

Machine Learning

Notes taken by Runqiu Ye
Carnegie Mellon University

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Contents

1	Probability and statistical inference	3
1.1	Basic probability theory	3
1.2	Statistical inference	4
2	Learning theory	6
2.1	PAC learning	6
2.1.1	Realizable learning	6
2.1.2	Agnostic learning	8
2.2	Infinite hypotheses space and VC dimension	10
3	Probability distributions	12
3.1	Binary variables	12
3.2	Multinomial variables	12
3.3	The Gaussian distribution	13
3.3.1	Conditionals and marginals of Gaussian distribution	14
3.3.2	Bayes' theorem for Gaussian distribution	15
3.3.3	Maximum likelihood for the Gaussian	15
3.3.4	Bayesian inference for the Gaussian	16
3.3.5	Student's t-distribution	18
3.4	The exponential family	19
4	Mixture models and EM	20
4.1	Kullback-Leibler (KL) Divergence	20
4.2	The EM Algorithm in General	23
5	Approximate inference	25
5.1	Variational inference	25
5.1.1	Factorized distributions	26
5.1.2	Properties of factorized approximations	26
5.1.3	Model comparison	27
5.2	Illustration: variational mixture of Gaussians	28

1 Probability and statistical inference

1.1 Basic probability theory

Definition (Convergence of random variables). Let $\{X_n\}_{n=1}^{\infty}$ be a sequence of random variables and X be another random variable. Let F_n be the CDF of X_n for each $n \in \mathbb{N}$ and F be the CDF of X .

1. X_n converges to X **in probability** and write $X_n \xrightarrow{P} X$ if for arbitrary $\varepsilon > 0$,

$$\mathbb{P}[|X_n - X| > \varepsilon] \rightarrow 0$$

as $n \rightarrow \infty$.

2. X_n converges to X **in distribution** and write $X_n \rightsquigarrow X$ if

$$\lim_{n \rightarrow \infty} F_n(t) = F(t)$$

for all t where F is continuous.

3. X_n converges to X in L^p if

$$\mathbb{E}[|X_n - X|^p] \rightarrow 0$$

as $n \rightarrow \infty$. In particular, say X_n converges to X in **quadratic mean** and write $X_n \xrightarrow{qm} X$ if X_n converges to X in L^2 .

4. X_n converges to X **almost surely** and write $X_n \xrightarrow{as} X$ if

$$\mathbb{P}\left[\lim_{n \rightarrow \infty} X_n = X\right] = 1.$$

Theorem. The following implication holds:

1. If X_n converges to X almost surely, then X_n converges to X in probability.
2. If X_n converges to X in L^p , then X_n converges to X in probability.

Proof. 1. If X_n converges to X almost surely, the set of points

$$O = \left\{ \omega : \lim_{n \rightarrow \infty} X_n(\omega) \neq X(\omega) \right\}$$

has measure zero. Now fix $\varepsilon > 0$ and consider the sequence of sets

$$A_n = \bigcup_{m=n}^{\infty} \{|X_m - X| > \varepsilon\}.$$

Note that $A_n \supset A_{n+1}$ for each $n \in \mathbb{N}$ and let $A_{\infty} = \bigcap_{n=1}^{\infty} A_n$. Now show $\mathbb{P}[A_{\infty}] = 0$. If $\omega \notin O$, then $\lim_{n \rightarrow \infty} X_n(\omega) = X(\omega)$ and thus $|X_n(\omega) - X(\omega)| < \varepsilon$ for some $n \in \mathbb{N}$. Therefore, $\omega \notin A_{\infty}$. It follows that $A_{\infty} \subset O$ and $\mathbb{P}[A_{\infty}] = 0$.

By monotone continuity, we have $\lim_{n \rightarrow \infty} \mathbb{P}[A_n] = \mathbb{P}[A_\infty]$. It follows that

$$\mathbb{P}[|X_n - X| > \varepsilon] \leq \mathbb{P}[A_n] \rightarrow 0$$

as $n \rightarrow \infty$. This completes the proof.

2. From Chebyshev's inequality, we have

$$\mathbb{P}[|X - X_n| > \varepsilon] \leq \frac{1}{\varepsilon^p} \mathbb{E}[|X - X_n|^p].$$

The claim follows directly. □

Theorem (Central Limit Theorem). Let X_1, \dots, X_n be i.i.d. with mean μ and variance σ^2 . Let $S_n = \frac{1}{n} \sum_{i=1}^n X_i$. Then

$$Z_n = \frac{S_n - \mu}{\sqrt{\text{var } S_n}} = \frac{\sqrt{n}(S_n - \mu)}{\sigma} \rightsquigarrow Z,$$

where $Z \sim \mathcal{N}(0, 1)$ and \rightsquigarrow represents convergence in distribution. In other words,

$$\lim_{n \rightarrow \infty} \mathbb{P}[Z_n < z] = \Phi(z) = \int_{-\infty}^z \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx.$$

Also write $Z_n \approx \mathcal{N}(0, 1)$.

1.2 Statistical inference

Definition. Let X_1, \dots, X_n be n i.i.d. data points observed from some distribution F with respect to parameter θ . A point estimator $\hat{\theta}_n$ of the parameter θ is some function of X_1, \dots, X_n :

$$\hat{\theta}_n = g(X_1, \dots, X_n).$$

The bias of an estimator is defined as

$$\text{bias}(\hat{\theta}_n) = \mathbb{E}_\theta[\hat{\theta}_n] - \theta.$$

The mean squared error is defined as

$$\text{MSE} = \mathbb{E}_\theta(\hat{\theta}_n - \theta)^2.$$

Definition (Consistent point estimator). A point estimator $\hat{\theta}_n$ of a parameter θ is **consistent** if $\hat{\theta}_n \xrightarrow{\text{P}} \theta$.

Next we an important relation between bias, variance, and MSE. This is a more rigorous way to express the **bias-variance tradeoff** of point estimators.

Theorem. The MSE can be written as

$$\text{MSE} = \text{bias}^2(\widehat{\theta}_n) + \text{var}_\theta(\widehat{\theta}_n).$$

Proof. Let $\bar{\theta}_n = \mathbb{E}_\theta(\widehat{\theta}_n)$. Then we have

$$\begin{aligned} \mathbb{E}_\theta(\theta - \widehat{\theta}_n)^2 &= \mathbb{E}_\theta(\theta - \bar{\theta}_n + \bar{\theta}_n - \widehat{\theta}_n)^2 \\ &= \mathbb{E}_\theta(\theta - \bar{\theta}_n)^2 - 2(\theta - \bar{\theta}_n)\mathbb{E}_\theta(\bar{\theta}_n - \widehat{\theta}_n) + \mathbb{E}_\theta(\bar{\theta}_n - \theta)^2 \\ &= (\theta - \bar{\theta}_n)^2 + \mathbb{E}_\theta(\bar{\theta}_n - \theta)^2 \\ &= \text{bias}^2(\widehat{\theta}_n) + \text{var}_\theta(\widehat{\theta}_n), \end{aligned}$$

where we have used the fact that $\mathbb{E}_\theta(\bar{\theta}_n - \widehat{\theta}_n) = \bar{\theta}_n - E_\theta(\widehat{\theta}_n) = \bar{\theta}_n - \bar{\theta}_n = 0$. \square

Below is the definition of a confidence set/interval.

Definition. A $1 - \alpha$ interval for a parameter θ is an interval $C_n = (a, b)$ where $a = a(X_1, \dots, X_n)$ and $b = b(X_1, \dots, X_n)$ are functions of data such that

$$\mathbb{P}_\theta[\theta \in C_n] \geq 1 - \alpha \text{ for all } \theta \in \Theta.$$

In other word, (a, b) traps θ with probability $1 - \alpha$.

Warning! In the above definition, C_n is random and θ is fixed.

2 Learning theory

2.1 PAC learning

PAC learning is short for Probably Approximate Correct learning, and the setting of PAC learning is as follows:

- We have data $x \in \mathbb{R}^d$ and label $y \in \{-1, +1\}$.
- We collect features x_1, \dots, x_n i.i.d. from some distribution D . Note that we make no assumption on the distribution D of the features.
- We collect corresponding labels y_1, \dots, y_n .
- Assume there exists some true classifier h^* .
- Let \mathcal{H} be the set of all hypotheses.

