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STATISTICAL MODELS WITH VARIATIONAL METHODS

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ABSTRACT

Some introduction about how important Variational methods are nowadays and what this project is about.

CONTENTS

I	BASIC CONCEPTS	5
1	PROBABILITY	6
2	DISTRIBUTIONS	11
2.1	Discrete Distributions	13
2.1.1	Bernoulli Distribution	13
2.1.2	Categorical Distribution	13
2.1.3	Binomial Distribution	13
2.1.4	Multinomial Distribution	13
2.2	Continuous Distributions	13
2.2.1	Uni-Variate Normal Distribution	13
2.2.2	Multi-Variate Normal Distribution	14
2.2.3	Gamma Distribution	15
2.2.4	Beta Distribution	15
2.2.5	Dirichlet Distribution	16
2.3	Kullback-Leibler Divergence	17
3	GRAPH THEORY	18
II	VARIATIONAL INFERENCE	20
4	INTRODUCTION	21
5	MEAN-FIELD VARIATIONAL INFERENCE	24
5.1	The mean-field variational family	24
5.2	CAVI Algorithm	25
6	EXPONENTIAL FAMILY	26
6.1	Latent Variable and Conditionally conjugate models	27
6.2	CAVI in Conditionally conjugate models	29
III	GRAPHICAL MODELS	31
7	BAYESIAN NETWORKS	32
8	MARKOV RANDOM FIELDS	36
9	APPLICATION TO VARIATIONAL INFERENCE	38
9.1	Gaussian Mixture	38
9.2	Latent Dirichlet allocation	39
9.3	From PCA to Variational auto-encoders	42
9.3.1	Artificial Neural networks	43
9.3.2	Variational Auto Encoders	43
IV	BAYESIAN NETWORKS LEARNING	45
10	INTRODUCTION	46
10.1	Utility	48
11	MAXIMUM LIKELIHOOD TRAINING	50

11.1	ML and KL divergence	51
12	BAYESIAN TRAINING	53
12.1	Global and local parameter independence	54
12.2	Learning binary variables	54
12.3	Learning discrete variables	56
12.3.1	No parents	56
12.3.2	Parents	57
13	STRUCTURE LEARNING	59
13.1	PC Algorithm	59
13.2	Independence Learning	60
14	VARIATIONAL INFERENCE IN BAYESIAN NETWORKS	61
14.1	Expectation Maximization	62
14.1.1	General case	62
14.1.2	EM increases the marginal likelihood	64
14.1.3	Bayesian Networks case	65
14.2	Distribution mixture example with EM	66
14.3	EM Extensions	68
14.3.1	Partial steps	68
14.4	Variational Bayes	69
14.4.1	VB is a generalization of the EM algorithm	70
V	PRACTICAL CASE WITH INFERPY	72
15	INFERPY USAGE	73
16	GAUSSIAN MIXTURE	74

Part I

BASIC CONCEPTS

In this part we will introduce the underlying concepts of probability and graph theory that we will need.

PROBABILITY

All our theory will be made under the assumption that there is a *referential set* Ω , set of all possible outcomes of an experiment. Any subset of Ω will be called an *event*.

Definition 1. Let $\mathcal{P}(\Omega)$ be the power set of Ω . Then, $\mathcal{F} \subset \mathcal{P}(\Omega)$ is called a σ -algebra if it satisfies:

- $\Omega \in \mathcal{F}$.
- \mathcal{F} is closed under complementation.
- \mathcal{F} is closed under countable unions.

From these properties it follows that $\emptyset \in \mathcal{F}$ and that \mathcal{F} is closed under countable intersections.

The tuple (Ω, \mathcal{F}) is called a *measurable space*.

Definition 2. A *probability* P over (Ω, \mathcal{F}) is a mapping $P : \mathcal{F} \rightarrow [0, 1]$ which satisfies

- $P(\alpha) \geq 0 \quad \forall \alpha \in \mathcal{F}$.
- $P(\Omega) = 1$.
- P is countably additive, that is, if $\{\alpha_i\}_{i \in \mathbb{N}} \subset \mathcal{F}$, is a countable collection of pairwise disjoint sets, then

$$P\left(\bigcup_{i \in \mathbb{N}} \alpha_i\right) = \sum_{i \in \mathbb{N}} P(\alpha_i).$$

The first condition guarantees non negativity. The second one states that the *trivial event* has the maximal possible probability of 1. The third condition implies that given a set of pairwise disjoint events, the probability of either one of them occurring is equal to the sum of the probabilities of each one.

From these conditions follows

- $P(\emptyset) = 0$.
- $P(\alpha \cup \beta) = P(\alpha) + P(\beta) - P(\alpha \cap \beta)$.

The triple (Ω, \mathcal{F}, P) is called a *probability space*.

Definition 3. Given two events $\alpha, \beta \in \mathcal{F}$, with $P(\beta) \neq 0$, the conditional probability of α given β is defined as the quotient of the probability of the joint events and the probability of β :

$$P(\alpha | \beta) = \frac{P(\alpha \cap \beta)}{P(\beta)}.$$

Theorem 1. (Bayes' theorem). Let α, β be two events of an experiment, given that $P(\beta) \neq 0$. Then

$$P(\alpha | \beta) = \frac{P(\beta | \alpha)P(\alpha)}{P(\beta)}.$$

Example 1. Consider a study where the relation of a disease d and an habit h is being investigated. Suppose that $P(d) = 10^{-5}$, $P(h) = 0.5$ and $P(h | d) = 0.9$. What is the probability that a person with habit h will have the disease d ?

$$P(d | h) = \frac{P(d \cap h)}{P(h)} = \frac{P(h | d)P(d)}{P(h)} = \frac{0.9 \times 10^{-5}}{0.5} = 1.8 \times 10^{-5}.$$

If we set the probability of having habit h to a much lower value as $P(h) = 0.001$, then the above calculation gives approximately $1/100$. Intuitively, a smaller number of people have the habit and most of them have the disease. This means that the relation between having the disease and the habit is stronger now compared with the case where more people had the habit.

Definition 4. We say that two events $\alpha, \beta \in \mathcal{F}$ are *independent* if knowing one of them does not give any extra information about the other. Mathematically,

$$P(\alpha \cap \beta) = P(\alpha)P(\beta), \quad P(\alpha | \beta) = P(\alpha).$$

Let $\gamma \in \mathcal{F}$, we say that α and β are *conditionally independent* on γ , $\alpha \perp\!\!\!\perp \beta | \gamma$ if and only if

$$P(\alpha \cup \beta | \gamma) = P(\alpha | \gamma)P(\beta | \gamma).$$

Otherwise, they are said to be *conditionally dependent* on γ , $\alpha \not\perp\!\!\!\perp \beta | \gamma$.

Now we are going to introduce the concept of *random variable* and some properties as we have done with events.

Definition 5. A function $f : \Omega_1 \rightarrow \Omega_2$ between two measurable spaces $(\Omega_1, \mathcal{F}_1)$ and $(\Omega_2, \mathcal{F}_2)$ is said to be *measurable* if $f^{-1}(\alpha) \in \mathcal{F}_1$ for every $\alpha \in \mathcal{F}_2$.

Definition 6. A *random variable* is a measurable function $X : \Omega \rightarrow E$ from a probability space (Ω, \mathcal{F}, P) to a measurable space (E, \mathcal{F}') verifying $X(\omega) \in \mathcal{F}' \forall \omega \in \Omega$.

The probability of X taking a value on a measurable set $S \in E$ is written as

$$P_X(S) = P(X \in S) = P(\{a \in \Omega \mid X(a) \in S\}).$$

We could make a question like “How likely is that the value of X equals a ?”. This is the same as asking for the probability of the set $\{\omega \in \Omega \mid X(\omega) = a\}$.

We will set the following notation that is going to be used, that is: random variables will be denoted with an upper case letter like X and a set of variables with a bold symbol like \mathbf{X} . The meaning of $P(\text{state})$ will be clear without a reference to the variable. Otherwise $P(X = \text{state})$ will be used. Using a lower case letter like $P(x)$ will denote the probability of the corresponding upper case variable X taking a specific value.

Definition 7. The *cumulative distribution function* of a real-valued random variable X is defined as

$$F_X(x) = P(X \leq x),$$

where the right-hand side represents the probability of the random variable taking value below or equal to x .

Definition 8. When the image of a random variable X is countable, the random variable is called a *discrete random variable* and its *probability mass function* p gives the probability of it being equal to some value:

$$p(x) = P(X = x).$$

In case the image is uncountable and real, then X is called a *continuous random variable* and if there exists a non-negative Lebesgue-integrable f such that

$$F_X(x) = P(X \leq x) = \int_{-\infty}^x f(u)du,$$

then it is called its *probability density function*.

A *mixed random variable* is a random variable who is neither discrete nor continuous, it can be realized as the sum of a discrete and continuous random variables. An example of a random variable of mixed type would be based on an experiment where a coin is flipped and a random positive number is chose only if the result of the coin toss is heads, -1 otherwise.

From now on, $P(x)$ will denote $f_X(x)$ when X is a continuous random variable. We define the *probability distribution* P_X of a random variable X over the probability space (Ω, \mathcal{F}, P) as the pushforward measure of it, that is, $P_X = PX^{-1}$.

