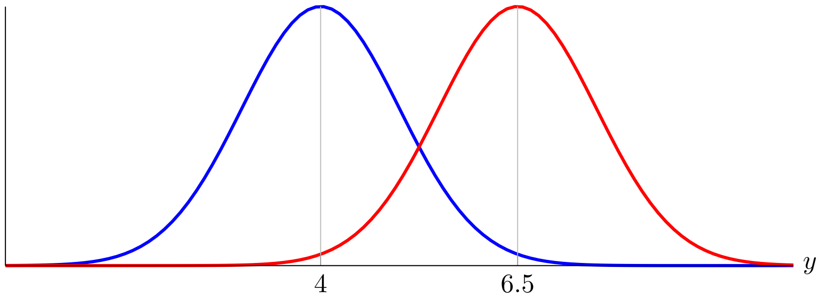
z_n	0	1
y_n	4.3	6.0

Problem definition - Example



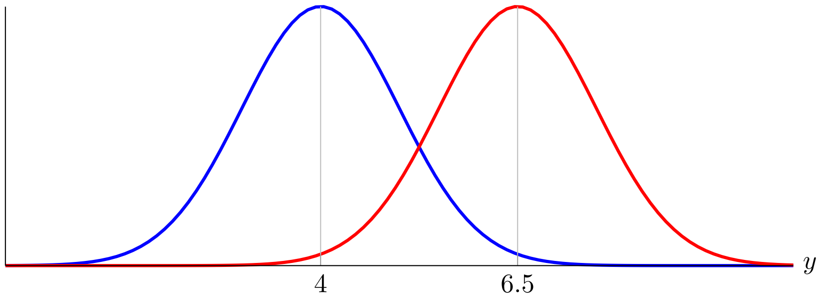
z_n	0	1	1
y_n	4.3	6.0	

Problem definition - Example



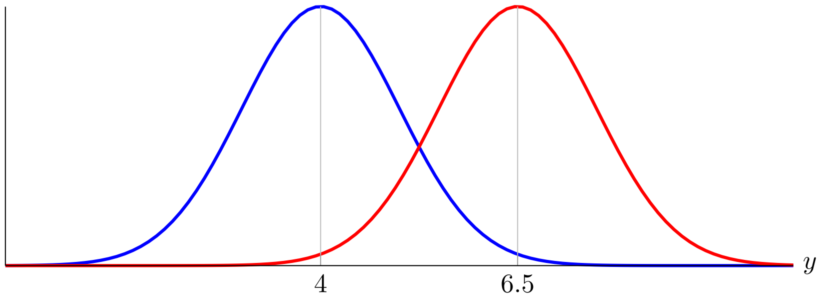
z_n	0	1	1
y_n	4.3	6.0	7.2

Problem definition - Example



z_n	0	1	1	0
y_n	4.3	6.0	7.2	

Problem definition - Example



z_n	0	1	1	0
y_n	4.3	6.0	7.2	3.8

Problem definition - Example

For z:

$$p(z) = \pi^z (1-\pi)^{1-z}, \quad p(z=1) = \pi, \quad p(z=0) = 1-\pi.$$

For y:

$$p(y|z) = \left(\mathcal{N}\left(y|\mu_1, \sigma_1^2\right)\right)^z \left(\mathcal{N}\left(y|\mu_2, \sigma_2^2\right)\right)^{1-z}.$$

The the joint probability:

$$p(y, z) = \left(\pi\mathcal{N}\left(y|\mu_1, \sigma_1^2\right)\right)^z \left((1-\pi)\mathcal{N}\left(y|\mu_2, \sigma_2^2\right)\right)^{1-z}.$$

Additionally:

$$\begin{aligned} p(z=1|y) &= \frac{p(y|z=1)p(z=1)}{p(y)} \\ &= \frac{\mathcal{N}(y|\mu_1, \sigma_1^2)\pi}{\pi\mathcal{N}\left(y|\mu_1, \sigma_1^2\right) + (1-\pi)\mathcal{N}\left(y|\mu_2, \sigma_2^2\right)} \end{aligned}$$

Problem definition - Example

Let's assume that we have $(\mathbf{y}, \mathbf{z}) = \{y_n, z_n\}_{n=1}^{N}$.
The parameters $\theta = \{\pi, \mu_1, \mu_2, \sigma_1^2, \sigma_2^2\}$, can be estimated as

$$\begin{aligned}
\theta_{\mathsf{ML}} &= \arg\max_{\theta} \; \ln\left(p(\mathbf{y}, \mathbf{z}|\theta)\right), \\
&= \arg\max_{\theta} \; \ln\left(\prod_{n=1}^{N} p(y_n, z_n|\theta)\right), \\
&= \arg\max_{\theta} \sum_{n=1}^{N} \ln\left(p(y_n, z_n|\theta)\right).
\end{aligned}$$