The goal of PAC learning is (ε, δ) -PAC, which is defined as follows.

Definition. An (ε, δ) -PAC learning algorithm refers to an algorithm that picks an hypothesis $h \in \mathcal{H}$ after observing training data $\{x_i, y_i\}_{i=1}^n$, where the hypothesis $h \in \mathcal{H}$ satisfies

$$\text{err}_D(\hat{h}) = \mathbb{P}_{x \sim D} [\hat{h}(x) \neq h^*(x)] < \varepsilon.$$

with probability at least $1 - \delta$, where the probability is with respect to the randomness of the training set.

Putting it more concretely, suppose g is a point estimator (the algorithm), then we want

$$\mathbb{P}_{x_i \sim D} [\text{err}_D(g(x_1, \dots, x_n)) < \varepsilon] \geq 1 - \delta.$$

Through the ε - δ definition of limit, it is not hard to notice the similarity between this definition and **convergence in probability**. As we observe more and more data ($n \rightarrow \infty$), we want the hypothesis produce by the algorithm to converge to the true classifier **in probability**. This is exactly the definition of a **consistent** point estimator in the previous section.

We also say the algorithm is a PAC learner if it uses n samples and the running time is at most $\text{poly}(d, \frac{1}{\varepsilon}, \log \frac{1}{\delta}, \text{bits}(h^*))$, but in this section we do not focus on the runtime of the algorithm.

There are two types of PAC learning – realizable PAC learning, in which case $h^* \in \mathcal{H}$, and agnostic PAC learning, in which case $h^* \notin \mathcal{H}$. We first discuss realizable PAC learning, and we will find out agnostic PAC learning is a more general setting but than PAC learning but a natural extension.

2.1.1 Realizable learning

For realizable PAC learning, we present a simple algorithm:

Algorithm (Consistent Learner). Pick any $\hat{h} \in \mathcal{H}$ such that $h(x_i) = y_i$ for all $1 \leq i \leq n$.

Now we analyze this algorithm in terms of the sample size needed to produce a desired hypothesis.

Theorem. Over the dataset of n i.i.d. samples, the consistent learning algorithm produces \hat{h} such that $\text{err}_D(\hat{h}) > \varepsilon$ with probability at most $|\mathcal{H}| e^{-n\varepsilon}$.

Proof. Suppose $h \in \mathcal{H}$ is such that $\text{err}_D(h) = \mathbb{P}_{x \sim D}[h(x) \neq h^*(x)] > \varepsilon$. For such an h and some data x_i , we have

$$\mathbb{P}_{x_i \sim D}[h(x_i) = y_i = h^*(x_i)] < 1 - \varepsilon.$$

Since $\{x_i, y_i\}_{i=1}^n$ are i.i.d., we have

$$\mathbb{P}_{x_{1:n} \sim D}[h(x_i) = h^*(x_i) \text{ for all } 1 \leq i \leq n] < (1 - \varepsilon)^n.$$

Note that our consistent learner do not make any mistake on the training set $\{x_i, y_i\}_{i=1}^n$

$$\mathbb{P}_{x_{1:n} \sim D}[h = \hat{h}] < (1 - \varepsilon)^n.$$

It follows that

$$\begin{aligned} \mathbb{P}_{x_{1:n} \sim D}[\text{err}_D(\hat{h}) > \varepsilon] &\leq \sum_{h \in \mathcal{H}: \text{err}_D(h) > \varepsilon} \mathbb{P}[\hat{h} = h] \\ &\leq |\mathcal{H}| (1 - \varepsilon)^n \\ &\leq |\mathcal{H}| e^{-n\varepsilon}, \end{aligned}$$

where in the last step we used the inequality $(1 - u)^n \leq e^{-nu}$. This completes the proof. \square

Corollary. If we want $\mathbb{P}_{x_{1:n} \sim D}[\text{err}_D(\hat{h}) > \varepsilon] \leq \delta$, we must have

$$n \geq \frac{\log(|\mathcal{H}|/\delta)}{\varepsilon}.$$

Technically speaking the implication should be the other direction, but this bound for sample size n **guarantees** (ε, δ) -PAC.

To illustrate how we should think of $|\mathcal{H}|$, we present an example.

Example. Consider the binary half-spaces hypotheses:

$$\mathcal{H} = \{h_w(x) = \text{sign}(\langle w, x \rangle) : w_i \in \{-1, 1\}\}.$$

In this case $|\mathcal{H}| = 2^d$, so $\log |\mathcal{H}| = \Theta(d)$.

We should always think of $|\mathcal{H}|$ as exponential with respect to the dimension, so $\log |\mathcal{H}|$ is linear with respect to dimension.

Now we move on to the setting of agnostic learning.

2.1.2 Agnostic learning

In agnostic learning, again we collect features $x_1, \dots, x_n \sim D$ i.i.d., and labels y_1, \dots, y_n . This forms a data set $S_n = \{x_i, y_i\}_{i=1}^n$. The goal is to use this dataset S_n to produce an hypothesis \hat{h} such that

$$\text{reg}_{D, \mathcal{H}}(\hat{h}) = \text{err}_D(\hat{h}) - \min_{h \in \mathcal{H}} \text{err}_D(h) < \varepsilon$$

with probability at least $1 - \delta$, where the probability is with respect to the randomness of the dataset S_n .

For this setting, we present an algorithm called the empirical loss minimizer (ERM).

Algorithm (empirical loss minimizer). Choose $\hat{h} \in \mathcal{H}$ by minimizing the $\{0, 1\}$ loss:

$$\hat{h} = \underset{h \in \mathcal{H}}{\text{argmin}} \sum_{i=1}^n \mathbf{1}\{h(x_i) \neq y_i\}.$$

In a more general setting, suppose $\ell(\cdot, \cdot)$ be any loss function bounded in $[0, 1]$, choose $\hat{h} \in \mathcal{H}$ by minimizing the loss:

$$\hat{h} = \underset{h \in \mathcal{H}}{\text{argmin}} \sum_{i=1}^n \ell(h(x_i), y_i).$$

We next prove a similar relation between the sample size and the performance of the hypothesis, evaluated in terms of risk. We first present the definition of risk.

Definition (risk). The **risk** of a hypothesis h is defined as

$$\text{risk}_D(h) = \mathbb{E}_{x \sim D}[\ell(h(x), y)].$$

Theorem. Over the dataset of n i.i.d. samples, the ERM algorithm produces \hat{h} such that

$$\text{reg}_{D, \mathcal{H}}(\hat{h}) = \text{risk}_D(\hat{h}) - \min_{h \in \mathcal{H}} \text{risk}_D(h) \leq 2\varepsilon.$$

with probability at least $1 - 2|\mathcal{H}|e^{-2n\varepsilon^2}$.

Proof. First we define

$$h^{\text{opt}} = \underset{h \in \mathcal{H}}{\text{argmin}} \text{risk}_D(h).$$

Note that $\text{reg}_{D, \mathcal{H}}(h^{\text{opt}}) = 0$. Define also the estimated risk of hypothesis h for data set S :

$$\widehat{\text{risk}}_S(h) := \frac{1}{n} \sum_{i=1}^n \ell(h(x_i), y_i).$$

Note that $\hat{h} = \operatorname{argmin}_{h \in \mathcal{H}} \widehat{\operatorname{risk}}_S(h)$ and $\mathbb{E}[\widehat{\operatorname{risk}}_S(h)] = \operatorname{risk}_D(h)$, where the expected value is with respect to the randomness of the dataset. Note that

$$\begin{aligned} \operatorname{reg}_{D,\mathcal{H}}(\hat{h}) &= \operatorname{risk}_D(\hat{h}) - \operatorname{risk}_D(h^{\operatorname{opt}}) \\ &= (\operatorname{risk}_D(\hat{h}) - \widehat{\operatorname{risk}}_S(\hat{h})) + (\widehat{\operatorname{risk}}_S(\hat{h}) - \widehat{\operatorname{risk}}_S(h^{\operatorname{opt}})) - (\operatorname{risk}_D(h^{\operatorname{opt}}) - \widehat{\operatorname{risk}}_S(h^{\operatorname{opt}})) \quad (*) \\ &\leq (\operatorname{risk}_D(\hat{h}) - \widehat{\operatorname{risk}}_S(\hat{h})) - (\operatorname{risk}_D(h^{\operatorname{opt}}) - \widehat{\operatorname{risk}}_S(h^{\operatorname{opt}})), \end{aligned}$$

where the inequality is because our algorithm always gives $\widehat{\operatorname{risk}}_S(\hat{h}) - \widehat{\operatorname{risk}}_S(h^{\operatorname{opt}}) \leq 0$.