Integrate notation will be used in both continuous and discrete cases, where the last one can be interpreted as integration with respect to the *counting measure* defined as

$$\#(dx) = \sum_{n \in \mathcal{I}} \delta(x - n)dx,$$

where \mathcal{I} is the set of values X can take, and δ is the Dirac distribution. Given this measure, integration corresponds to summation as

$$\int_x P(x)\#(dx) = \sum_{n \in \mathcal{I}} \int_x P(x)\delta(x - n)dx = \sum_{n \in \mathcal{I}} P(n).$$

Where we used that $\int f(x)\delta(x - x_0) = f(x_0)$. Given this, from now on, we will use the integration notation for both discrete and continuous variables given that the integrals will be respect to the counting measure when needed.

Definition 9. As we did for events, we can define the *conditional probability* over random variables, let X, Y be two random variables, then

$$P(x | y) = \frac{P(x, y)}{P(y)}.$$

It is required that $P(y) \neq 0$ for the conditional probability to be defined.

We can also enunciate the *Bayes' theorem* as

$$P(x, y) = \frac{P(y | x)P(x)}{P(y)}$$

Clearly an arbitrary number of variables can be considered in both cases.

Definition 10. The *marginal distribution* of a subset of random variables is the probability distribution of the variables contained in that subset.

Let X, Y be two random variables, it follows that

$$P(x) = \int_y P(x, y).$$

Definition 11. Let $\mathbf{X} = \{X_1, X_2, \dots, X_n\}$ be a set of random variables, the *joint probability distribution* for \mathbf{X} is function that gives the probability of each random variable X_i falling in a particular range or discrete set of values for that variable. It is called a *multi-variate distribution*.

When using only two random variables, then is called a *bi-variate distribution*.

This distribution can be expressed either in terms of a joint cumulative distribution function

$$F_{\mathbf{X}}(\mathbf{x}) = F_{X_1, \dots, X_n}(x_1, \dots, x_n) = P(X_1 \leq x_1, \dots, X_n \leq x_n)^1,$$

or using a probability density or mass function.

Definition 12. We say that two random variables X and Y are *independent* if knowing one of them doesn't give any extra information about the other. Mathematically,

$$P(x, y) = P(x)P(y).$$

From this it follows that if X and Y are independent, then $P(x | y) = P(x)$.

Definition 13. Let X, Y and Z be three random variables, then X and Y are *conditionally independent* given Z if and only if

$$P(x, y | z) = P(x | z)P(y | z),$$

in that case we will denote $X \perp\!\!\!\perp Y | Z$. If X and Y are not conditionally independent, they are *conditionally dependent* $X \not\perp\!\!\!\perp Y | Z$

¹ Where $\mathbf{x} = (x_1, \dots, x_n)$

Both independence definitions can be made over sets of variables \mathbf{X}, \mathbf{Y} and \mathbf{Z} in a straight forward way.

Definition 14. We say that a set of n random variables $\{X_1, \dots, X_n\}$ defined to assume values in $I \subset \mathbb{R}$ are *independent and identically distributed (i.i.d)* if and only if they are independent, i.e,

$$F_{X_1, \dots, X_n}(x_1, \dots, x_n) = F_{X_1}(x_1) \dots F_{X_n}(x_n) \quad \forall x_1, \dots, x_n \in I,$$

and are identically distributed

$$F_{X_1}(x_1) = F_{X_k}(x_k) \quad \forall k \in \{2, \dots, n\} \text{ and } \forall x \in I.$$

Definition 15. A *multi-variate random variable* or *random vector* is a column vector $\mathbf{X} = (X_1, \dots, X_n)^T$ whose components are random variables that can be defined over different probability spaces.

Note that we use the same symbol \mathbf{X} for random vectors and sets of variables, but the meaning will be clear within the context.

DISTRIBUTIONS

In this section we will summarize some concepts concerning probability distributions among with some of the most used ones.

From now on, let X be a random variable and P its probability distribution.

Definition 16. The *mode* X_* of the probability distribution P is the state of X where the distribution takes it's highest value

$$X_* = \arg \max_x P(x).$$

A distribution could have more than one mode, in this case we say it is *multi-modal*.

Definition 17. The notation $\mathbb{E}[X]$ is used to denote the *average* or *expectation* of the values a real-valued variable takes respect to its distribution. It is worth mentioning that it might not exists. If X is non-negative, it is defined as

$$\mathbb{E}[X] = \int_{\Omega} X(\omega) dP(\omega)^1.$$

For a general variable X it is defined as $\mathbb{E}[X] = \mathbb{E}[X^+] - \mathbb{E}[X^-]$. Where

$$X^+(\omega) = \max(X(\omega), 0), \quad X^-(\omega) = \min(X(\omega), 0).$$

Suppose now that X is a real-valued random variable, in case it is also continuous, the expectation is

$$\mathbb{E}[X] = \int_{-\infty}^{+\infty} xf(x)dx.$$

And if it is discrete, let x_i be the values X can take, the expectation takes the form

$$\mathbb{E}[X] = \sum_{i=1}^{+\infty} x_i p(x_i)dx.$$

Let $g : \mathbb{R} \rightarrow \mathbb{R}$ be a measurable function, then $g \circ X$ is another random variable and we can talk about $\mathbb{E}[g(X)]$, so in case X is continuous, we have that

$$\mathbb{E}[g(X)] = \int_{-\infty}^{+\infty} g(x)f(x)dx.$$

¹ P is a measure over Ω

In the above definition, the expectation is calculated over the probability distribution P of the random variable, in future sections this distribution is unknown and a guessed distribution Q will be used. In this cases when the distribution is not clear from the context the notation $\mathbb{E}_Q[X]$ will be used.

Definition 18. We define the k^{th} moment of a distribution as the average of X^k over the distribution

$$\mu_k = \mathbb{E}[X^k]$$

For $k = 1$ it is typically denoted as μ . Note μ_k can also denote the k^{th} element in the mean vector of a multi-variate variable.

Definition 19. The *variance* of a distribution is defined as

$$\text{Var}(X) = \sigma^2 = \mathbb{E}[(X - \mathbb{E}[X])^2] = \mathbb{E}[X]^2 - \mathbb{E}[X^2]$$

The square root of the variance σ is called the *standard deviation*.

When using a multi-variate distribution $\mathbf{X} = (X_1, \dots, X_n)^T$ we can talk about the *covariance matrix* Σ whose elements are

$$\begin{aligned} \Sigma_{ij} &= \mathbb{E}[(X_i - \mathbb{E}[X_i])(X_j - \mathbb{E}[X_j])] = \mathbb{E}[(X_i - \mu_i)(X_j - \mu_j)] \\ &= \mathbb{E}[X_i X_j] - \mathbb{E}[X_i] \mathbb{E}[X_j] \end{aligned}$$

The following result will be helpful later on.

Proposition 1. Let $\mathcal{X} = \{X_1, \dots, X_n\}$ be a set of random variables, $\mathcal{X}_0 \subset \mathcal{X}$ and $P(\mathcal{X}), P(\mathcal{X}_0)$ their probability distributions. It follows that the expectation of a function g over \mathcal{X}_0 , verifies

$$\mathbb{E}_{P(\mathcal{X})}[g(\mathcal{X}_0)] = \mathbb{E}_{P(\mathcal{X}_0)}[g(\mathcal{X}_0)].$$

That is, we only need to know the marginal distribution of the subset in order to carry out the average.

Proof. Let $\mathcal{I} = (i_1, \dots, i_k)$ be the indexes corresponding to \mathcal{X}_0 , then

$$\begin{aligned} \mathbb{E}_{P(\mathcal{X})}[g(\mathcal{X}_0)] &= \int_{x_1} \cdots \int_{x_n} g(x_{i_1}, \dots, x_{i_k}) f(x_1, \dots, x_n) \\ &= \int_{x_{i_1}} \cdots \int_{x_{i_k}} g(x_{i_1}, \dots, x_{i_k}) \int \cdots \int f(x_1, \dots, x_n) dx_1, \dots, dx_n \\ &= \int_{x_{i_1}} \cdots \int_{x_{i_k}} g(x_{i_1}, \dots, x_{i_k}) f(x_{i_1}, \dots, x_{i_k}) = \mathbb{E}_{P(\mathcal{X}_0)}[g(\mathcal{X}_0)]. \end{aligned}$$

Where in the second-last equality we used marginalization. □

We are going to discuss now some examples of probability distributions that are going to be used from now on.

2.1 DISCRETE DISTRIBUTIONS

2.1.1 Bernoulli Distribution

The Bernoulli distribution describes a discrete binary variable X that takes the value 1 with probability p and the value 0 with probability $1 - p$.

$$P(x) = \begin{cases} p & \text{if } x = 1 \\ 1 - p & \text{if } x = 0 \end{cases}.$$

2.1.2 Categorical Distribution

A generalization of the Bernoulli Distribution when the variable can take more than two states is the *Categorical Distribution*. Let $\text{Dom}(X) = \{1, \dots, N\}$, then X follows a categorical distribution of parameters $\theta = (\theta_1, \dots, \theta_N)$ if and only if

$$P(x \mid \theta) = \prod_{i=1}^N \theta_i^{\mathbb{I}[x=i]} \text{ and } \sum_{i=1}^N \theta_i = 1.$$

2.1.3 Binomial Distribution

The binomial distribution describes the number of successes in a sequence of independent Bernoulli Trials. A discrete binary random variable X follows a *binomial distribution* of parameters $n \in \mathbb{N}$ and $p \in [0, 1]$, denoted as $X \sim B(n, p)$ if and only if

$$P(x = k) = \binom{n}{k} p^k (1 - p)^{n-k}.$$

2.1.4 Multinomial Distribution

The multinomial distribution is a generalization of the binomial distribution which describes the result of a sequence of independent trials in a categorical distribution. A discrete random variable X follows a *multinomial distribution* of parameters $n \in \mathbb{N}$, $\mathbf{p} = (p_1, \dots, p_K)$ such that $\sum p_k = 1$ if and only if

$$P(\mathbf{x} = x_1, \dots, x_K) = \begin{cases} \frac{n!}{x_1! \dots x_K!} \prod_{k=1}^K p_k^{x_k} & \text{if } \sum_k x_k = n \\ 0 & \text{otherwise} \end{cases}$$

2.2 CONTINUOUS DISTRIBUTIONS

2.2.1 Uni-Variate Normal Distribution

The *normal* or *Gaussian distribution* is a type of continuous probability distribution for real-valued random variables.