Where:

$$\begin{aligned}
\ln p(y_n, z_n|\theta) =& z_n \left(\color{red}{\ln(\pi) + \ln\mathcal{N}\left(y_n|\mu_1, \sigma_1^2\right)}\right) \\
&+ (1 - z_n)\left(\color{blue}{\ln(1-\pi) + \ln\mathcal{N}\left(y_n|\mu_2, \sigma_2^2\right)}\right).
\end{aligned}$$

Problem definition - Example

Let's assume that $\mathbf{y} = \{y_n\}_{n=1}^N$, y $\mathbf{z}$ is unknown (latent).
The parameters $\theta = \{\pi, \mu_1, \mu_2, \sigma_1^2, \sigma_2^2\}$, can be estimated as

$$
\begin{aligned}
\theta_{\text{ML}} &= \arg\max_{\theta} \sum_{n=1}^{N} \ln\left(p(y_n|\theta)\right), \\
&= \arg\max_{\theta} \sum_{n=1}^{N} \ln\left(\sum_{z} p(y_n, z_n|\theta)\right).
\end{aligned}
$$

Where:

$$
\ln\left(\sum_{z} p(y_n, z_n|\theta)\right) = \ln\left(\pi\mathcal{N}\left(y_n|\mu_1, \sigma_1^2\right) + (1-\pi)\mathcal{N}\left(y_n|\mu_2, \sigma_2^2\right)\right).
$$

Problem definition - General

The model consists of observations $\mathbf{y}$ and a latent random variable $\mathbf{z}$. Then

$$
\begin{aligned}
p(\mathbf{y}|\theta) &= \prod_{n=1}^{N} p(y_n|\theta) \\
&= \prod_{n=1}^{N} \sum_{\mathbf{z}} p(y_n, \mathbf{z}|\theta) = \prod_{n=1}^{N} \sum_{\mathbf{z}} p(y_n|\mathbf{z}, \theta) p(\mathbf{z}|\theta)
\end{aligned}
$$

The estimation of θ_{ML} is given by

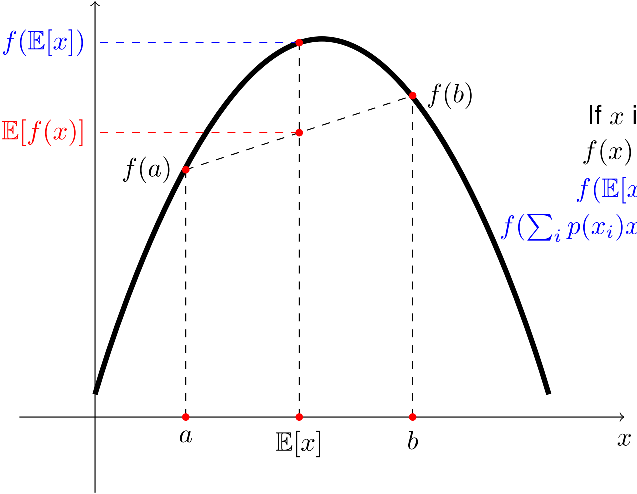
$$
\begin{aligned}
\theta_{\text{ML}} &= \arg\max_{\theta} \ln\left(p(\mathbf{y}|\theta)\right) \\
&= \arg\max_{\theta} \sum_{n=1}^{N} \ln\left(\sum_{\mathbf{z}} p(y_n|\mathbf{z}, \theta) p(\mathbf{z}|\theta)\right)
\end{aligned}
$$

Problem definition

$$\theta_{\mathsf{ML}} = \arg\max_{\theta} \sum_{n=1}^{N} \ln \left(\sum_{\mathbf{z}} p(y_n, |\mathbf{z}, \theta) p(\mathbf{z}|\theta) \right)$$

- The sum over $\mathbf{z}$ couples the parameters θ.
- Gradients have no closed form.
- $\mathbf{z}$ and θ are also coupled.

Jensen's Inequality



If x is a r.v. and
$f(x)$ is concave:

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

$$f(\sum_i p(x_i)x_i) \geq \sum_i p(x_i)f(x_i)$$

EM algorithm - Jensen's Inequality

$$\log p(\mathbf{y}|\theta) = \sum_{n=1}^{N} \ln \left(\sum_{\mathbf{z}} p(y_n, \mathbf{z}|\theta) \right)$$

EM algorithm - Jensen's Inequality

$$
\begin{aligned}
\log p(\mathbf{y}|\theta) &= \sum_{n=1}^{N} \ln \left(\sum_{\mathbf{z}} p(y_n, \mathbf{z}|\theta) \right) \\
&= \sum_{n=1}^{N} \ln \left(\sum_{\mathbf{z}} q(\mathbf{z}) \frac{p(y_n, \mathbf{z}|\theta)}{q(\mathbf{z})} \right)
\end{aligned}
$$