For any $h \in \mathcal{H}$, we have

$$\begin{aligned} \widehat{\operatorname{risk}}_S(h) - \operatorname{risk}_D(h) &= \frac{1}{n} \sum_{i=1}^n \ell(h(x_i), y_i) - \operatorname{risk}_D(h) \\ &= \frac{1}{n} \sum_{i=1}^n (\ell(h(x_i), y_i) - \mathbb{E}_{x,y \sim D}[\ell(h(x), y)]). \end{aligned}$$

Define now random variable $Z_i := \ell(h(x_i), y_i) - \mathbb{E}_{x,y \sim D}[\ell(h(x), y)]$. Notice that Z_i i.i.d., $\mathbb{E}[Z_i] = 0$, and $|Z_i| \leq 1$. Therefore, we can utilize the **Hoeffding bound** to get

$$\mathbb{P} \left[\frac{1}{n} \sum_{i=1}^n Z_i > \varepsilon \right] \leq e^{-2n\varepsilon^2} \quad \text{and} \quad \mathbb{P} \left[\frac{1}{n} \sum_{i=1}^n Z_i < -\varepsilon \right] \leq e^{-2n\varepsilon^2}$$

This implies that for any fixed $h \in \mathcal{H}$,

$$\mathbb{P} \left[\left| \widehat{\operatorname{risk}}_S(h) - \operatorname{risk}_D(h) \right| > \varepsilon \right] \leq 2e^{-2n\varepsilon^2}.$$

It follows from the union bound that

$$\mathbb{P} \left[\exists h \in \mathcal{H} : \left| \widehat{\operatorname{risk}}_S(h) - \operatorname{risk}_D(h) \right| > \varepsilon \right] \leq 2|\mathcal{H}| e^{-2n\varepsilon^2}.$$

Notice that if $\left| \widehat{\operatorname{risk}}_S(h) - \operatorname{risk}_D(h) \right| \leq \varepsilon$ for all $h \in \mathcal{H}$, we must have $\operatorname{reg}_{D,\mathcal{H}}(\hat{h}) \leq 2\varepsilon$ by inequality (*). above. Therefore, $\operatorname{reg}_{D,\mathcal{H}}(\hat{h}) \leq 2\varepsilon$ with probability at least $1 - 2|\mathcal{H}| e^{-2n\varepsilon^2}$. \square

Corollary. Let $\delta > 0$ be given. Then, setting $n = \frac{1}{2\varepsilon^2} \log(2|\mathcal{H}|/\delta)$, we obtain that $\operatorname{reg}_{D,\mathcal{H}}(\hat{h}) \leq 2\varepsilon$ with probability at least $1 - \delta$. Therefore, if we want $\operatorname{reg}_{D,\mathcal{H}}(\hat{h}) \leq \varepsilon$ with probability at least $1 - \delta$, we must have

$$n \geq \frac{2 \log(2|\mathcal{H}|/\delta)}{\varepsilon^2}.$$

As a comparison between realizable learning and agnostic learning, we can see the sample size needed to achieve the same (ε, δ) -PAC bound is

$$n = \Theta \left(\frac{\log(|\mathcal{H}|/\delta)}{\varepsilon} \right)$$

for realizable learning, and

$$n = \Theta\left(\frac{\log(|\mathcal{H}|/\delta)}{\varepsilon^2}\right)$$

for agnostic learning. Since $\varepsilon < 1$, we can deduce that agnostic learning needs **more sample** for the estimator to achieve the same (ε, δ) -PAC bound.

Theorem (Hoeffding inequality). Let X_1, \dots, X_n be independent random variables such that $a_i \leq X_i \leq b_i$ almost surely. Let

$$S = X_1 + \dots + X_n.$$

Then for all $t > 0$, we have

$$\begin{aligned}\mathbb{P}[S - \mathbb{E}[S] \geq t] &\leq \exp\left[\frac{2t^2}{\sum_{i=1}^n (b_i - a_i)^2}\right], \\ \mathbb{P}[|S - \mathbb{E}[S]| \geq t] &\leq 2 \exp\left[\frac{2t^2}{\sum_{i=1}^n (b_i - a_i)^2}\right].\end{aligned}$$

2.2 Infinite hypotheses space and VC dimension

In last section, we discussed PAC learning with finite hypotheses space \mathcal{H} . However, we often need to deal with situations where the hypotheses space is infinite. Consider the following example.

Example. Consider the binary half space hypotheses:

$$\mathcal{H} = \{h_w(x) = \text{sign}(\langle w, x \rangle) : w \in \mathbb{R}^d\}.$$

Then, $|\mathcal{H}| = \infty$ since each $w \in \mathbb{R}^d$ gives a different decision boundary.

However, on some fixed dataset S , not all of the hypotheses in the hypotheses space \mathcal{H} gives a different prediction. This leads to the following definition and theorem, which characterize the “effective size” of the hypotheses space.

Definition. Let S be a dataset with n points $\{x_1, \dots, x_n\}$. Define $|\mathcal{H}(S)|$ as the number of distinct labeling $\{(x_i, y_i)\}_{i=1}^n$, where each $y_i = h(x_i)$ for a fixed $h \in \mathcal{H}$.

With this definition, we can derive a similar confidence bound for our learned hypotheses.

Theorem. Define the effective size

$$\mathcal{H}[n] = \sup_{x_1, \dots, x_n} |\mathcal{H}(\{x_1, \dots, x_n\})|,$$

and let \hat{h}_n denote the consistency learner from n examples. Then we have

$$\mathbb{P}_{x \sim D}[\text{err}_D(\hat{h}) \geq \varepsilon] \leq \delta,$$

where

$$\varepsilon = O\left(\frac{\log \mathcal{H}[n] + \log(1/\delta)}{n}\right).$$

Example. Consider the threshold hypotheses space:

$$\mathcal{H} = \{h_w(x) = 2 \cdot \mathbf{1}\{x > w\} - 1 : w \in \mathbb{R}\}.$$

Then it is easy to see that $\mathcal{H}[n] = n$. It follows that

$$\varepsilon = O\left(\frac{\log \mathcal{H}[n] + \log(1/\delta)}{n}\right) = O\left(\frac{\log n + \log(1/\delta)}{n}\right),$$

which approaches to 0 as $n \rightarrow \infty$.

Another way to characterize the “effective size” of the hypotheses space is **VC dimension**.

Definition (VC dimension). For a hypotheses space \mathcal{H} , we say \mathcal{H} **shatters** a dataset $\{x_1, \dots, x_n\}$ if for any choice of labels $\{-1, 1\}^n$, there exists $h \in \mathcal{H}$ such that $h(x_i) = y_i$ for all $1 \leq i \leq n$.

The **VC dimension** of a hypotheses space \mathcal{H} is defined as the largest n such that there exists a dataset S of size n such that \mathcal{H} shatters S . Denote this as $\text{VC}(\mathcal{H}) = n$.

The VC dimension of a hypotheses space \mathcal{H} is related to $\mathcal{H}[n]$ by the following lemma by Sauer:

Theorem (Sauer’s Lemma). For any hypotheses class \mathcal{H} , we have

$$\log \mathcal{H}[n] \leq O(\text{VC}(\mathcal{H}) \cdot \log n).$$

Recalling our bound for realizable learning, we get (ε, δ) -PAC with

$$\varepsilon = O\left(\frac{\log \mathcal{H}[n] + \log(1/\delta)}{n}\right) = O\left(\frac{\text{VC}(\mathcal{H}) \cdot \log n + \log(1/\delta)}{n}\right).$$

3 Probability distributions

3.1 Binary variables

Definition (binomial distribution). The binomial distribution is given by

$$\text{Binomial}(m \mid N, \mu) = \binom{N}{m} \mu^m (1 - \mu)^{N-m},$$

where

$$\binom{N}{m} = \frac{N!}{(N-m)!m!}$$

is the binomial coefficient.