Definition 20. We say the real valued random variable X follows a *normal distribution* of parameters $\mu, \sigma \in \mathbb{R}$, denoted as $X \sim N(\mu, \sigma)$ if and only if, its probability density function exists and is

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}.$$

The parameter μ is the mean or expectation of the distribution and σ is its standard deviation.

The simplest case of a normal distribution is known as *standard normal distribution*, denoted as Z . It is a special case where $\mu = 0$ and $\sigma = 1$, then its density function is

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}.$$

One of the properties of the normal distribution is that if $X \sim N(\mu, \sigma)$, $a, b \in \mathbb{R}$ and $f : \mathbb{R} \rightarrow \mathbb{R}$ be defined as $f(x) = ax + b$, then $f(X) \sim N(\mu + b, a^2\sigma)$.

2.2.2 Multi-Variate Normal Distribution

This distribution plays a fundamental role in this project so we will discuss its properties in more detail.

This distribution is an extension of the uni-variate one when having a multi-variate random variable.

Definition 21. We say that a random vector $\mathbf{X} = (X_1, \dots, X_p)$ follows a *multi-variate normal distribution* of parameters $\boldsymbol{\mu} \in \mathbb{R}^p$ and $\boldsymbol{\Sigma} \in \mathbb{M}_n(\mathbb{R})$, denoted as $\mathbf{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ if and only if its probability density function is

$$f(\mathbf{x}) = \frac{1}{\sqrt{\det(2\pi\boldsymbol{\Sigma})}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}.$$

Where $\boldsymbol{\mu}$ is the mean vector of the distribution, and $\boldsymbol{\Sigma}$ the covariance matrix. The inverse matrix $\boldsymbol{\sigma}^{-1}$ is called *precision*. It also satisfies that

$$\boldsymbol{\mu} = \mathbb{E}[\mathbf{X}], \quad \boldsymbol{\Sigma} = \mathbb{E}\left[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T\right].$$

As $\boldsymbol{\Sigma}$ is a real symmetric matrix, it can be eigendecomposed

$$\boldsymbol{\Sigma} = \mathbf{E}\boldsymbol{\Delta}\mathbf{E}^T,$$

where $\mathbf{E}^T \mathbf{E} = \mathbf{I}$ and $\boldsymbol{\Delta} = \text{diag}(\lambda_1, \dots, \lambda_n)$.

Using the transformation

$$\mathbf{y} = \boldsymbol{\Delta}^{\frac{1}{2}} \mathbf{E}^T (\mathbf{x} - \boldsymbol{\mu}),$$

we get that

$$(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma} (\mathbf{x} - \boldsymbol{\mu}) = \mathbf{y}^T \mathbf{y}.$$

Using this, the multi-variate Normal Distribution reduces to a product of n uni-variate standard normal distributions.

2.2.3 Gamma Distribution

Another continuous distribution that we are going to use is the *Gamma distribution*.

Definition 22. We say that a continuous random variable X defined on \mathbb{R}^+ follows a *Gamma distribution* of parameters $\alpha, \beta > 0$, denoted as $X \sim \text{Gamma}(\alpha, \beta)$ if and only if its density function is

$$f(x) = \frac{\beta^\alpha x^{\alpha-1} e^{-\beta x}}{\Gamma(\alpha)},$$

where Γ is the Gamma function defined as

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

The mean is given by $\mathbb{E}[X] = \frac{\alpha}{\beta}$.

Definition 23. The *inverse gamma distribution* is defined by the density function

$$f(x) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{-\alpha-1} e^{-\beta/x}.$$

2.2.4 Beta Distribution

Definition 24. We say that a continuous random variable X defined on the interval $[0, 1]$ follows a *Beta distribution* of parameters $\alpha, \beta > 0$, denoted as $X \sim \text{Beta}(\alpha, \beta)$ if and only if its density function is

$$f(x) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1},$$

where $B(\alpha, \beta)$ is the *beta function* defined as

$$B(\alpha, \beta) = \int_0^1 x^{\alpha-1} (1-x)^{\beta-1} dx.$$

The mean is given by $\mathbb{E}[X] = \frac{\alpha}{\alpha+\beta}$.

2.2.5 Dirichlet Distribution

The Dirichlet distribution is a family of continuous multi-variate probability distributions parameterized by a vector α of positive reals. It is a multi-variate generalization of the Beta Distribution.

Definition 25. We say that a continuous random multi-variate variable \mathbf{X} with order $K \geq 2$, follows a *Dirichlet Distribution* with parameters $\alpha = (\alpha_1, \dots, \alpha_K)$, if and only if its density function is defined as

$$f(\mathbf{x}) = \frac{1}{B(\alpha)} \prod_{k=1}^K x_k^{\alpha_k-1},$$

and it satisfies that

$$\sum_{k=1}^K x_k = 1 \text{ and } x_k > 0 \ \forall k = 1, \dots, K.$$

Where the normalization constant is the multi-variate beta function

$$B(\alpha) = \frac{\prod_k \Gamma(\alpha_k)}{\Gamma(\sum_k \alpha_k)}.$$

When the vector parameter α is filled with the same value α_0 , the distribution is called Symmetric-Dirichlet with parameter α_0 .

Proposition 2. Let $(X_0, \dots, X_n) \sim \text{Dirichlet}(\alpha_0, \dots, \alpha_n)$, then $X_0 \sim \text{Beta}(\alpha_0, \alpha_1 + \dots + \alpha_n)$.

Proof. Following [Farrow (2008)], we can write the joint probability as

$$f(x_1, \dots, x_n) = f_1(x_1) f_2(x_2 | x_1) \dots f_{n-1}(x_{n-1} | x_1, \dots, x_{n-2}).$$

We do not need the last term because it is fixed given the others. In fact, let $A = \sum_i \alpha_i$, we can write it as

$$\begin{aligned} & \left(\frac{\Gamma(A)}{\Gamma(\alpha_1)\Gamma(A-\alpha_1)} x_1^{\alpha_1-1} (1-x_1)^{A-\alpha_1-1} \right) \left(\frac{\Gamma(A-\alpha_1)}{\Gamma(\alpha_2)\Gamma(A-\alpha_1-\alpha_2)} \frac{x_2^{\alpha_2-1} (1-x_1-x_2)^{A-\alpha_2-\alpha_1-1}}{(1-x_1)^{A-\alpha_1-1}} \right) \\ & \dots \left(\frac{\Gamma(A-\alpha_1-\dots-\alpha_{n-2})}{\Gamma(\alpha_{n-1})\Gamma(A-\alpha_1-\dots-\alpha_{n-1})} \frac{x_{n-1}^{\alpha_{n-1}-1} x_n^{\alpha_n-1}}{(1-x_1-\dots-x_{n-2})^{\alpha_{n-1}+\alpha_n-1}} \right). \end{aligned}$$

From this, we get that

$$f_1(x_1) = \frac{\Gamma(A)}{\Gamma(\alpha_1)\Gamma(A-\alpha_1)} x_1^{\alpha_1-1} (1-x_1)^{A-\alpha_1-1} \implies X_1 \sim \text{Beta}(\alpha_1, A-\alpha_1).$$

Making the decomposition over any other X_j , results on $X_j \sim \text{Beta}(\alpha_j, A-\alpha_j)$. □

2.3 KULLBACK-LEIBLER DIVERGENCE

Definition 26. Let P and Q be two probability distributions over the same set of random variables \mathbf{X} , the *Kullback-Leibler divergence* $KL(Q \mid P)$ measures the “difference” between both distributions as

$$KL(Q \mid P) = \mathbb{E}_Q[\log Q(x) - \log P(x)].$$

Remark 1. A random variable can not have two different distributions, in this case it must be understood that one or both distributions are “guessed” and we want to calculate the differences between them. For example, consider P the real distribution of the variable and Q an approximation.

Proposition 3. *The Kullback-Leibler divergence is always non-negative.*

Proof. As the logarithm is bounded by $x - 1$, we can bound $\log \frac{P(x)}{Q(x)}$

$$\log x \leq x - 1 \implies \frac{P(x)}{Q(x)} - 1 \geq \log \frac{P(x)}{Q(x)}.$$

Since probabilities are non-negative, we can multiply by $Q(x)$

$$P(x) - Q(x) \geq Q(x) \log P(x) - Q(x) \log Q(x).$$

Now we integrate (sum in case of discrete variables) both sides

$$0 \geq \mathbb{E}_Q[\log P(x) - \log Q(x)] \implies \mathbb{E}_Q[\log Q(x) - \log P(x)] \geq 0.$$

□

As a result, the Kullback-Leibler divergence is 0 if and only if the two distributions are equal almost everywhere.

GRAPH THEORY

Definition 27. A graph $G = (V, E)$ is a set of vertices or nodes V and edges $E \subset V \times V$ between them. If V is a set of ordered pairs then the graph is called a *directed graph*, otherwise if V is a set of unordered pairs it is called an *undirected graph*.