EM algorithm - Jensen's Inequality

$$
\begin{aligned}
\log p(\mathbf{y}|\theta) &= \sum_{n=1}^{N} \ln\left(\sum_{\mathbf{z}} p(y_n, \mathbf{z}|\theta)\right) \\
&= \sum_{n=1}^{N} \ln\left(\sum_{\mathbf{z}} q(\mathbf{z}) \frac{p(y_n, \mathbf{z}|\theta)}{q(\mathbf{z})}\right) \\
&\geq \sum_{n=1}^{N} \sum_{\mathbf{z}} q(\mathbf{z}) \ln\left(\frac{p(y_n, \mathbf{z}|\theta)}{q(\mathbf{z})}\right)
\end{aligned}
$$

Distribution $q(\mathbf{z})$

Assuming a value of $\theta^{(t)}$, what form $q(\mathbf{z})$ should have to maximize

$$\ln p(\mathbf{y}|\theta^{(t)}) \geq \sum_{n=1}^{N} \sum_{\mathbf{z}} q(\mathbf{z}) \ln \left(\frac{p(\mathbf{z}|y_n, \theta^{(t)}) p(y_n|\theta^{(t)})}{q(\mathbf{z})} \right)$$

Distribution $q(\mathbf{z})$

Assuming a value of $\theta^{(t)}$, what form $q(\mathbf{z})$ should have to maximize

$$\begin{aligned}
\ln p(\mathbf{y}|\theta^{(t)}) &\geq \sum_{n=1}^{N} \sum_{\mathbf{z}} q(\mathbf{z}) \ln \left(\frac{p(\mathbf{z}|y_n, \theta^{(t)}) p(y_n|\theta^{(t)})}{q(\mathbf{z})} \right) \\
&\geq \sum_{n=1}^{N} \sum_{\mathbf{z}} q(\mathbf{z}) \left[\ln \left(\frac{p(\mathbf{z}|y_n, \theta^{(t)})}{q(\mathbf{z})} \right) + \ln p(y_n|\theta^{(t)}) \right]
\end{aligned}$$

Distribution $q(\mathbf{z})$

Assuming a value of $\theta^{(t)}$, what form $q(\mathbf{z})$ should have to maximize

$$\ln p(\mathbf{y}|\theta^{(t)}) \geq \sum_{n=1}^{N}\sum_{\mathbf{z}} q(\mathbf{z}) \ln\left(\frac{p(\mathbf{z}|y_n,\theta^{(t)})p(y_n|\theta^{(t)})}{q(\mathbf{z})}\right)$$

$$\geq \sum_{n=1}^{N}\sum_{\mathbf{z}} q(\mathbf{z}) \left[\ln\left(\frac{p(\mathbf{z}|y_n,\theta^{(t)})}{q(\mathbf{z})}\right) + \ln p(y_n|\theta^{(t)})\right]$$

organizing,

$$\sum_{n=1}^{N} \ln p(y_n|\theta^{(t)}) \geq \sum_{n=1}^{N}\sum_{\mathbf{z}} q(\mathbf{z}) \ln\left(\frac{p(\mathbf{z}|y_n,\theta^{(t)})}{q(\mathbf{z})}\right) + \sum_{n=1}^{N} \ln p(y_n|\theta^{(t)}),$$

Distribution $q(\mathbf{z})$

Assuming a value of $\theta^{(t)}$, what form $q(\mathbf{z})$ should have to maximize

$$\ln p(\mathbf{y}|\theta^{(t)}) \geq \sum_{n=1}^{N} \sum_{\mathbf{z}} q(\mathbf{z}) \ln \left(\frac{p(\mathbf{z}|y_n, \theta^{(t)}) p(y_n|\theta^{(t)})}{q(\mathbf{z})} \right)$$

$$\geq \sum_{n=1}^{N} \sum_{\mathbf{z}} q(\mathbf{z}) \left[\ln \left(\frac{p(\mathbf{z}|y_n, \theta^{(t)})}{q(\mathbf{z})} \right) + \ln p(y_n|\theta^{(t)}) \right]$$

organizing,

$$\sum_{n=1}^{N} \ln p(y_n|\theta^{(t)}) \geq \sum_{n=1}^{N} \sum_{\mathbf{z}} q(\mathbf{z}) \ln \left(\frac{p(\mathbf{z}|y_n, \theta^{(t)})}{q(\mathbf{z})} \right) + \sum_{n=1}^{N} \ln p(y_n|\theta^{(t)}),$$