Definition (beta distribution). The beta distribution is given by

$$\text{Beta}(\mu \mid a, b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \mu^{a-1} (1-\mu)^{b-1},$$

where $\Gamma(x)$ is the Gamma function given by

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt.$$

The mean and variance of the beta distribution is given by

$$\mathbb{E}[\mu] = \frac{a}{a+b} \quad \text{and} \quad \text{var}[\mu] = \frac{ab}{(a+b)^2(a+b+1)}.$$

Definition (conjugate distribution). In Bayesian probability theory, if, given a likelihood function $p(x \mid \theta)$, the posterior distribution $p(\theta \mid x)$ is in the same probability distribution family as the prior probability distribution $p(\theta)$, the prior and posterior are then called **conjugate distributions** with respect to that likelihood function and the prior is called a **conjugate prior** for the likelihood function $p(x \mid \theta)$.

It is easy to verify that the beta distribution $\text{Beta}(\mu \mid a, b)$ is the **conjugate prior** of the binomial distribution $\text{Binomial}(m \mid N, \mu)$.

3.2 Multinomial variables

Definition (multinomial distribution). The multinomial distribution is given by

$$\text{Multinomial}(m_1, \dots, m_K \mid \mu, N) = \binom{N}{m_1 \ m_2 \ \dots \ m_K} \prod_{k=1}^K \mu_k^{m_k},$$

where $\sum_{k=1}^K m_k = N$, $\mu = (\mu_1, \dots, \mu_K)$ is such that $\sum_{k=1}^K \mu_k = 1$, and

$$\binom{N}{m_1 \ m_2 \ \dots \ m_K} = \frac{N!}{m_1! \ m_2! \ \dots \ m_K!}$$

is the multinomial coefficient.

Definition (Dirichlet distribution). The Dirichlet is a multivariate distribution over K random variables $0 \leq \mu_k \leq 1$, where $k = 1, \dots, K$, subject to the constraints

$$0 \leq \mu_k \leq 1 \quad \text{and} \quad \sum_{k=1}^K \mu_k = 1.$$

Denoting $\mu = (\mu_1, \dots, \mu_K)$ and $\alpha = (\alpha_1, \dots, \alpha_K)$, the PDF of Dirichlet distribution is given by

$$\text{Dirichlet}(\mu \mid \alpha) = C(\alpha) \prod_{k=1}^K \mu_k^{\alpha_k - 1},$$

where $C(\alpha)$ is a normalizing constant given by

$$C(\alpha) = \frac{\Gamma(\alpha_1 + \dots + \alpha_K)}{\Gamma(\alpha_1) \dots \Gamma(\alpha_K)}.$$

It is easy to verify that the Dirichlet distribution is the **conjugate prior** of the multinomial distribution. Indeed,

$$p(\mu \mid \mathcal{D}, \alpha) \propto p(\mathcal{D} \mid \mu) p(\mu \mid \alpha) \propto \prod_{k=1}^K \mu_k^{\alpha_k + m_k - 1},$$

so $p(\mu \mid \mathcal{D}, \alpha) = \text{Dirichlet}(\mu \mid \alpha + m)$, where we denote $m = (m_1, \dots, m_K)$.

3.3 The Gaussian distribution

Definition (Gaussian distribution). The D -dimensional multivariate **Gaussian distribution** is given by

$$\mathcal{N}(x \mid \mu, \Sigma) = \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right],$$

where μ is the **mean** and Σ is the **covariance matrix**. The inverse of the covariance matrix $\Lambda = \Sigma^{-1}$ is called the **precision matrix**.

The moment and covariance of the Gaussian distribution is given by

$$\mathbb{E}[x] = \mu \quad \text{and} \quad \mathbb{E}[xx^T] = \mu\mu^T + \Sigma.$$

Therefore, the covariance (or variance) is

$$\text{cov}[x] = \mathbb{E}[(x - \mathbb{E}[x])(x - \mathbb{E}[x])^T] = \Sigma.$$

Note that the functional dependence of the Gaussian on x is through the quadratic form

$$\Delta^2 = (x - \mu)^T \Sigma^{-1} (x - \mu)$$

which appears in the exponent. It is usually the case that we can identify some distribution is Gaussian by noting the quadratic form in the exponent. We can then identify the mean and variance of the distribution by **completing the square**. When completing the square, the following identity is very helpful:

$$-\frac{1}{2}(x - \mu)^T \Sigma^{-1} (x - \mu) = -\frac{1}{2}x^T \Sigma^{-1} x + x^T \Sigma^{-1} \mu + \text{const},$$

where the constant is independent of x . This can help us read off the precision matrix and the mean from quadratic term and linear term of the expression.

3.3.1 Conditionals and marginals of Gaussian distribution

When considering the conditional and marginals of Gaussian distributions, we often need to deal with **partitioned matrix**. The inverse of a partitioned matrix and itself is related through the following identity:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} M & -MBD^{-1} \\ -D^{-1}CM & D^{-1} + D^{-1}CMBD^{-1} \end{bmatrix},$$

where

$$M = (A - BD^{-1}C)^{-1}.$$

Theorem. Given a joint Gaussian distribution $\mathcal{N}(x \mid \mu, \Sigma)$ with $\Lambda = \Sigma^{-1}$, and

$$x = \begin{bmatrix} x_a \\ x_b \end{bmatrix}, \quad \mu = \begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix}, \quad \Sigma = \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix}, \quad \Lambda = \begin{bmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{bmatrix}.$$

We have the conditional distribution:

$$p(x_a \mid x_b) = \mathcal{N}(x_a \mid \mu_{a|b}, \Lambda_{aa}^{-1}),$$

where

$$\mu_{a|b} = \mu_a - \Lambda_{aa}^{-1} \Lambda_{ab} (x_b - \mu_b),$$

and the marginal distribution

$$p(x_a) = \mathcal{N}(x_a \mid \mu_a, \Sigma_{aa}).$$

3.3.2 Bayes' theorem for Gaussian distribution

Theorem. Given a marginal Gaussian distribution for x and a conditional Gaussian distribution for y given x in the form

$$p(x) = \mathcal{N}(x \mid \mu, \Lambda^{-1}),$$

$$p(y \mid x) = \mathcal{N}(y \mid Ax + b, L^{-1}),$$

the marginal distribution of y and the conditional distribution of x given y are given by

$$p(y) = \mathcal{N}(y \mid A\mu + b, L^{-1} + A\Lambda^{-1}A),$$

$$p(x \mid y) = \mathcal{N}(x \mid \Sigma(A^T L(y - b) + \Lambda\mu), \Sigma),$$

where

$$\Sigma = (\Lambda + A^T L A)^{-1}.$$

3.3.3 Maximum likelihood for the Gaussian

Given a data set $X = \{x_1, \dots, x_N\}$ of observations drawn independent from a Gaussian distribution, we can estimate the parameters of the distribution by maximum likelihood. The log likelihood function is given by

$$\log p(X \mid \mu, \Sigma) = -\frac{ND}{2} \log(2\pi) - \frac{N}{2} \log |\Sigma| - \frac{1}{2} \sum_{n=1}^N (x_n - \mu)^T \Sigma^{-1} (x_n - \mu).$$

It is easy to notice that this only depends on $\sum_{n=1}^N x_n$ and $\sum_{n=1}^N x_n x_n^T$. These quantities are called the **sufficient statistics** for the Gaussian distribution. We can easily derive the maximum likelihood estimation by setting the corresponding partial derivative to zero:

$$\mu_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N x_n, \quad \Sigma_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N (x_n - \mu_{\text{ML}})(x_n - \mu_{\text{ML}})^T.$$

Recall the moment of the Gaussian distribution $\mathbb{E}[x] = \mu$ and $\mathbb{E}[xx^T] = \mu\mu^T + \Sigma$. It follows that

$$\mathbb{E}[x_n] = \mu, \quad \mathbb{E}[x_n \mu_{\text{ML}}^T] = \frac{N-1}{N} \mu\mu^T + \frac{1}{N} \Sigma$$

for any $1 \leq n \leq N$, and

$$\mathbb{E}[\mu_{\text{ML}} \mu_{\text{ML}}^T] = \frac{N^2 - 1}{N^2} \mu\mu^T + \frac{N}{N^2 - 1} \Sigma.$$

Therefore, if we evaluate the maximum likelihood estimation under the true distribution, we obtain

$$\mathbb{E}[\mu_{\text{ML}}] = \mu, \quad \mathbb{E}[\Sigma_{\text{ML}}] = \frac{N-1}{N} \Sigma,$$

We can see that the estimation for mean is unbiased but the estimation for variance is biased. We can correct this by

$$\tilde{\Sigma} = \frac{1}{N-1} \sum_{n=1}^N (x_n - \mu_{\text{ML}})(x_n - \mu_{\text{ML}})^T.$$

It is clear that now

$$\mathbb{E}[\tilde{\Sigma}] = \Sigma,$$

and $\tilde{\Sigma}$ is called the **unbiased estimator** for the Gaussian distribution.