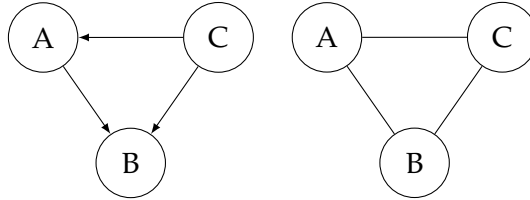


Figure 1: Example of directed and undirected graph, respectively.

Definition 28. In a directed graph $G = (V, E)$, a *directed path* $A \rightarrow B$ is a sequence of vertices $A = A_0, A_1, \dots, A_{n-1}, A_n = B$ where $(A_i, A_{i+1}) \in E \forall i \in 0, \dots, n-1$.

If G is a undirected graph, $A \rightarrow B$ is an *undirected path* if $\{A_i, A_{i+1}\} \in E \forall i \in 0, \dots, n-1$

Definition 29. Let A, B be two vertices of a directed graph G . If $A \rightarrow B$ is a directed path and $B \not\rightarrow A$ (meaning there isn't a directed path from B to A), then A is called an *ancestor* of B and B is called a *descendant* of A .

For example, in the figure 1, C is an ancestor of B .

Definition 30. A *directed acyclic graph (DAG)* is a directed graph such that no directed path between any two nodes revisits a vertex.

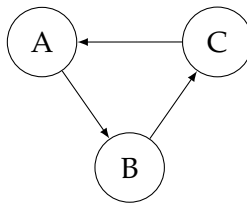


Figure 2: Example of graph which isn't a DAG.

As we can see in the figure 2, $A \rightarrow B \rightarrow C \rightarrow A \rightarrow B$ is a path from A to B that revisits A .

Now where are going to define some relations between nodes in a DAG.

Definition 31. The *parents* of a node A is the set of nodes B such that there is a directed edge from B to A . The same applies for the *children* of a node.

The *Markov blanket* of a node is composed by the node itself, its children, its parents and the parents of its children.

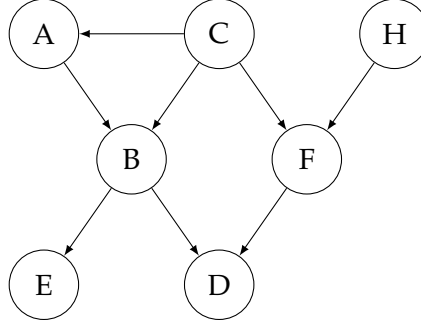


Figure 3: Directed acyclic graph

Definition 32. In a graph, the *neighbors* of a node are those directly connected to it.

We can use figure 3 to reflect on these definitions. The parents of B are $pa(B) = \{A, C\}$ and its children are $ch(B) = \{E, D\}$. Taking this into account, its neighbors are $ne(B) = \{A, C, E, D\}$ and its Markov blanket is $\{A, B, C, D, E, F\}$.

Definition 33. Let G be a DAG, U be a path between two vertex and $A \in U$

- A is called a *collider* if $\forall B \in ne(A) \cap U, (B, A) \in E$.
- A is called a *fork* if $\forall B \in ne(A) \cap U, (A, B) \in E$.

Notice, a vertex can be a collider for a path but not for others. A vertex is said to be a collider or a fork without any reference to the path when it is for any path that goes through it. This happens when the edge direction condition is satisfied for every neighbor.

For example in figure 3, D is a collider and C is a fork.

Definition 34. Let G be an undirected graph, a *clique* is a maximally connected subset of vertices. That is, all the members of the clique are connected to each others and there is no bigger clique that contains another.

Formally, $S \subset V$ is a *clique* if and only if $\forall A, B \in S, \{A, B\} \in E$ and $\nexists C \in V \setminus S$ such that $\forall A \in S, \{A, C\} \in E$.

Part II

VARIATIONAL INFERENCE

INTRODUCTION

Statistical inference is the process of using data analysis to deduce properties of an underlying distribution.

The following elements are being considered: a random variable X with its corresponding set of observations $\mathbf{x} = (x_1, \dots, x_N)$ and a *hidden or latent variable* Z , which means that it is unobserved and the values $\mathbf{z} = (z_1, \dots, z_N)$ are unknown. The samples are governed by the joint distribution $P(\mathcal{V}, \mathbf{z})$. Where \mathbf{z} represents a vector with length N with a possible configuration of the unknown values, then, it is not fixed as \mathbf{x} .

In *classical inference* the conditional is calculated as

$$P(\mathbf{z} \mid \mathbf{x}) = \frac{P(\mathbf{x}, \mathbf{z})}{\int_{\mathbf{z}} P(\mathbf{x}, \mathbf{z})},$$

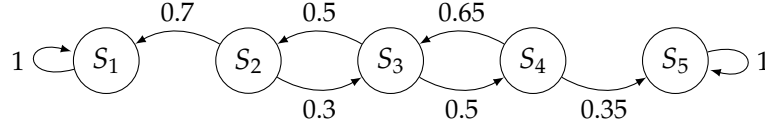
but for many models this integral is computationally hard to solve.

By comparison, *Bayesian inference* is a method of statistical inference in which Bayes' theorem is used, it derives the posterior probability $P(\mathbf{z} \mid \mathbf{x})$ as a consequence of two antecedents: a prior probability $P(\mathbf{z})$ and a *likelihood function* $P(\mathbf{x} \mid \mathbf{z})$ derived from a statistical model for the observed data.

Other methods as *Markov chain Monte Carlo* (MCMC) and *variational Bayesian inference* try a different approach when solving the given inference problem.

On one hand, *Variational Bayesian inference* or *variational inference*, is a machine learning method whose main goal is to approximate probability distributions (Jordan *et al.* (1999), Wainwright & Jordan (2008)). On the other hand, MCMC approximates the posterior distribution using a Markov chain. Let us introduce briefly the main idea behind this method, we need to introduce two concepts: *Markov chain* and MCMC.

A *Markov Chain* is formally defined as a stochastic process, i.e, a family of random variables, that satisfies the *Markov property* also known as the *memoryless property*: *the conditional probability distribution of future states of the process (conditional on both present and past values) depends only on the present state*. To fully understand it, imagine a system with a number of possible states S_1, \dots, S_5 and the probabilities of going from one state to another as in the following diagram.



Consider a sequence of random variables X_t that symbolize the current state at the step t . The Markov property means that the probability of moving to the next state depends only on the present one, i.e.,

$$P(X_{n+1} = x \mid X_1 = x_1 \dots, X_n = x_n) = P(X_{n+1} = x \mid X_n = x_n).$$

We need two concepts to define the process of MCMC:

- **Ergodic Markov chain.** A Markov chain where it exists a number $N \in \mathbb{N}$ such that any state can be reached from any other state in any number of steps less or equal than N .
- **Stationary Distribution.** The probability distribution to which the process converges over time.

In MCMC, an ergodic Markov chain over the latent variable whose stationary distribution is the posterior $P(z \mid \mathbf{x})$, samples are taken from the chain to approximate the posterior with them.

Instead, *variational inference* changes the inference problem with an optimization one. We fix a family of distributions \mathcal{Q} over the latent variable \mathbf{Z} and find the element that minimizes its Kullback-Leibler divergence with the posterior $P(z \mid \mathbf{x})$.

$$Q^{opt} = \arg \min_{Q \in \mathcal{Q}} KL(Q(z) \mid P(z \mid \mathbf{x})).$$

Compared to *Markov Chain Monte Carlo (MCMC)*, variational inference tends to be faster and scale easier to large data.

We can further analyze the Kullback-Leibler divergence we want to minimize, it may be decomposed the following way:

$$\begin{aligned} KL(Q(z) \mid P(z \mid \mathbf{x})) &= \mathbb{E}_{Q(z)} [\log Q(z)] - \mathbb{E}_{Q(z)} [\log P(z \mid \mathbf{x})] \\ &= \mathbb{E}_{Q(z)} [\log Q(z)] - \mathbb{E}_{Q(z)} [\log P(\mathbf{x}, z)] + \log P(\mathbf{x}). \end{aligned}$$

Given that the Kullback-Leibler divergence cannot be computed (as $P(z \mid \mathcal{V})$ is unknown), we can optimize an equivalent objective: we already saw that the divergence is always positive so we have the following lower bound to the evidence, defined as *evidence lower bound* or *ELBO*.

$$\log P(\mathbf{x}) \geq -\mathbb{E}_{Q(z)} [\log Q(z)] + \mathbb{E}_{Q(z)} [\log P(\mathbf{x}, z)] = \text{ELBO}(Q).$$

So that minimizing the Kullback-Leibler divergence is equivalent to maximize the ELBO. We can rewrite this bound as

$$\begin{aligned} \text{ELBO}(Q) &= \mathbb{E}_{Q(z)} [\log P(z)] + \mathbb{E}_{Q(z)} [\log P(\mathbf{x} \mid z)] - \mathbb{E}_{Q(z)} [\log Q(z)] \\ &= \mathbb{E}_{Q(z)} [\log P(\mathbf{x} \mid z)] - KL(Q(z) \mid P(z)), \end{aligned}$$

where it is expressed as the sum of the log likelihood of the observations and the Kullback-Leibler divergence between the prior $P(z)$ and $Q(z)$.

The *Expectation Maximization algorithm* is designed to optimize this lower bound in order to solve the optimization problem we are focusing. We will go deep into this algorithm in Section [14.1](#).