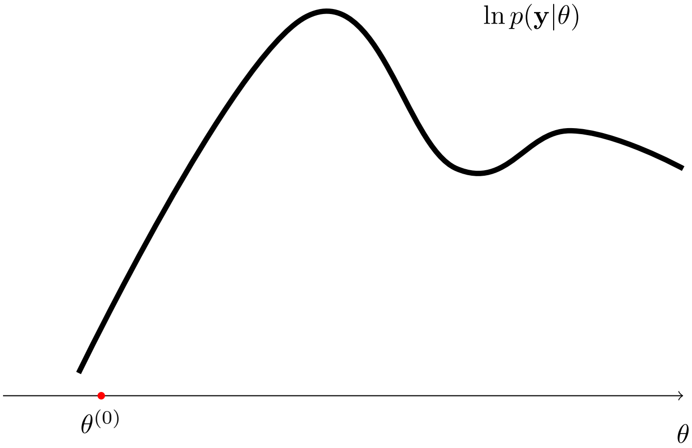
then, $q(\mathbf{z}) = p(\mathbf{z}|y_n, \theta^{(t)})$.

Parameter estimation

If $q(\mathbf{z}) = p(\mathbf{z}|y_n, \theta^{(t)})$,

$$
\begin{aligned}
\theta^{(t+1)} &= \arg\max_{\theta} \sum_{n=1}^{N} \sum_{\mathbf{z}} p(\mathbf{z}|y_n, \theta^{(t)}) \ln \left(\frac{p(y_n, \mathbf{z}|\theta)}{p(\mathbf{z}|y_n, \theta^{(t)})} \right) \\
&= \arg\max_{\theta} \sum_{n=1}^{N} \mathbb{E}_{q(\mathbf{z})} \left[\ln \left(p(y_n, \mathbf{z}|\theta) \right) \right] \\
&= \arg\max_{\theta} \mathcal{Q}\left(\theta, \theta^{(t)} \right)
\end{aligned}
$$

EM algorithm - Visual explanation



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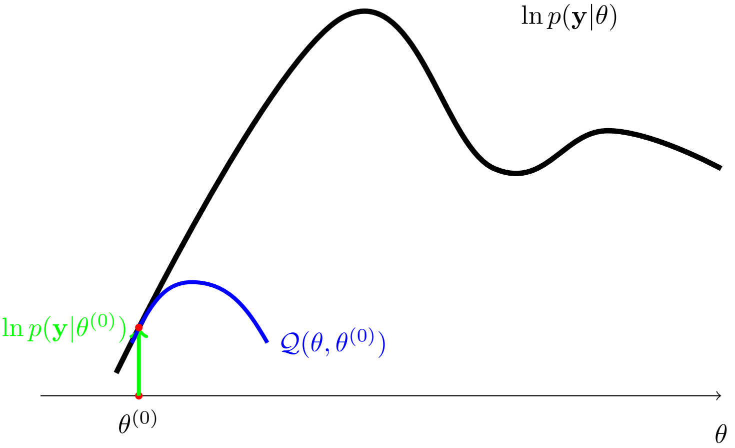

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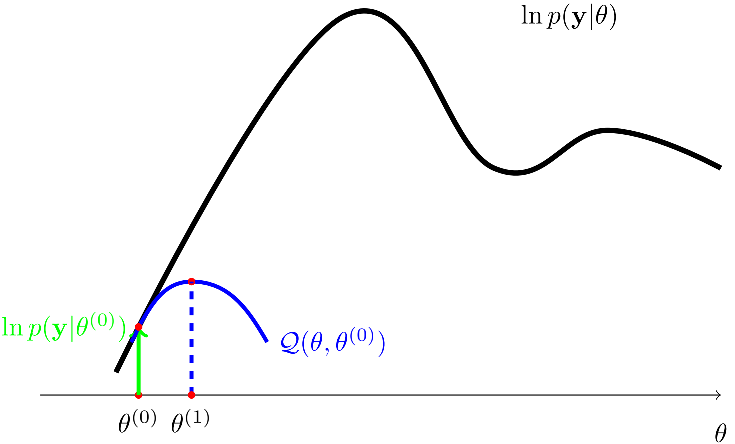

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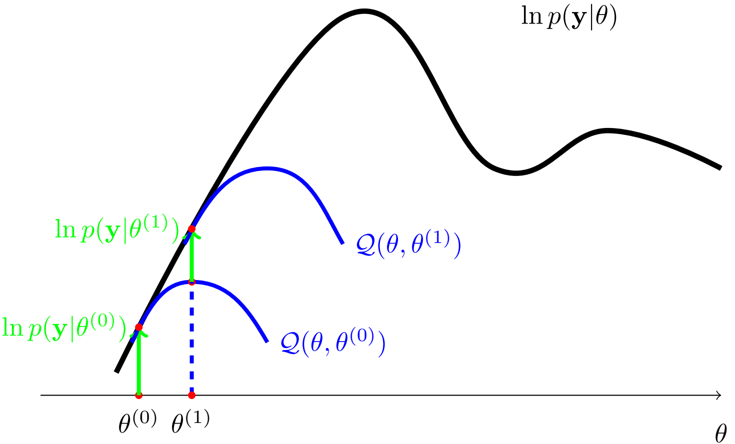