3.3.4 Bayesian inference for the Gaussian

Now consider a Bayesian model for Gaussian distribution. Suppose first the variance σ^2 of a Gaussian distribution is known and we want to infer the mean μ with observed data $X = \{x_1, \dots, x_N\}$. The likelihood function is given by

$$p(X | \mu) = \frac{1}{(2\pi\sigma^2)^{N/2}} \exp \left[-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 \right].$$

It is important to note that this is not a probability distribution over μ . If we take the prior to be also Gaussian, then it will be conjugate to this likelihood function. Therefore, we take our prior distribution to be

$$p(\mu) = \mathcal{N}(\mu | \mu_0, \sigma_0^2).$$

Then the posterior is given by $p(\mu | X) \propto p(X | \mu)p(\mu)$. Through calculation, we can obtain that $p(\mu | X) = \mathcal{N}(\mu | \mu_N, \sigma_N^2)$, where

$$\begin{aligned} \mu_N &= \frac{\sigma^2}{N\sigma_0^2 + \sigma^2} \mu_0 + \frac{N\sigma_0^2}{N\sigma_0^2 + \sigma^2} \mu_{\text{ML}}, \\ \frac{1}{\sigma_N^2} &= \frac{1}{\sigma_0^2} + \frac{N}{\sigma^2}, \end{aligned}$$

in which μ_{ML} is the maximum likelihood estimation given by

$$\mu_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N x_n.$$

Note that as we increase the number of observed data points (taking the limit as $N \rightarrow \infty$), the precision steadily increases, corresponding to a posterior distribution with steadily decreasing variance.

Now suppose the mean μ is known and we hope to infer the variance. It turns out working with the precision $\lambda = \frac{1}{\sigma^2}$ is more convenient. We again write down the likelihood function:

$$p(X | \lambda) \propto \lambda^{N/2} \exp \left[-\frac{\lambda}{2} \sum_{n=1}^N (x_n - \mu)^2 \right].$$

To choose a conjugate prior, we introduce the gamma distribution.

Definition (gamma distribution). The **gamma distribution** is given by

$$\text{Gamma}(\lambda \mid a, b) = \frac{1}{\Gamma(a)} b^a \lambda^{a-1} \exp(-b\lambda).$$

In particular, we have the following integral:

$$\int_0^\infty \lambda^{a-1} \exp(-b\lambda) d\lambda = \int_0^\infty \frac{1}{b^a} u^{a-1} e^{-u} du = \frac{1}{b^a} \Gamma(a),$$

where we used change of variable $u = b\lambda$ in the first equality.

Through more gamma function calculation, we can obtain the mean and variance of the gamma distribution:

$$\mathbb{E}[\lambda] = \frac{a}{b}, \quad \text{var}[\lambda] = \frac{a}{b^2}.$$

Now consider a prior distribution $\text{Gamma}(\lambda \mid a_0, b_0)$. We can then obtain the posterior

$$p(\lambda \mid X) \propto \lambda^{a_0-1} \lambda^{N/2} \exp \left[-b_0 \lambda - \frac{\lambda}{2} \sum_{n=1}^N (x_n - \mu)^2 \right],$$

which is easily identified as a gamma distribution with

$$\begin{aligned} a_N &= a_0 + \frac{N}{2}, \\ b_N &= b_0 + \frac{1}{2} \sum_{n=1}^N (x_n - \mu)^2 = b_0 + \frac{N}{2} \sigma_{\text{ML}}^2, \end{aligned}$$

and the normalization constant then follows easily.

Now suppose both the mean and the variance is unknown. Consider the likelihood function:

$$\begin{aligned} p(X \mid \mu, \lambda) &= \prod_{n=1}^N \frac{\lambda^{1/2}}{(2\pi)^{1/2}} \exp \left[-\frac{\lambda}{2} (x_n - \mu)^2 \right] \\ &\propto \left[\lambda^{1/2} \exp \left(-\frac{\lambda \mu^2}{2} \right) \right]^N \exp \left[\lambda \mu \sum_{n=1}^N x_n - \frac{\lambda}{2} \sum_{n=1}^N x_n^2 \right]. \end{aligned}$$

Therefore, we should be looking for a conjugate prior in the form of

$$\begin{aligned} p(\mu, \lambda) &\propto \left[\lambda^{1/2} \exp \left(-\frac{\lambda \mu^2}{2} \right) \right]^\beta \exp(c\lambda\mu - d\lambda) \\ &= \exp \left[-\frac{\lambda\beta}{2} \left(\mu - \frac{c}{\beta} \right)^2 \right] \lambda^{\beta/2} \exp \left[-\left(d - \frac{c^2}{2\beta} \right) \lambda \right]. \end{aligned}$$

This is the **Gaussian-gamma distribution**:

$$p(\mu, \lambda) = \mathcal{N}(\mu \mid \mu_0, (\beta\lambda)^{-1}) \text{Gamma}(\lambda \mid a, b),$$

where $\mu_0 = \frac{c}{\beta}$, $a = \frac{\beta}{2} + 1$, and $b = d - \frac{c^2}{2\beta}$.

In the case of a multivariate Gaussian $\mathcal{N}(x \mid \mu, \Lambda^{-1})$ for a D -dimensional variable x , the conjugate prior for the mean is again Gaussian if we assume the variance is known. If the mean is known and the variance is unknown, the conjugate prior is a **Wishart distribution** given by

$$\mathcal{W}(\Lambda \mid W, \nu) = B |\Lambda|^{(\nu-D-1)/2} \exp \left[-\frac{1}{2} \text{tr}(W^{-1}\Lambda) \right],$$

where ν is the degrees of freedom and W is a $D \times D$ scale matrix. The normalization constant B is given by

$$B(W, \nu) = |W|^{-\nu/2} \left[2^{\nu D/2} \pi^{D(D-1)/4} \prod_{i=1}^D \Gamma \left(\frac{\nu + 1 - i}{2} \right) \right]^{-1}.$$

For unknown mean and unknown precision, the conjugate prior is the **Gaussian-Wishart distribution** given by

$$p(\mu, \Lambda \mid \mu_0, \beta, W, \nu) = \mathcal{N}(\mu \mid \mu_0, (\beta\Lambda)^{-1}) \mathcal{W}(\Lambda \mid W, \nu).$$

3.3.5 Student's t-distribution

We have seen the conjugate prior for the precision of a Gaussian is given by the gamma distribution. Now suppose we have a univariate Gaussian $\mathcal{N}(x \mid \mu, \tau^{-1})$ together with a gamma prior $\text{Gamma}(\tau \mid a, b)$, we integrate over the precision to get

$$\begin{aligned} p(x \mid \mu, a, b) &= \int_0^\infty \mathcal{N}(x \mid \mu, \tau^{-1}) \text{Gamma}(\tau \mid a, b) d\tau \\ &= \int_0^\infty \frac{\tau^{1/2}}{(2\pi)^{1/2}} \exp \left[-\frac{\tau}{2} (x - \mu)^2 \right] \frac{1}{\Gamma(a)} b^a \tau^{a-1} \exp(-\tau b) d\tau \\ &= \frac{b^a}{\Gamma(a)} \frac{1}{(2\pi)^{1/2}} \left[b + \frac{(x - \mu)^2}{2} + b \right]^{-a-1/2} \Gamma(a + 1/2). \end{aligned}$$

Now we introduce a new distribution.