MEAN-FIELD VARIATIONAL INFERENCE

5.1 THE MEAN-FIELD VARIATIONAL FAMILY

The *mean-field variational family* \mathcal{Q} is defined as the family of distributions where the variables are mutually independent, i.e, any $Q \in \mathcal{Q}$ verifies

$$Q(z) = \prod_{n=1}^N Q_n(z_n),$$

where $z = \{z_1, \dots, z_N\}$ is the considered set of variables. The mean-field family is commonly used to model the family of distributions over the latent variables in our optimization problem. Notice that each *factor* Q_n can be different and this family does not depend on the observed data.

The mean-field family can capture any marginal of the latent variables but not correlation between them, as it assumes they are independent. For example, consider a two dimensional Gaussian distribution where a high percentage of the density is inside the blue ellipse shown in the next figure. Any mean-field approximation would factorize as a product of two Gaussian distributions, condensing its density in a circle as shown in purple.

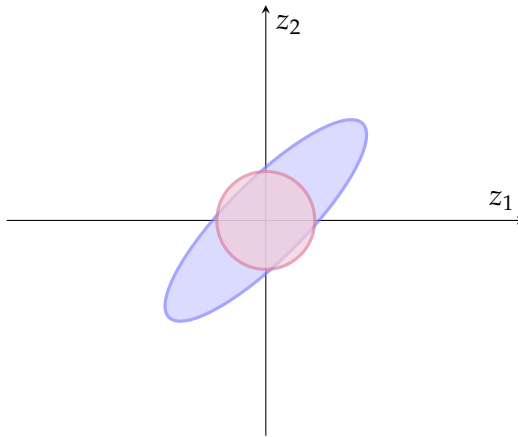


Figure 4: Mean-field family distribution (purple) approximating a Gaussian distribution (blue)

Notice the parametric form of each factor Q_n is not specified and the appropriate configuration depends on the variable. For example, a continuous variable might have a Gaussian factor and a categorical variable have a categorical factor.

Algorithm 1: Coordinate Ascent Variational Inference**Data:** A distribution $P(\mathcal{V}, \mathbf{z})$ with a dataset \mathcal{V} **Result:** A distribution of the mean-field family $Q(\mathbf{z}) = \prod_{n=1}^N Q_n(z_n)$ Initialize $Q(\mathbf{z})$;**while** *Convergence stop criteria* **do** **for** $n \in 1, \dots, N$ **do** $\mathbf{z}_{\setminus n} = (z_1, \dots, z_{n-1}, z_{n+1}, \dots, z_M)$; Set $Q_n(z_n) \propto \exp \mathbb{E}_{Q(\mathbf{z}_{\setminus n})} [\log P(z_n | \mathbf{z}_{\setminus n}, \mathcal{V})]$; **end** Compute $ELBO(Q)$;**end****return** Q ;

5.2 CAVI ALGORITHM

In this section, we describe a widely used algorithm to solve the optimization problem we discussed in the previous section using the mean-field family. It is *coordinate ascent variational inference* or *CAVI* and its procedure is to iteratively optimize each factor of the mean-field family distribution, while fixing the others. With this, the ELBO reaches a local optimum.

Let us see the main idea behind this iterative process, consider the n^{th} variable z_n and the denote $\mathbf{z}_{\setminus n} = (z_1, \dots, z_{n-1}, z_{n+1}, \dots, z_N)$, the full set of variables without the focused one. Let the other factors $Q_m, m \neq n$ be fixed. Under this assumptions, the ELBO has the form

$$\begin{aligned}
 ELBO(Q) &= \mathbb{E}_{Q_n} \left[\mathbb{E}_{Q_{\mathbf{z}_{\setminus n}}} [\log P(\mathbf{x}, \mathbf{z})] \right] - \mathbb{E}_{Q_n} [\log Q_n(z_n)] + \text{const.} \\
 &= \mathbb{E}_{Q_n} \left[\mathbb{E}_{Q_{\mathbf{z}_{\setminus n}}} [\log P(z_n | \mathbf{z}_{\setminus n}, \mathbf{x}) + \log P(\mathbf{z}_{\setminus n}, \mathbf{x})] \right] - \mathbb{E}_{Q_n} [\log Q_n(z_n)] + \text{const.} \\
 &= \mathbb{E}_{Q_n} \left[\mathbb{E}_{Q_{\mathbf{z}_{\setminus n}}} [\log P(z_n | \mathbf{z}_{\setminus n}, \mathbf{x})] \right] - \mathbb{E}_{Q_n} [\log Q_n(z_n)] + \text{const.} \\
 &= -KL(Q_n(z_n) | \exp \mathbb{E}_{Q(\mathbf{z}_{\setminus n})} [\log P(z_n | \mathbf{z}_{\setminus n}, \mathbf{x})]) + \text{const.}
 \end{aligned}$$

Minimizing the ELBO corresponds to setting the new distribution Q_n^{new} as:

$$Q_n^{new}(z_n) \propto \exp \mathbb{E}_{Q(\mathbf{z}_{\setminus n})} [\log P(z_n | \mathbf{z}_{\setminus n}, \mathcal{V})].$$

Notice that the proportionality restriction is enough to fully determine the distribution as its integral is normalized. Equivalently, the distribution is proportional to

$$Q_n^{new}(z_n) \propto \exp \mathbb{E}_{Q(\mathbf{z}_{\setminus n})} [\log P(z_n, \mathbf{z}_{\setminus n}, \mathcal{V})].$$

As the ELBO is generally a non-convex function and the CAVI algorithm converges to a local optimum, the initialization values of the algorithm play an important role on its performance. The convergence criteria is usually a threshold for the ELBO.

EXPONENTIAL FAMILY

The exponential family is a parametric set of probability distributions of a certain form. This form is chosen based on some useful algebraic properties and generality (figure 5).

Let X be a random variable and θ a set of parameters. A family of distributions is said to belong to the exponential family if its probability distribution is

$$P(x | \theta) = h(x) \exp \left(\sum_{i=1}^S \eta_i(\theta) T_i(x) - \psi(\theta) \right),$$

where $h(x)$, $T_i(x)$, $\eta_i(\theta)$ and $\psi(\theta)$ are known functions such that h is called a *base measure*, $\eta_i(\theta)$ are called the *parameters*, $T_i(x)$ the *test statistics* and ψ is the *log normalizer* as it ensures logarithmic normalization due to

$$\begin{aligned} 1 &= \int_x h(x) \exp \left(\sum_{i=1}^S \eta_i(\theta) T_i(x) - \psi(\theta) \right) \\ &= \int_x e^{-\psi(\theta)} h(x) \exp \left(\sum_{i=1}^S \eta_i(\theta) T_i(x) \right) \\ &= e^{-\psi(\theta)} \int_x h(x) \exp \left(\sum_{i=1}^S \eta_i(\theta) T_i(x) \right), \end{aligned}$$

so ψ verifies

$$\psi(\theta) = \log \int_x h(x) \exp \left(\sum_{i=1}^S \eta_i(\theta) T_i(x) \right).$$

Naming η and T the corresponding vector functions, the parameters can always be transformed as $\theta^{new} = \eta(\theta)$, in which case we say the distribution is in *canonical form* (notice ψ has changed but we are not differentiating it from the other since it is determined by the other functions):

$$P(x | \theta) = h(x) e^{\theta^T T(x) - \psi(\theta)}.$$

In this form, it is easier to see that T is the sufficient statistic for θ . This is a consequence of *Fisher–Neyman factorization theorem* which says that T is sufficient for θ if and only if the probability distribution P can be factored into a product such that one factor, h , does not depend on θ and the other factor, which does depend on θ , depends on x only through T .

An important property of the exponential family is that they have *conjugate priors*, when the posterior distribution is in the same probability distribution family as the prior distribution,

Distribution	Parameter set θ	Base measure h	Parameter function η	Statistics T
Bernoulli	p	1	$\log \frac{p}{1-p}$	x
Binomial	p	$\binom{n}{x}$	$\log \frac{p}{1-p}$	x
Categorical	p_1, \dots, p_K	1	$\begin{pmatrix} \log p_1 \\ \vdots \\ \log p_K \end{pmatrix}$	$\begin{pmatrix} [x = 1] \\ \vdots \\ [x = K] \end{pmatrix}$
Gaussian	μ, σ^2	$\frac{1}{\sqrt{2\pi}}$	$\begin{pmatrix} \frac{\mu}{\sigma^2} \\ -\frac{1}{2\sigma^2} \end{pmatrix}$	$\begin{pmatrix} x \\ x^2 \end{pmatrix}$
Beta	α, β	$\frac{1}{x(1-x)}$	$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$	$\begin{pmatrix} \log x \\ \log(1-x) \end{pmatrix}$
Dirichlet	$\alpha_1, \dots, \alpha_K$	1	$\begin{pmatrix} \alpha_1 - 1 \\ \vdots \\ \alpha_K - 1 \end{pmatrix}$	$\begin{pmatrix} \log x_1 \\ \vdots \\ \log x_K \end{pmatrix}$

Figure 5: Some distributions in the exponential family

they are called *conjugate distributions*, and the prior is called a *conjugate prior* of the likelihood distribution.