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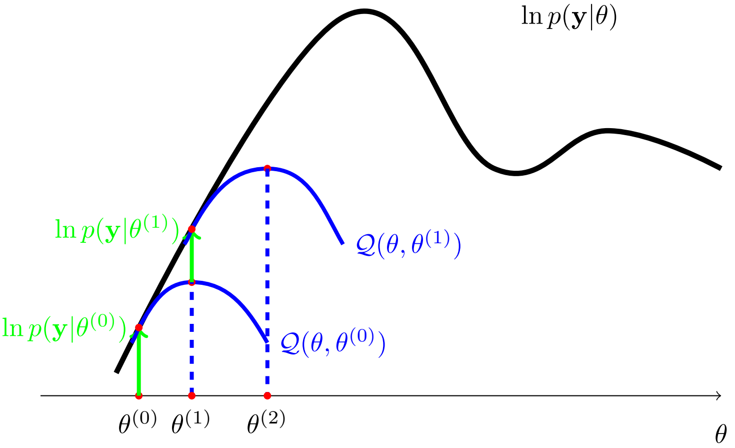
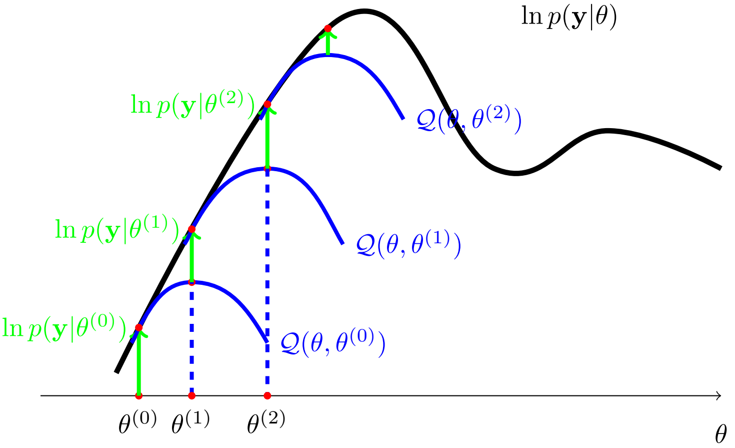


EM algorithm - Visual explanation



EM Algorithm - Pseudo-code

Given the joint distribution $p(\mathbf{y}, \mathbf{z}|\theta)$, the objective is to maximize $p(\mathbf{y}|\theta)$ w.r.t. θ.

1. Select the initial parameters $\theta^{(t)} \leftarrow \theta^{(0)}$.
2. Evaluate E-step, $q(\mathbf{z}) = p(\mathbf{z}|\mathbf{y}, \theta^{(t)})$.
3. Evaluate M-step,
$$\theta^{(\text{t+1})} = \arg\max_{\theta} \mathcal{Q}\left(\theta, \theta^{(t)}\right)$$
4. Verify convergence. If it doesn't satisfy, then
$$\theta^{(t)} \leftarrow \theta^{(t+1)},$$
return to step 2.

EM algorithm - Remark

$$\log p(\mathbf{y}|\theta) \geq \sum_{n=1}^{N} \sum_{\mathbf{z}} q(\mathbf{z}) \ln \left(\frac{p(y_n, \mathbf{z}|\theta)}{q(\mathbf{z})} \right)$$

$$\sum_{n=1}^{N} \ln p(y_n|\theta) \geq \sum_{n=1}^{N} \sum_{\mathbf{z}} q(\mathbf{z}) \ln \left(\frac{p(\mathbf{z}|y_n, \theta)}{q(\mathbf{z})} \right) + \sum_{n=1}^{N} \ln p(y_n|\theta),$$

$$\sum_{n=1}^{N} \ln p(y_n|\theta) \geq \sum_{n=1}^{N} \sum_{\mathbf{z}} q(\mathbf{z}) \ln \left(p(y_n|\mathbf{z}, \theta) \right) + \sum_{\mathbf{z}} q(\mathbf{z}) \ln \left(\frac{p(\mathbf{z}|\theta)}{q(\mathbf{z})} \right).$$

$$\sum_{n=1}^{N} \ln p(y_n|\theta) \geq \sum_{n=1}^{N} \sum_{\mathbf{z}} q(\mathbf{z}) \ln \left(p(y_n, \mathbf{z}|\theta) \right) - \sum_{\mathbf{z}} q(\mathbf{z}) \ln \left(q(\mathbf{z}) \right).$$

EM algorithm - Summary

1. We just need to calculate the expected value of the joint distribution w.r.t. the posterior of the latent variables.
2. We are able to estimate the parameters θ by maximizing an easier objective function.