Definition (student's t-distribution). The **student's t-distribution** is given by

$$\text{St}(x \mid \mu, \lambda, \nu) = \frac{\Gamma(\nu/2 + 1/2)}{\Gamma(\nu/2)} \left(\frac{\lambda}{\pi\nu} \right)^{1/2} \left[1 + \frac{\lambda(x - \mu)^2}{\nu} \right]^{-\nu/2-1/2},$$

where ν is called the **degrees of freedom** of the distribution.

Student's t-distribution have longer tails than the Gaussian distribution, so it is more **robust** – much less sensitive to a few outliers.

It is easy to verify that

$$\text{St}(x \mid \mu, \lambda, \nu) = \int_0^\infty \mathcal{N}(x \mid \mu, (\eta\lambda)^{-1}) \text{Gamma}(\eta \mid \nu/2, \nu/2) d\eta.$$

We can then generalize this to a **multivariate student's t-distribution**:

$$\text{St}(x \mid \mu, \Lambda, \nu) = \int_0^\infty \mathcal{N}(x \mid \mu, (\eta\Lambda)^{-1}) \text{Gamma}(\eta \mid \nu/2, \nu/2) d\eta.$$

Through computation, we obtain

$$\text{St}(x \mid \mu, \Lambda, \nu) = \frac{\Gamma(D/2 + \nu/2)}{\Gamma(\nu/2)} \frac{|\Lambda|^{1/2}}{(\pi\nu)^{D/2}} \left(1 + \frac{\Delta^2}{\nu}\right)^{-D/2 - \nu/2},$$

where D is the dimensionality of x and

$$\Delta^2 = (x - \mu)^T \Lambda (x - \mu).$$

We also have

$$\begin{aligned} \mathbb{E}[x] &= \mu & \text{if } \nu > 1, \\ \text{cov}[x] &= \frac{\nu}{(\nu - 2)} \Lambda^{-1} & \text{if } \nu > 2, \\ \text{mode}[x] &= \mu. \end{aligned}$$

3.4 The exponential family

Definition. The exponential family of distributions over x , given parameters η , is defined to be the set of distributions of the form

$$p(x \mid \eta) = h(x)g(\eta) \exp [\eta^T u(x)].$$

Here η is called the **natural parameters** of the distribution, $u(x)$ is some function of x and $g(\eta)$ can be interpreted as a normalization constant so that

$$g(\eta) \int h(x) \exp [\eta^T u(x)] dx = 1.$$

4 Mixture models and EM

4.1 Kullback-Leibler (KL) Divergence

In this section, we adopt the convention that $0 \log 0 = 0$.

Definition (KL divergence). The **Kullback-Leibler (KL) divergence** of two distributions $P(X)$ and $Q(X)$ over the outcome space X is defined as follows:

$$D_{\text{KL}}(P \parallel Q) = \sum_{x \in X} P(x) \log \frac{P(x)}{Q(x)}.$$

To understand the significance of KL-divergence better, we first discuss some related concepts in information theory, starting with the definition of **entropy**.

Definition. The **entropy** of a distribution $P(X)$ is defined as

$$H(P) = - \sum_{x \in X} P(x) \log P(x)$$

Intuitively, entropy measures how dispersed a probability distribution is. For example, a uniform distribution is considered to have very high entropy (i.e. a lot of uncertainty), whereas a distribution that assigns all its mass on a single point is considered to have zero entropy (i.e. no uncertainty). Notably, it can be shown that among continuous distributions over \mathbb{R} , the Gaussian distribution $\mathcal{N}(\mu, \sigma^2)$ has the highest entropy (highest uncertainty) among all possible distributions that have the given mean μ and variance σ^2 .

To further solidify our intuition, we present motivation from communication theory. Suppose we want to communicate from a source to a destination, and our messages are always (a sequence of) discrete symbols over space X (for example, X could be letters $\{a, b, \dots, z\}$). We want to construct an encoding scheme for our symbols in the form of sequences of binary bits that are transmitted over the channel. Further, suppose that in the long run the frequency of occurrence of symbols follow a probability distribution $P(X)$. This means, in the long run, the fraction of times the symbol x gets transmitted is $P(x)$.

A common desire is to construct an encoding scheme such that the average number of bits per symbol transmitted remains as small as possible. Intuitively, this means we want very frequent symbols to be assigned to a bit pattern having a small number of bits. Likewise, because we are interested in reducing the average number of bits per symbol in the long term, it is tolerable for infrequent words to be assigned to bit patterns having a large number of bits, since their low frequency has little effect on the long term average. The encoding scheme can be as complex as we desire, for example, a single bit could possibly represent a long sequence of multiple symbols (if that specific pattern of symbols is very common). The entropy of a probability distribution $P(X)$ is its optimal bit rate, i.e., the lowest average bits per message that can possibly be achieved if the symbols $x \in X$ occur according to $P(X)$. It does not specifically tell us how to construct

that optimal encoding scheme. It only tells us that no encoding can possibly give us a lower long term bits per message than $H(P)$.

To see a concrete example, suppose our messages have a vocabulary of $K = 32$ symbols, and each symbol has an equal probability of transmission in the long term (i.e, uniform probability distribution). An encoding scheme that would work well for this scenario would be to have $\log_2 K$ bits per symbol, and assign each symbol some unique combination of the $\log_2 K$ bits. In fact, it turns out that this is the most efficient encoding one can come up with for the uniform distribution scenario.

It may have occurred to you by now that the long term average number of bits per message depends only on the frequency of occurrence of symbols. The encoding scheme of scenario A can in theory be reused in scenario B with a different set of symbols (assume equal vocabulary size for simplicity), with the same long term efficiency, as long as the symbols of scenario B follow the same probability distribution as the symbols of scenario A. It might also have occurred to you, that reusing the encoding scheme designed to be optimal for scenario A, for messages in scenario B having a different probability of symbols, will always be suboptimal for scenario B. To be clear, we do not need know what the specific optimal schemes are in either scenarios. As long as we know the distributions of their symbols, we can say that the optimal scheme designed for scenario A will be suboptimal for scenario B if the distributions are different.

Concretely, if we reuse the optimal scheme designed for a scenario having symbol distribution $Q(X)$, into a scenario that has symbol distribution $P(X)$, the long term average number of bits per symbol achieved is called the cross entropy, denoted by $H(P, Q)$:

Definition. The cross-entropy of two distributions $P(X)$ and $Q(X)$ is defined as

$$H(P, Q) = - \sum_{x \in X} P(x) \log Q(x)$$

To recap, the entropy $H(P)$ is the best possible long term average bits per message (optimal) that can be achieved under a symbol distribution $P(X)$ by using an encoding scheme (possibly unknown) specifically designed for $P(X)$. The cross entropy $H(P, Q)$ is the long term average bits per message (suboptimal) that results under a symbol distribution $P(X)$, by reusing an encoding scheme (possibly unknown) designed to be optimal for a scenario with symbol distribution $Q(X)$.

Now, KL divergence is the penalty we pay, as measured in average number of bits, for using the optimal scheme for $Q(X)$, under the scenario where symbols are actually distributed as $P(X)$. It is straightforward to see this:

$$\begin{aligned} D_{\text{KL}}(P \parallel Q) &= \sum_{x \in X} P(x) \log \frac{P(x)}{Q(x)} \\ &= \sum_{x \in X} P(x) \log P(x) - \sum_{x \in X} P(x) \log Q(x) \\ &= H(P, Q) - H(P). \quad (\text{difference in average number of bits}) \end{aligned}$$

If the cross entropy between P and Q is zero (and hence $D_{\text{KL}}(P \parallel Q) = 0$) then it necessarily means $P = Q$. In Machine Learning, it is a common task to find a distribution Q that is “close” to another distribution P . To achieve this, we use $D_{\text{KL}}(P \parallel Q)$ to be the loss function to be optimized. As we will see in this below, Maximum Likelihood Estimation, which is a commonly used optimization objective, turns out to be equivalent minimizing KL divergence between the training data (i.e. the empirical distribution over the data) and the model.

Now we present some useful properties of KL divergence.