6.1 LATENT VARIABLE AND CONDITIONALLY CONJUGATE MODELS

One important case of exponential family are *latent variable models* or *LVMs*. In this models, the following assumptions are made:

1. There set of i.i.d random variables $\{X_1, \dots, X_N\}$ and a set of observations $\mathbf{x} = (x_1, \dots, x_N)$.
2. Both global θ and local parameters $\mathbf{Z} = \{Z_1, \dots, Z_n\}$ govern the data (both seen as latent variables). We refer to *global latent variables* when they affect the whole distribution and *local latent variables* when they affect only to a subset, in this case each Z_i affects only x_i . Given this, the joint probability is

$$P(\mathbf{x}, \theta, \mathbf{z}) = P(\theta) \prod_{n=1}^N P(z_n, x_n \mid \theta).$$

3. The n^{th} observation x_n and the n^{th} local hidden variable z_n are conditionally independent, given the global variables θ , of all other observations and local hidden variables,

$$P(x_n, z_n \mid \theta, \mathbf{x}_{\setminus n}, \mathbf{z}_{\setminus n}) = P(x_n, z_n \mid \theta).$$

Remark 2. These models are widely used to discover patterns in data sets (Blei (2014)). LVMs include popular models like *Latent Dirichlet Allocation* models used to uncover the hidden topics in text corpora (cite?), mixture of Gaussian models to discover hidden clusters in data (cite) and probabilistic principal component analysis for dimensionality reduction (cite).

One important case of LVMs and exponential family models are *Conditionally conjugate models*, where the following assumptions are made.

1. The prior for the global latent variable $P(\boldsymbol{\theta})$ is in the exponential family with an hyper-parameter $\alpha = [\alpha_1, \alpha_2]$, where α_1 is a vector and α_2 is a scalar, and statistics that concatenate the global latent variable and its log normalizer $[\boldsymbol{\theta}, -\psi(\boldsymbol{\theta})]$,

$$P(\boldsymbol{\theta}) = h(\boldsymbol{\theta}) \exp \left(\alpha^T [\boldsymbol{\theta}, -\psi(\boldsymbol{\theta})] - \psi(\alpha) \right).$$

2. Each local term $P(z_n, x_n \mid \boldsymbol{\theta})$ is in the exponential family of the form

$$P(z_n, x_n \mid \boldsymbol{\theta}) = h(z_n, x_n) \exp \left(\boldsymbol{\theta}^T T(z_n, x_n) - \psi(\boldsymbol{\theta}) \right).$$

3. The complete conditional of a local latent variable verifies

$$P(z_n \mid \boldsymbol{\theta}, \mathbf{x}, \mathbf{z}_{\setminus n}) = P(z_n \mid x_n, \boldsymbol{\theta})$$

and is also in the exponential family

$$P(z_n \mid x_n, \boldsymbol{\theta}) = h(z_n) \exp \left(\eta(\boldsymbol{\theta}, x_n)^T T(z_n) - \psi(\boldsymbol{\theta}, x_n) \right).$$

As conjugacy holds, the posterior $P(\boldsymbol{\theta} \mid \mathcal{V}, \mathbf{z})$ is in the same family with parameter

$$\bar{\alpha} = [\alpha_1 + \sum_{n=1}^N T(z_n, x_n), \alpha_2 + N]^T.$$

This can be calculated as follows,

$$\begin{aligned} P(\boldsymbol{\theta} \mid \mathbf{x}, \mathbf{z}) &= \frac{P(\mathbf{x}, \mathbf{z} \mid \boldsymbol{\theta}) P(\boldsymbol{\theta})}{P(\mathbf{x}, \mathbf{z})} \propto P(\mathbf{x}, \mathbf{z} \mid \boldsymbol{\theta}) P(\boldsymbol{\theta}) = P(\boldsymbol{\theta}) \prod_{n=1}^N h(x_n, z_n) \exp \left(\boldsymbol{\theta}^T T(z_n, x_n) - \psi(\boldsymbol{\theta}) \right) \\ &\propto h(\boldsymbol{\theta}) \exp \left(\alpha^T [\boldsymbol{\theta}, -\psi(\boldsymbol{\theta})] \right) \prod_{n=1}^N h(x_n, z_n) \exp \left(\boldsymbol{\theta}^T T(z_n, x_n) - \psi(\boldsymbol{\theta}) \right) \\ &\propto h(\boldsymbol{\theta}) \exp \left(\alpha^T [\boldsymbol{\theta}, -\psi(\boldsymbol{\theta})] + \sum_{n=1}^N \boldsymbol{\theta}^T T(z_n, x_n) - \psi(\boldsymbol{\theta}) \right) \\ &\propto h(\boldsymbol{\theta}) \exp \left(\alpha_1^T \boldsymbol{\theta} - \alpha_2^T \psi(\boldsymbol{\theta}) - N \psi(\boldsymbol{\theta}) + \sum_{n=1}^N T(z_n, x_n)^T \boldsymbol{\theta} \right) \\ &\propto h(\boldsymbol{\theta}) \exp \left(\left(\alpha_1 + \sum_{n=1}^N T(z_n, x_n) \right)^T \boldsymbol{\theta} - (\alpha_2 + N)^T \psi(\boldsymbol{\theta}) \right). \end{aligned}$$

The inverse reasoning can be done, therefore if the complete conditional of the global hidden variable is in the exponential family with hyper-parameter $\bar{\alpha}$, the prior is in the same family with the corresponding hyper-parameter α .

6.2 CAVI IN CONDITIONALLY CONJUGATE MODELS

Set aside the conditionally conjugate models and consider the following situation where we fit a distribution $Q(z) = \prod_{n=1}^N Q_n(z_n)$ in the mean-field family, using an exponential family distribution for the marginal $P(z_n | z_{\setminus n}, x)$, where $z_{\setminus n}$ indicates the rest of hidden variables in the full model.

$$P(z_n | z_{\setminus n}, x) = h(z_n) \exp \left(\eta_n(z_{\setminus n}, x)^T T(z_n) - \psi(z_{\setminus n}, x) \right).$$

Notice that $(z_{\setminus n}, x)$ are the parameters for the exponential family.

The update of the CAVI algorithm is then given by

$$\begin{aligned} Q(z_n) &\propto \exp \mathbb{E}_{Q(z_{\setminus n})} \left[\log P(z_n | z_{\setminus n}, x) \right] \\ &= h(z_n) \exp \left(\mathbb{E}_{Q(z_{\setminus n})} \left[\eta_n(z_{\setminus n}, x) \right]^T T(z_n) - \mathbb{E}_{Q(z_{\setminus n})} \left[\psi(z_{\setminus n}, x) \right] \right) \\ &\propto h(z_n) \exp \left(\mathbb{E}_{Q(z_{\setminus n})} \left[\eta_n(z_{\setminus n}, x) \right]^T T(z_n) \right) = h(z_n) e^{v_n^T T(z_n)}, \end{aligned} \quad (1)$$

where

$$v_n = \mathbb{E}_{Q(z_{\setminus n})} \left[\eta_n(z_{\setminus n}, x) \right].$$

Summarizing, the factor is in the exponential family with the same base measure h and updating it is equivalent to setting the parameter η to the expected one of the complete conditional $\mathbb{E} \left[\eta_n(x, z_{\setminus n}) \right]$. This expression facilitates deriving CAVI algorithm for many complex models.

Going back to the conditionally conjugate models, we set both the local and global hidden variable update. Our variational distribution is in the mean-field family with $Q(\theta | \lambda)$ where λ is called the *global variational parameter*, and the posterior on each local variable is $Q(z_n | \gamma_n)$, where γ_n is called a *local variational parameter*. As we already have seen, these distributions are in the exponential family:

$$Q(z_n | \gamma_n) \propto h(z_n) e^{\gamma_n^T T(z_n)},$$

$$Q(\theta | \lambda) = h(\theta) \exp \left(\lambda^T [\theta, -\psi(\theta)] - \psi(\lambda) \right).$$

As we already know, CAVI iteratively updates each local variational parameter and the global variational parameter.

The local variational parameter update is

$$\gamma_n^{new} = \mathbb{E}_{Q(\theta | \lambda)} \left[\eta(\theta, x_n) \right],$$

following the steps done in 1, where we take the expectation of the natural parameter of the complete conditional. In this case, the local hidden variable conditional does not depend on the other local hidden variables, neither other data-points.

The global variational parameter update is calculated as

$$\begin{aligned}
Q^{new}(\boldsymbol{\theta} \mid \lambda) &\propto \exp \mathbb{E}_{Q(\mathbf{z})} \left[\log P(\boldsymbol{\theta} \mid \mathbf{z}, \mathbf{x}) \right] \propto h(\boldsymbol{\theta}) \exp \mathbb{E}_{Q(\mathbf{z})} \left[\left[\lambda_1 + \sum_{n=1}^N T(x_n, z_n), \lambda_2 + N \right]^T [\boldsymbol{\theta}, \psi(\boldsymbol{\theta})] \right] \\
&\propto h(\boldsymbol{\theta}) \exp \left(\left[\lambda_1 + \sum_{n=1}^N \mathbb{E}_{Q(\mathbf{z})} \left[T(x_n, z_n) \right], \lambda_2 + N \right]^T [\boldsymbol{\theta}, -\psi(\boldsymbol{\theta})] \right) \\
&= Q(\boldsymbol{\theta}, \lambda^{new}).
\end{aligned}$$

Then, the parameter updated is

$$\lambda^{new} = \left[\lambda_1 + \sum_{n=1}^N \mathbb{E}_{Q(z_n|\gamma_n)} \left[T(x_n, z_n) \right], \lambda_2 + N \right].$$

We can compute the ELBO at each iteration up to a constant that does not depend on the variational parameters,

$$\begin{aligned}
ELBO &= \left(\lambda_1 + \sum_{n=1}^N \mathbb{E}_{Q(z_n|\gamma_n)} \left[T(x_n, z_n) \right] \right)^T \mathbb{E}_{Q(\boldsymbol{\theta}|\lambda)} [\boldsymbol{\theta}] - (\lambda_2 + N) \mathbb{E}_{Q(\boldsymbol{\theta}|\lambda)} [\psi(\boldsymbol{\theta})] \\
&\quad + \lambda^T \mathbb{E}_{Q(\boldsymbol{\theta}, \lambda)} [T(\boldsymbol{\theta})] - \psi(\lambda) + \sum_{n=1}^N \gamma_n^T \mathbb{E}_{Q(z_n, \gamma_n)} [z_n] - \psi(\gamma_n) + \text{const.}
\end{aligned}$$

Part III

GRAPHICAL MODELS

A *graphical model* is a statistical model for which a graph expresses the conditional dependence structure between random variables.