Outline

1. EM algorithm

2. **Variational EM**

3. Approximate inference for Neural Networks
   - Bayesian Deep Neural Networks
   - Laplace Approximation

Problem formulation

In this case,

$$p(\mathbf{z}|\mathbf{y}) = \frac{p(\mathbf{y}, \mathbf{z})}{p(\mathbf{y})}$$

is intractable. Most of the time because

$$\begin{aligned} p(\mathbf{y}) &= \int_{\mathbf{z}} p(\mathbf{y}, \mathbf{z}) \, \mathrm{d}\, \mathbf{z} \\ &= \int_{\mathbf{z}} p(\mathbf{y}|\mathbf{z}) p(\mathbf{z}) \, \mathrm{d}\, \mathbf{z} \\ &= \mathbb{E}_{p(\mathbf{z})} \left[p(\mathbf{y}|\mathbf{z}) \right] \end{aligned}$$

is difficult to calculate.

Variational EM - Objective

We are interested in estimating $p(\mathbf{z}|\mathbf{y})$. This can be achieved by solving the following optimization problem,

$$q^*(\mathbf{z}) = \text{arg min } \mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{y}))$$

where

$$\mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{y})) = \int q(\mathbf{z}) \ln \frac{q(\mathbf{z})}{p(\mathbf{z}|\mathbf{y})} \mathrm{d}\mathbf{z}$$

Variational EM - Objective

Analysing the KL divergence between $q(\mathbf{z})$ and $p(\mathbf{z}|\mathbf{y})$,

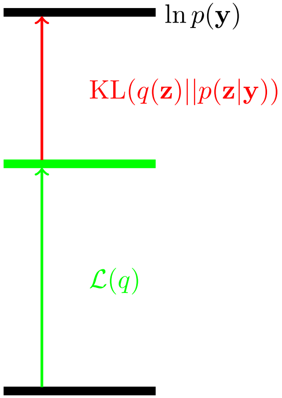
$$\begin{aligned}
\mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{y})) &= \int q(\mathbf{z}) \ln \frac{q(\mathbf{z})}{p(\mathbf{z}|\mathbf{y})} \mathrm{d}\mathbf{z} \\
&= \int q(\mathbf{z}) \ln q(\mathbf{z}) \mathrm{d}\mathbf{z} - \int q(\mathbf{z}) \ln p(\mathbf{z}|\mathbf{y}) \mathrm{d}\mathbf{z} \\
&= \int q(\mathbf{z}) \ln q(\mathbf{z}) \mathrm{d}\mathbf{z} - \int q(\mathbf{z}) \ln \frac{p(\mathbf{z},\mathbf{y})}{p(\mathbf{y})} \mathrm{d}\mathbf{z} \\
&= \int q(\mathbf{z}) \ln q(\mathbf{z}) \mathrm{d}\mathbf{z} - \int q(\mathbf{z}) \ln p(\mathbf{z},\mathbf{y}) \mathrm{d}\mathbf{z} + \ln {\color{red} p(\mathbf{y})}
\end{aligned}$$

From previous equation we have,

$$\begin{aligned}\ln p(\mathbf{y}) &= \mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{y})) + \int q(\mathbf{z}) \ln p(\mathbf{z}, \mathbf{y}) \mathsf{d}\mathbf{z} - \int q(\mathbf{z}) \ln q(\mathbf{z}) \mathsf{d}\mathbf{z} \\ &= \mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{y})) + \mathcal{L}(q).\end{aligned}$$

Given that $\mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{y})) \geq 0$, then the lower bound of $\ln p(\mathbf{y})$ is $\mathcal{L}(q)$.

Variational EM - The evidence lower bound



Variational EM - Summary

1. If the posterior $p(\mathbf{z}|\mathbf{y})$ is intractable or complex (main issue is to calculate $p(\mathbf{y})$).
2. We can approximate the posterior by minimizing KL$(q(\mathbf{z})||p(\mathbf{z}|\mathbf{y}))$, which results in maximizing $\mathcal{L}(q)$.
3. The E-step is an iterative process.

Variational EM - Remark

$$\mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{y})) = \int q(\mathbf{z}) \ln \frac{q(\mathbf{z})}{p(\mathbf{z}|\mathbf{y})} \mathsf{d}\mathbf{z}$$

$$\mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{y})) = \int q(\mathbf{z}) \ln q(\mathbf{z}) \mathsf{d}\mathbf{z} - \int q(\mathbf{z}) \ln p(\mathbf{z}, \mathbf{y}) \mathsf{d}\mathbf{z} + \ln {\color{red} p(\mathbf{y})}$$

$$\mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{y})) = -\int q(\mathbf{z}) \ln p(\mathbf{y}|\mathbf{z}) \mathsf{d}\mathbf{z} + \int q(\mathbf{z}) \ln \frac{q(\mathbf{z})}{p(\mathbf{z})} \mathsf{d}\mathbf{z} + \ln {\color{red} p(\mathbf{y})}$$