Theorem (Non-negativity). For any distribution P and Q , we have

$$D_{\text{KL}}(P \parallel Q) \geq 0,$$

and $D_{\text{KL}}(P \parallel Q) = 0$ if and only if $P = Q$ (almost everywhere).

Proof. By definition,

$$D_{\text{KL}}(P \parallel Q) = \sum_{x \in X} P(x) \log \frac{P(x)}{Q(x)} = - \sum_{x \in X} P(x) \log \frac{Q(x)}{P(x)}.$$

Since $-\log x$ is strictly convex, by Jensen’s inequality, we have

$$D_{\text{KL}}(P \parallel Q) = - \sum_{x \in X} P(x) \log \frac{Q(x)}{P(x)} \geq - \log \sum_{x \in X} P(x) \frac{Q(x)}{P(x)} = 0.$$

When the equality holds,

$$\log \frac{Q(x)}{P(x)} = 0$$

almost everywhere. That is, $Q = P$ almost everywhere. This completes the proof. \square

Definition (KL divergence of conditional distribution). The KL divergence between 2 conditional distributions $P(X \mid Y)$, $Q(X \mid Y)$ is defined as follows:

$$D_{\text{KL}}(P(X \mid Y) \parallel Q(X \mid Y)) = \sum_y P(y) \left(\sum_x P(x \mid y) \log \frac{P(x \mid y)}{Q(x \mid y)} \right).$$

This can be thought of as the expected KL divergence between the corresponding conditional distributions on x . That is, between $P(X \mid Y = y)$ and $Q(X \mid Y = y)$, where the expectation is taken over the random y .

Theorem (Chain rule for KL divergence). The following equality holds:

$$D_{\text{KL}}(P(X, Y) \parallel Q(X, Y)) = D_{\text{KL}}(P(X) \parallel Q(X)) + D_{\text{KL}}(P(Y \mid X) \parallel Q(Y \mid X)).$$

Proof.

$$\begin{aligned}
\text{LHS} &= \sum_x \sum_y P(x, y) \log \frac{P(x, y)}{Q(x, y)} \\
&= \sum_x \sum_y P(y | x) P(x) \left[\log \frac{P(y | x)}{Q(y | x)} + \log \frac{P(x)}{Q(x)} \right] \\
&= \sum_x \sum_y P(y | x) P(x) \log \frac{P(y | x)}{Q(y | x)} + \sum_x P(x) \log \frac{P(x)}{Q(x)} \sum_y P(y | x) \\
&= \sum_x \sum_y P(y | x) P(x) \log \frac{P(y | x)}{Q(y | x)} + \sum_x P(x) \log \frac{P(x)}{Q(x)} \\
&= D_{\text{KL}}(P(X) \parallel Q(X)) + D_{\text{KL}}(P(Y | X) \parallel Q(Y | X)) \\
&= \text{RHS}.
\end{aligned}$$

□

4.2 The EM Algorithm in General

Consider a probabilistic model in which we collectively denote all of the observed variables by X and all of the hidden variables by Z . The joint distribution $p(X, Z | \theta)$ is governed by a set of parameters denoted θ . Our goal is to maximize the likelihood function that is given by

$$p(X | \theta) = \sum_Z p(X, Z | \theta).$$

Assume direct optimization of $p(X | \theta)$ is difficult but optimization of $p(X, Z | \theta)$ is easy. Introduce distribution $q(Z)$ for the latent variable Z , we then have

$$\log p(X | \theta) = \mathcal{L}(q, \theta) + D_{\text{KL}}(q \parallel p),$$

where

$$\begin{aligned}
\mathcal{L}(q, \theta) &= \sum_Z q(Z) \log \frac{p(X, Z | \theta)}{q(Z)}, \\
D_{\text{KL}}(q \parallel p) &= - \sum_Z q(Z) \log \frac{p(Z | X, \theta)}{q(Z)}.
\end{aligned}$$

Note that \mathcal{L} is a functional of the distribution $q(Z)$. Note also that $D_{\text{KL}}(q \parallel p)$ is the KL divergence of $q(Z)$ and $p(Z | X, \theta)$ so $D_{\text{KL}}(q \parallel p) \geq 0$. Therefore, $\mathcal{L}(q, \theta) \leq \log p(X | \theta)$. In other word, $\mathcal{L}(q, \theta)$ is a **lower bound** for $\log p(X | \theta)$.

Therefore, for the EM algorithm, suppose currently the model parameter is θ_t . In the E step, the lower bound $\mathcal{L}(q, \theta)$ is maximized with respect to $q(Z)$ while holding θ fixed. Note that

$\log p(X | \theta_t)$ is not dependent on $q(Z)$, so the lower bound will be maximized when $D_{\text{KL}}(q \| p) = 0$. This is equivalent to when $q(Z) = p(Z | X, \theta)$. Therefore, in the E step we simply set

$$q(Z) = p(Z | X, \theta_t).$$

In the subsequent M step, the distribution $q(Z)$ is fixed and the lower bound $\mathcal{L}(q, \theta)$ is maximized with respect to θ to give some new model parameter θ_{t+1} . Because the distribution q is determined using the old parameter values rather than the new values and is held fixed during the M step, it will not equal the new posterior distribution $p(Z | X, \theta_{t+1})$, and hence there will be a nonzero KL divergence. Substituting the result from E step, we have the following expression for the lower bound of M step:

$$\begin{aligned} \mathcal{L}(q, \theta) &= \sum_Z p(Z | X, \theta_t) \log p(X, Z | \theta) - \sum_Z p(Z | X, \theta_t) \log p(Z | X, \theta_t) \\ &= \mathcal{Q}(\theta_t, \theta) + \text{const}, \end{aligned}$$

where

$$\mathcal{Q}(\theta_t, \theta) = \sum_Z p(Z | X, \theta_t) \log(X, Z | \theta)$$

and the constant is simply the negative entropy of the q distribution. Note that the variable θ over which we are optimizing appears only inside the logarithm.

The EM algorithm can also be used to maximize the **posterior** $p(\theta | X)$ with a prior $p(\theta)$ of the parameters. This is done by noting that

$$\begin{aligned} \log p(\theta | X) &= \log p(\theta, X) - \log p(X) \\ &= \mathcal{L}(q, \theta) + D_{\text{KL}}(q \| p) + \log p(\theta) - \log p(X) \\ &\geq \mathcal{L}(q, \theta) + \log p(\theta) - \log p(X), \end{aligned}$$

where $\log p(X)$ is a constant.

5 Approximate inference

A central task in the application of probabilistic models is the evaluation of the posterior distribution $p(Z \mid X)$ of the latent variables Z given the observed (visible) data variables X , and the evaluation of expectations computed with respect to this distribution. For many models of practical interest, it will be infeasible to evaluate the posterior distribution or indeed to compute expectations with respect to this distribution. This could be because the dimensionality of the latent space is too high to work with directly or because the posterior distribution has a highly complex form for which expectations are not analytically tractable. In the case of continuous variables, the required integrations may not have closed-form analytical solutions, while the dimensionality of the space and the complexity of the integrand may prohibit numerical integration. For discrete variables, the marginalizations involve summing over all possible configurations of the hidden variables, and though this is always possible in principle, we often find in practice that there may be exponentially many hidden states so that exact calculation is prohibitively expensive. The following table summarizes the properties of the mentioned distributions:

Concept	Known?	Tractable?	Notes
$p(Z)$	✓	✓	Chosen prior distribution
$p(X \mid Z)$	✓	✓	Likelihood model (possibly NN)
$p(X, Z)$	✓	✓	Product of above two
$p(Z \mid X)$	✗	✗	Intractable posterior
$p(X)$	✗	✗	Intractable marginals

In this chapter, we introduce a range of deterministic approximation schemes, some of which scale well to large applications. These are based on analytical approximations to the posterior distribution, for example by assuming that it factorizes in a particular way or that it has a specific parametric form such as a Gaussian. As such, they can never generate exact results, and so their strengths and weaknesses are complementary to those of sampling methods.