Commonly, they provide a graph-based representation for encoding a multi-dimensional distribution representing a set of independences that hold in the specific distribution. The most commonly used are *Bayesian networks* and *Markov random fields*, which differ in the set of independences they can encode and the factorization of the distribution that they include.

BAYESIAN NETWORKS

Consider we have N variables with the corresponding distribution $P(x_1, \dots, x_N)$. Let \mathcal{E} be a set of indexes such as $\text{evidence} = \{X_e = x_e \mid e \in \mathcal{E}\}$. Inference could be made by brute force:

$$P(X_i = x_i \mid \text{evidence}) = \frac{\int_{j \notin \mathcal{E}, j \neq i} P(\text{evidence}, x_j, X_i = x_i)}{\int_{j \notin \mathcal{E}} P(\text{evidence}, x_j)}$$

Let us suppose all these variables are binary, this calculation will require $O(2^{N-\#\mathcal{E}})$ operations. Also, all entries of a table $P(x_1, \dots, x_N)$ take $O(2^N)$ space.

This is unpractical when taking into account millions of variables. The underlying idea of belief networks is to specify which variables are independent of others, factoring the joint probability distribution.

Definition 35. Let $G = (V, E)$ be a graph where $V = \{X_1, \dots, X_n\}$ is a set of random variables. We say that the joint probability $P(x_1, \dots, x_n)$ *factorizes* according to G if and only if

$$P(x_1, \dots, x_N) = \prod_{i=1}^N P(x_i \mid pa(x_i))$$

Definition 36. A *belief network* or *Bayesian network* is a pair (G, P) where P factorizes over G . It is a probabilistic graphical model that represents conditional dependencies of a set of variables X_1, \dots, X_n .

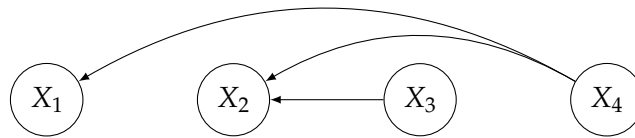


Figure 6: Bayesian Network factorizing $P(x_1, x_2, x_3, x_4) = P(x_1|x_4)P(x_2|x_3, x_4)P(x_3)P(x_4)$

Any probability distribution can be written as a Bayesian Network, even though it may end up been a fully-connected DAG. To set the specification of the Belief Network, we need to define all elements of the probability tables $P(x_i \mid pa(x_i))$. When the number of variables is large, this is still intractable so the tables are generally parameterized in a low dimensional manner.

Bayesian Networks are good for encoding conditional independence over the variables, but aren't for encoding dependence. For example, with the following network

$$P(x, y) = P(y | x)P(x)$$

represented as $x \rightarrow y$ in a DAG (a Bayesian network can be defined giving the graph or the joint probability equally). It may appear to encode dependence between both variables but the conditional $P(y|x)$ could happen to equal $P(y)$, giving $P(x, y) = P(x)P(y)$.

How could we check if two variables are conditionally independent given a Bayesian Network? For example in figure 3, $X_1 \perp\!\!\!\perp X_2 | X_4$ as¹:

$$\begin{aligned} P(x_2|x_4) &= \frac{1}{P(x_4)} \int_{x_1, x_3} P(x_1, x_2, x_3, x_4) = \frac{1}{P(x_4)} \int_{x_1, x_3} P(x_1|x_4)P(x_2|x_3, x_4)P(x_3)P(x_4) \\ &= \int_{x_3} P(x_2|x_3, x_4)P(x_3) \\ P(x_1, x_2|x_4) &= \frac{1}{P(x_4)} \int_{x_3} P(x_1, x_2, x_3, x_4) = \frac{1}{P(x_4)} \int_{x_3} P(x_1|x_4)P(x_2|x_3, x_4)P(x_3)P(x_4) \\ &= P(x_1|x_4) \int_{x_3} P(x_2|x_3, x_4)P(x_3) = P(x_1|x_4)P(x_2|x_4) \end{aligned}$$

Now we are going to define two central concepts to determine conditional independence in any Bayesian Network, these are *d-connection* and *d-separation*.

Definition 37. Let G be a DAG where X, Y and Z are disjoint sets of vertices. We say that X and Y are *d-connected* by Z if and only if there exists an undirected path U from any vertex in X to any vertex in Y such that:

- For any collider C , itself or any it's descendants is in Z
- No non-collider on U is on Z

Definition 38. Let G be a DAG where X, Y and Z are disjoint sets of vertices. X and Y are *d-separated* by Z if and only if they are not d-connected by Z in G

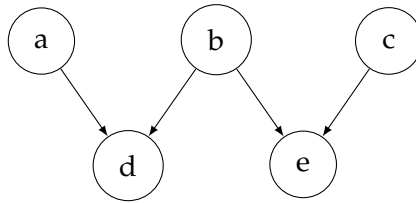


Figure 7: D-separation example

For example, in figure 7 d d-separates a and c (b is a collider in the path that isn't in $\{d\}$), and $\{d, e\}$ d-connect them.

Theorem 2 (Pearl & Dechter (2013)). Let G be a DAG where X, Y and Z are disjoint sets of vertices. If X and Y are d-separated by Z , then they are independent conditional on Z in all probability distributions that G can represent.

¹ Continuous variable notation is used

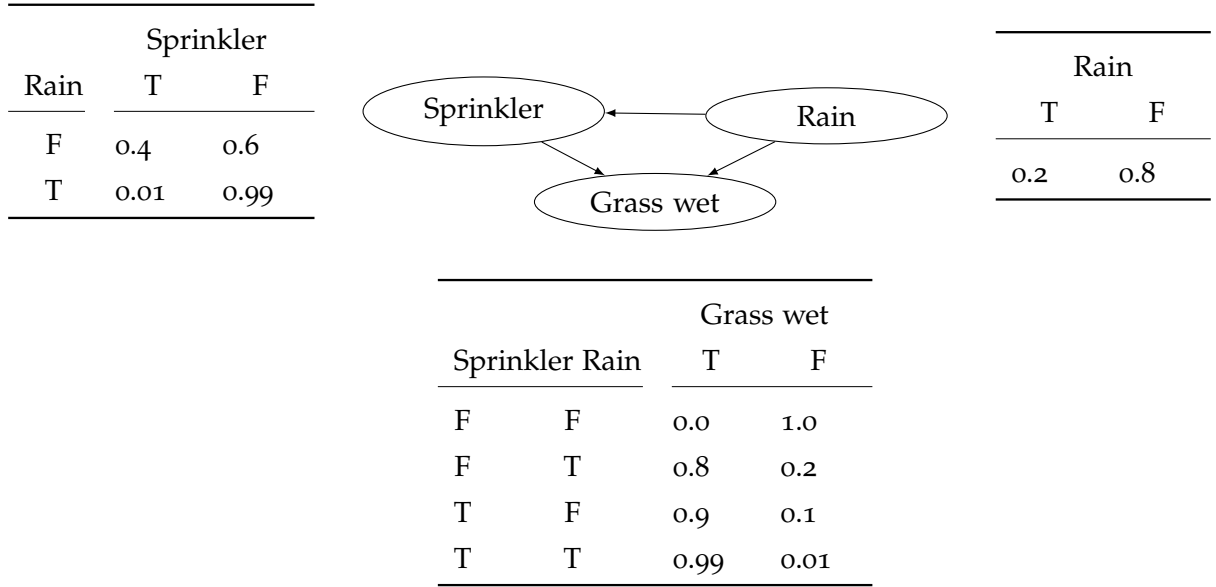
The Bayes Ball algorithm [Shachter (2013)] provides a linear time complexity algorithm that computes conditional independent using this theorem.

Example 2. In this example we are modeling three discrete random variables: Sprinkler (S), Rain (R) and Grass wet (G).

The joint probability function is:

$$P(s, r, g) = P(s|r)P(g|s, r)P(r)$$

The following DAG illustrates the Bayesian Network among with the probability tables we are using.



This model can answer questions about the presence of a cause given the presence of an effect. For example, What is the probability that it has being raining given the grass is wet?

$$P(R = T|G = T) = \frac{P(G = T, R = T)}{P(G = T)} = \frac{\sum_s P(G = T, R = T, s)}{\sum_{r,s} P(G = T, r, s)}$$

Using the expression of the joint probability among with the tables we can compute every term. For example:

$$\begin{aligned} P(G = T, R = T, S = T) &= P(S = T|R = T)P(G = T|R = T, S = T)P(R = T) \\ &= 0.01 * 0.99 * 0.2 = 0.00198 \end{aligned}$$

In some situations our Belief Networks will contain a number of nodes that are essentially the same but repeated a number of times, for this, we are going to introduce the *plate notation*. Suppose we have the situation that figure 8 shows on the left. The we can collapse all B_i variables in a box, indicating there number of variables inside it.