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1. **EM algorithm**
2. **Variational EM**
3. **Approximate inference for Neural Networks**
   - Bayesian Deep Neural Networks
   - Laplace Approximation

Approx. NNs - Problem definition

Let's assume we have a dataset $\mathcal{D} = \{\mathbf{X}, \mathbf{Y}\}$, with $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ and $\mathbf{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_N\}$

$$\begin{aligned}
\mathrm{KL}\left(q_\theta(\boldsymbol{\omega}) \| p(\boldsymbol{\omega}|\mathcal{D})\right) &\propto -\int q_\theta(\boldsymbol{\omega}) \log p(\mathbf{Y}|\mathbf{X}, \boldsymbol{\omega}) \mathrm{d}\boldsymbol{\omega} + \mathrm{KL}\left(q_\theta(\boldsymbol{\omega}) \| p(\boldsymbol{\omega})\right), \\
&= -\sum_{i=1}^{N} \int q_\theta(\boldsymbol{\omega}) \log p\left(\mathbf{y}_i | \mathbf{f}^{\omega}\left(\mathbf{x}_i\right)\right) \mathrm{d}\boldsymbol{\omega} + \mathrm{KL}\left(q_\theta(\boldsymbol{\omega}) \| p(\boldsymbol{\omega})\right),
\end{aligned}$$

where ω is a vector composed by the stacking of all weights.

Approx. NNs - Problem definition

1. The summed-over terms log-likelihood are not tractable for BNNs with more than a single hidden layer.
2. This objective requires us to perform computations over the entire dataset, which can be too costly for large N.

Approx. NNs - Data size solution

We can reduce the data size problem by data sub-sampling (also referred to as mini-batch optimization).

$$\widehat{\mathcal{L}}_{\mathrm{VI}}(\theta) := -\frac{N}{M} \sum_{i \in S} \int q_\theta(\boldsymbol{\omega}) \log p\left(\mathbf{y}_i | \mathbf{f}^{\boldsymbol{\omega}}\left(\mathbf{x}_i\right)\right) \mathrm{d}\boldsymbol{\omega} + \mathrm{KL}\left(q_\theta(\boldsymbol{\omega}) \| p(\boldsymbol{\omega})\right)$$

with a random index set S of size M.

Approx. NNs - Expected value solution

We can reduce the data size problem by data sub-sampling (also referred to as mini-batch optimization).

$$\mathbb{E}_{q_\theta(\boldsymbol{\omega})}[\log p(\mathbf{y}_i|\mathbf{f}^{\boldsymbol{\omega}}(\mathbf{x}_i))] = \int q_\theta(\boldsymbol{\omega}) \log p(\mathbf{y}_i|\mathbf{f}^{\boldsymbol{\omega}}(\mathbf{x}_i))\, \mathrm{d}\boldsymbol{\omega}$$

$$q_\theta(\boldsymbol{\omega}) = \prod_{i=1}^{L} q_\theta(\mathbf{W}_i) = \prod_{i=1}^{L}\prod_{j=1}^{K_i}\prod_{k=1}^{K_{i+1}} q(w_{ijk}) = \prod_{i,j,k} \mathcal{N}\left(w_{ijk}; m_{ijk}, \sigma_{ijk}^2\right)$$

$$\mathbb{E}_{q_\theta(\boldsymbol{\omega})}[\log p(\mathbf{y}_i|\mathbf{f}^{\boldsymbol{\omega}}(\mathbf{x}_i))] \approx \frac{1}{M}\sum_{m=1}^{M} q_\theta(\boldsymbol{\omega}_j) \log p(\mathbf{y}_i|\mathbf{f}^{\boldsymbol{\omega}}(\mathbf{x}_i))$$

Approx. NNs - Expected value solution

A better way is to use Pathwise Gradient Estimator

$$\mathbb{E}_{q_{\boldsymbol{\theta}}(\boldsymbol{\omega})}\left[f_{\boldsymbol{\theta}}(\boldsymbol{\omega})\right] \longrightarrow \mathbb{E}_{q_0(\boldsymbol{\epsilon})}\left[f_{\boldsymbol{\theta}}(g(\boldsymbol{\theta};\boldsymbol{\epsilon}))\right]$$

$$q\left(w_{ijk}\right) = g(\theta_{ijk}, \epsilon_{ijk}) = m_{ijk} + \sigma_{ijk}\epsilon_{ijk}$$

then

$$\widehat{\mathcal{L}}_{\mathrm{VI}}(\theta) := -\frac{N}{M}\sum_{i\in S}\int q_{\theta}(\boldsymbol{\omega})\log p\left(\mathbf{y}_i|\mathbf{f}^{\boldsymbol{\omega}}\left(\mathbf{x}_i\right)\right)\mathrm{d}\boldsymbol{\omega} + \mathrm{KL}\left(q_{\theta}(\boldsymbol{\omega})\|p(\boldsymbol{\omega})\right)$$