5.1 Variational inference

Suppose we have a fully Bayesian model in which every parameter is given prior distributions. Denote all latent variable with Z and all observed variable with X . As before we have

$$\log p(X) = \mathcal{L}(q) + D_{\text{KL}}(q \parallel p),$$

where

$$\begin{aligned} \mathcal{L}(q) &= \int q(Z) \log \frac{p(X, Z)}{q(Z)} dZ, \\ D_{\text{KL}}(q \parallel p) &= - \int q(Z) \log \frac{p(Z \mid X)}{q(Z)} dZ. \end{aligned}$$

It is well known that the KL divergence $D_{\text{KL}}(q \parallel p)$ is maximized when $q(Z) = p(Z \mid X)$. However, here we assume the posterior $p(Z \mid X)$ is intractable. We therefore consider instead a restricted family of distributions $q(Z)$ and then seek the member of this family for which the KL divergence is minimized.

5.1.1 Factorized distributions

Suppose partitioning the latent variables Z into disjoint groups Z_1, \dots, Z_m , and assume the q distribution factorizes in the form

$$q(Z) = \prod_{i=1}^M q_i(Z_i).$$

This factorized form of variational inference corresponds to an approximation framework developed in physics called **mean field theory**.

We now wish to optimize $\mathcal{L}(q)$ with respect to all distributions $q_i(Z_i)$. We first compute

$$\begin{aligned} \mathcal{L}(q) &= \int \prod_i q_i(Z_i) \left[\log p(X, Z) - \sum_i \log q_i(Z_i) \right] dZ \\ &= \int q_j \left[\int \log p(X, Z) \prod_{i \neq j} q_i(Z_i) dZ_i \right] dZ_j - \int q_j \log q_j dZ_j + \text{const} \\ &= \int q_j \log \tilde{p}(X, Z_j) dZ_j - \int q_j \log q_j dZ_j + \text{const}, \end{aligned}$$

where we have defined

$$\log \tilde{p}(X, Z_j) = \mathbb{E}_{i \neq j} [\log p(X, Z)] + \text{const}.$$

Suppose we keep $\{q_{i \neq j}\}$ fixed and maximize $\mathcal{L}(q)$ with respect to one of the factor $q_j(Z_j)$. Note that this is equivalent to minimizing the KL divergence of $q_j(Z_j)$ and $\tilde{p}(X, Z_j)$. Indeed, we have

$$D_{\text{KL}}(q_j(Z_j) \parallel \tilde{p}(X, Z_j)) = \int q_j \log q_j dZ_j - \int q_j \log \tilde{p}(X, Z_j) dZ_j.$$

The minimum is thus achieved at $q_j(Z_j) = \tilde{p}(X, Z_j)$. Hence, the general solution is

$$\log q_j^*(Z_j) = \mathbb{E}_{i \neq j} [\log p(X, Z)] + \text{const}, \quad (*)$$

and the constant is set by normalizing:

$$q_j^*(Z_j) = \frac{\exp(\mathbb{E}_{i \neq j} [\log p(X, Z)])}{\int \exp(\mathbb{E}_{i \neq j} [\log p(X, Z)]) dZ_j}.$$

The algorithm is then to first initialize each $q_i(Z_i)$ appropriately and cycling through all the factors and replacing each with a revised estimate given by (*). Convergence is guaranteed because the bound is convex with respect to each factor $q_i(Z_i)$.

5.1.2 Properties of factorized approximations

Alternatively, consider instead that we have been minimizing the reverse KL divergence $D_{\text{KL}}(p \parallel q)$ with respect to factorized distribution q . The KL divergence take the form

$$D_{\text{KL}}(p \parallel q) = - \int p(Z) \left[\sum_{i=1}^M \log q_i(Z_i) \right] dZ + \text{const}.$$

To optimize this, consider the Lagrangian

$$L[q_j] = - \int p(Z) \log q_j(Z_j) dZ + \lambda \int q_j(Z_j) dZ_j,$$

where we have kept only the terms dependent on q_j . Note also

$$\int p(Z) \left[\sum_{i=1}^M \log q_i(Z_i) \right] dZ = \int \log q_j(Z_j) \left[\int p(Z) \prod_{i \neq j} dZ_i \right] dZ_j.$$

It follows that

$$L[q_j] = - \int \log q_j(Z_j) \left[\int p(Z) \prod_{i \neq j} dZ_i \right] dZ_j + \lambda \int q_j(Z_j) dZ_j.$$

Taking the functional derivative, we can then obtain

$$\lambda = - \frac{1}{q_j(Z_j)} \int p(Z) \prod_{i \neq j} dZ_i.$$

Therefore,

$$q_j^*(Z_j) = \int p(Z) \prod_{i \neq j} dZ_i = p(Z_j).$$

To compare the two results, note that we have

$$\begin{aligned} D_{\text{KL}}(q \parallel p) &= - \int q(Z) \log \frac{p(Z)}{q(Z)} dZ, \\ D_{\text{KL}}(p \parallel q) &= - \int p(Z) \log \frac{q(Z)}{p(Z)} dZ. \end{aligned}$$

Note that for $D_{\text{KL}}(q \parallel p)$, there is a large positive contribution in region where $p(Z)$ is small. Therefore, minimizing $D_{\text{KL}}(q \parallel p)$ avoids region where $p(Z)$ is near 0. Conversely, $D_{\text{KL}}(p \parallel q)$ is minimized by having $q(Z)$ nonzero in region where $p(Z)$ is nonzero. It follows that minimizing $D_{\text{KL}}(q \parallel p)$ often leads to a more **compact** distribution, while minimizing $D_{\text{KL}}(p \parallel q)$ tends to give an **average across a large region** (see PRML page 469, 472).

5.1.3 Model comparison

As well as performing inference over the hidden variables Z , we may also wish to compare a set of candidate models, labelled by the index m , and having prior probabilities $p(m)$. Our goal is then to approximate the posterior probabilities $p(m \mid X)$, where X is the observed data.

We must recognize that the posterior over Z must be conditioned on m , and so we must consider $q(Z, m) = q(Z | m)q(m)$. We then have the following variational distribution:

$$\log p(X) = \mathcal{L}_m - \sum_m \sum_Z q(Z | m)q(m) \log \frac{p(Z, m | X)}{q(Z | m)q(m)},$$

where \mathcal{L}_m is a lower bound for $\log p(X)$ given by

$$\mathcal{L}_m = \sum_m \sum_Z q(Z | m)q(m) \log \frac{p(X, Z, m)}{q(Z | m)q(m)}.$$

Now, if we consider a specific model M and assign equal prior $p(m)$ to each model m , then

$$\mathcal{L} = \sum_Z q(Z | M) \log \frac{p(X, Z | M)}{q(Z | M)}$$

is a lower bound for $\log p(X | M)$. Note that we also have

$$p(M | X) \propto p(X | M)p(M).$$

However, $p(m)$ are equal for each m . This implies that we can interpret \mathcal{L} as an approximation to the posterior $p(M | X)$, and we can do model selection using the value of \mathcal{L} for each model. This should be contrasted with a maximum likelihood approach, which tend to overfit models (see PRML page 489-490).

5.2 Illustration: variational mixture of Gaussians

Consider the following model: for each observation x_n , we have a corresponding latent variable z_n , which is a 1-of- K binary vector with elements z_{nk} for $k = 1, \dots, K$. Denote $X = \{x_1, \dots, x_n\}$ and $Z = \{z_1, \dots, z_n\}$. We have the following likelihood model:

$$p(Z | \pi) = \prod_{n=1}^N \prod_{k=1}^K \pi_k^{z_{nk}},$$

$$p(X | Z, \mu, \Lambda) = \prod_{n=1}^N \prod_{k=1}^K \mathcal{N}(x_n | \mu_k, \Lambda_k^{-1})^{z_{nk}}.$$

Now we choose conjugate priors for each parameter. For the mixing coefficient π , we have

$$p(\pi) = \text{Dirichlet}(\pi | \alpha_0) = C(\alpha_0) \prod_{k=1}^K \pi_k^{\alpha_0 - 1},$$

where we choose the same parameter α_0 for each component by symmetry. For the mean μ and precision Λ , we have

$$p(\mu, \Lambda) = p(\mu | \Lambda)p(\Lambda) = \prod_{k=1}^K \mathcal{N}(\mu_k | m_0, (\beta_0 \Lambda_k^{-1})) \mathcal{W}(\Lambda_k | W_0, \nu_0),$$

where we often choose $m_0 = 0$ by symmetry.

TODO: do the calculation