becomes

$$\widehat{\mathcal{L}}_{\mathrm{MC}}(\theta) = -\frac{N}{M}\sum_{i\in S}\log p\left(\mathbf{y}_i|\mathbf{f}^{g(\theta,\epsilon)}\left(\mathbf{x}_i\right)\right) + \mathrm{KL}\left(q_{\theta}(\boldsymbol{\omega})\|p(\boldsymbol{\omega})\right)$$

where $\mathbb{E}_{S,\epsilon}\left[\hat{\mathcal{L}}_{\mathrm{MC}}(\theta)\right] = \mathcal{L}_{\mathrm{VI}}(\theta)$.

Algorithm 1 Minimise divergence between $q_\theta(\boldsymbol{\omega})$ and $p(\boldsymbol{\omega}|X, Y)$

```
Given dataset X, Y,
Define learning rate schedule η,
Initialise parameters θ randomly.
repeat
    Sample M random variables ε̂_i ~ p(ε), S a random subset of {1, .., N} of size M.
    Calculate stochastic derivative estimator w.r.t. θ:
    Update θ:
until θ has converged.
```

Given dataset $\mathbf{X}, \mathbf{Y}$,

Define learning rate schedule η,

Initialise parameters θ randomly.

repeat

  Sample M random variables $\widehat{\boldsymbol{\epsilon}}_i \sim p(\boldsymbol{\epsilon})$, S a random subset of $\{1, .., N\}$ of size M.

  Calculate stochastic derivative estimator w.r.t. θ:

$$\widehat{\Delta\theta} \leftarrow -\frac{N}{M}\sum_{i\in S}\frac{\partial}{\partial\theta}\log p(\mathbf{y}_i|\mathbf{f}^{g(\theta,\widehat{\boldsymbol{\epsilon}}_i)}(\mathbf{x}_i)) + \frac{\partial}{\partial\theta}\mathrm{KL}(q_\theta(\boldsymbol{\omega})||p(\boldsymbol{\omega})).$$

  Update θ:

$$\theta \leftarrow \theta + \eta\widehat{\Delta\theta}.$$

until θ has converged.

Approx. NNs - Dropout

$$
\begin{aligned}
\widehat{\mathbf{y}} &= \widehat{\mathbf{h}}\mathbf{M}_2 \\
&= (\mathbf{h} \odot \widehat{\boldsymbol{\epsilon}}_2)\mathbf{M}_2 \\
&= (\mathbf{h} \cdot \mathrm{diag}(\widehat{\boldsymbol{\epsilon}}_2))\mathbf{M}_2 \\
&= \mathbf{h}(\mathrm{diag}(\widehat{\boldsymbol{\epsilon}}_2)\mathbf{M}_2) \\
&= \sigma\Big(\widehat{\mathbf{x}}\mathbf{M}_1 + \mathbf{b}\Big)(\mathrm{diag}(\widehat{\boldsymbol{\epsilon}}_2)\mathbf{M}_2) \\
&= \sigma\Big((\mathbf{x} \odot \widehat{\boldsymbol{\epsilon}}_1)\mathbf{M}_1 + \mathbf{b}\Big)(\mathrm{diag}(\widehat{\boldsymbol{\epsilon}}_2)\mathbf{M}_2) \\
&= \sigma\Big(\mathbf{x}(\mathrm{diag}(\widehat{\boldsymbol{\epsilon}}_1)\mathbf{M}_1) + \mathbf{b}\Big)(\mathrm{diag}(\widehat{\boldsymbol{\epsilon}}_2)\mathbf{M}_2)
\end{aligned}
$$

Ountline

1. **EM algorithm**

2. **Variational EM**

3. **Approximate inference for Neural Networks**
   - Bayesian Deep Neural Networks
   - Laplace Approximation

Approx. NNs - Laplace approximation

The standard Laplace approximation is obtained by taking the second-order Taylor expansion around a mode of a distribution.
If we approximate the log posterior over the weights of a network given some data $\mathcal{D}$ around a MAP estimate ω^*, we obtain

$$\log p(\boldsymbol{\omega}|\mathcal{D}) \approx \log p\left(\boldsymbol{\omega}^*|\mathcal{D}\right) - \frac{1}{2}\left(\boldsymbol{\omega} - \boldsymbol{\omega}^*\right)^\top \overline{H}\left(\boldsymbol{\omega} - \boldsymbol{\omega}^*\right),$$

where $\overline{H} = \mathbb{E}[H]$ is the average Hessian of the negative log posterior. The posterior over the weights is then approximated as Gaussian:

$$\boldsymbol{\omega} \sim \mathcal{N}\left(\boldsymbol{\omega}^*, \overline{H}^{-1}\right)$$

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