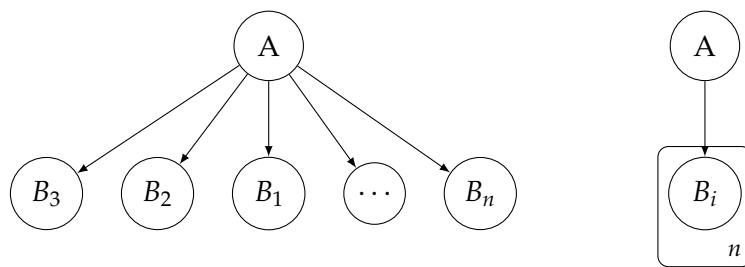


Figure 8: Plate notation example. Standard notation on the left and plate on the right

MARKOV RANDOM FIELDS

Definition 39. A *potential* ϕ is a non-negative function. It is worth to mention that a probability distribution is a special case of a potential.

Definition 40. Let \mathbf{X} be a set of random variables, G an undirected graph, $\mathbf{X}_c, c \in \{1, \dots, C\}$ be the maximal cliques of G and P a probability distribution over \mathbf{X} . The pair (G, P) is said to be a *Markov network* or *Markov random field* if, and only if

$$P(x_1, \dots, x_n) = \frac{1}{Z} \prod_{c=1}^C \phi_c(\mathbf{X}_c)$$

where Z is a constant that ensures normalization.

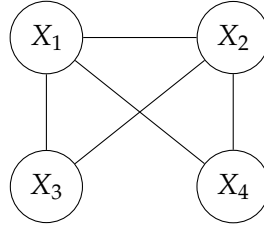


Figure 9: Markov Network $P(x_1, x_2, x_3, x_4) = \phi(x_1, x_2, x_3)\phi(x_2, x_3, x_4)/Z$

In figure 9 we can see an example of the factorization, without giving any reference of the potentials.

Let (G, P) be a Markov network, then it satisfies the following properties known as Markov properties:

- Pairwise Markov property. Any two non-adjacent variables are conditionally independent given all other variables.
- Local Markov property. A variable is conditionally independent over all other variables given it's neighbors. That is,

$$P(x_i | x_{\setminus i}) = p(x_i | ne(x_i))$$
¹

- Global Markov property. Any two subsets of variables are conditionally independent given a separating subset (any path from one set to the other passes through this one).

¹ $X_{\setminus i} = \{X_j \mid j \neq i\} \subset \mathbf{X}$

Remark 3. A Markov network can also be defined as a pair (G, P) such as all Markov properties are satisfied. The clique factorization definition is a special case of these properties.

Definition 41. Let G be an undirected graph and P a probability distribution over a set of random variables \mathbf{X} . The pair (G, P) is called a Markov Random Field if and only if it follows the local Markov Property.

APPLICATION TO VARIATIONAL INFERENCE

We are now in a situation where we can show the Bayesian network of a LVM (figure 10). Two central problems using these type of models are *Gaussian mixtures* and *latent Dirichlet allocation*.

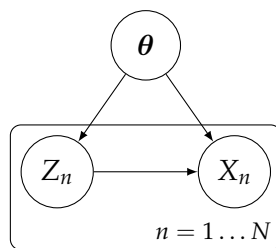


Figure 10: Bayesian network of a Latent Variable Model

9.1 GAUSSIAN MIXTURE

A Gaussian mixture model (figure 12) is a probabilistic model that assumes all the data points are generated from a mixture of a finite number of Gaussian distributions with unknown parameters. We will discuss another mixture example with the EM algorithm in Section 14.2.

The following elements are being considered (using Bishop (2006) notation):

- K mixture components and N observations.
- A set of i.i.d real valued random variables $\mathbf{X} = \{X_1, \dots, X_N\}$ and a corresponding set of observations $\mathbf{x} = \{x_1, \dots, x_n\}$.
- The cluster assignment latent variables $\mathbf{Z} = \{Z_1, \dots, Z_N\}$, where each z_n is a indicator vector.
- We choose a Dirichlet distribution over the mixing coefficients π

$$\pi \sim \text{Symmetric-Dirichlet}(\alpha_0) \implies P(\pi) \propto \prod_{k=1}^K \pi_k^{\alpha_0-1}$$

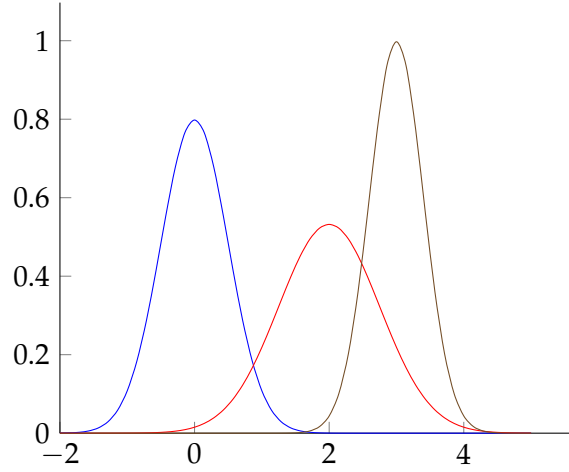


Figure 11: One-dimensional Gaussian mixture with 3 clusters.

The hyper-parameter α_0 is the effective prior of each mixture component. Then $\pi = \{\pi_1, \dots, \pi_K\}$ are the mixture weights, i.e, prior probability of a particular component k .

$$P(z | \pi) = \prod_{n=1}^N \prod_{k=1}^K \pi_k^{z_{n,k}} \implies (Z_n | \pi) \sim \text{Categorical}(\pi)$$

- $\mu = \{\mu_1, \dots, \mu_K\}$ and $\Lambda = \{\Lambda_1, \dots, \Lambda_K\}$ are the distribution parameters of each observation full conditional

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

- The prior governing μ and Λ is an independent Gaussian, Inverse-Gamma distribution with hyper parameters m_0, β_0, w_0 and v_0 :

$$P(\mu, \Lambda) = P(\mu | \Lambda)P(\Lambda) \text{ where } \begin{cases} (\mu | \Lambda) & \sim \prod_{k=1}^K \mathcal{N}(m_0, \beta_0 \Lambda_k) \\ \Lambda & \sim \prod_{k=1}^K \text{Inverse-Gamma}(w_0, v_0) \end{cases}$$

The joint probability factorizes as

$$P(x, z, \pi, \mu, \Lambda) = P(x | z, \mu, \Lambda)P(z | \pi)P(\pi)P(\mu | \Lambda)P(\Lambda).$$

[Bishop \(2006\)](#) uses a Gaussian-Wishart prior for μ and Λ and gives the explicit update for the CAVI algorithm.

9.2 LATENT DIRICHLET ALLOCATION

Latent Dirichlet allocation or *LDA* is a conditionally conjugate model (figure 13) in natural language processing that allows set of observations to be explained by unobserved groups that explain why some parts of the data are similar.

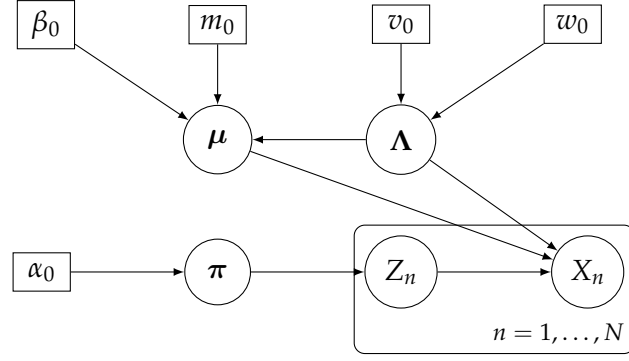


Figure 12: Gaussian mixture model. Squares represent hyper-parameters.

For example, observations may be words in a document, which is a mixture of a small number of topics and each word's presence is attributable to one of the document's topics. Learning corresponds to extract information as the set of topics, their associated word probabilities, the topic of each word, and the particular topic mixture of each document.

The considered elements are (using [Hoffman et al. \(2013\)](#) and [Blei et al. \(2003\)](#) notation):

- K number of topics, V number of words in the vocabulary, M number of documents, N_d number of words in document d and N total number of words.
- $\beta = \{\beta_1, \dots, \beta_K\}$, where a topic β_k the distribution of words in topic k . Each component $\beta_{k,n}$ is the probability of the n^{th} word in topic k .
- Each document d is associated with a vector of topic proportions θ_d , which is a $K - 1$ simplex. Then each component $\theta_{d,k}$ is the probability of topic k in document d . Note $\theta = \{\theta_1, \dots, \theta_K\}$.
- Each word in each document is assumed to be related with a single topic. The variable $Z_{d,n}$ indexes the topic of the n^{th} word in the d^{th} document.

LDA model assumes that each document is generated with the following generative process:

1. Draw topics from a Dirichlet distribution, for each $k = 1, \dots, K$:

$$P(\beta_k) = \frac{1}{B(\eta)} \prod_{v=1}^V \beta_{k,v}^{\eta-1} \implies \beta_k \sim \text{Symmetric-Dirichlet}_V(\eta)$$

2. For each document $d = 1, \dots, D$:

- a) Draw topic proportions,

$$P(\theta_d) = \frac{1}{B(\alpha)} \prod_{k=1}^K \theta_{d,k}^{\alpha-1} \implies \theta_d \sim \text{Symmetric-Dirichlet}_K(\alpha)$$

- b) For each word in the document $n = 1, \dots, N_d$:

- i. Draw a topic,

$$P(z_{d,n} \mid \theta_d) = \prod_{k=1}^K \theta_{d,k}^{\mathbb{I}[z_{d,n}=k]} \implies (Z_{d,n} \mid \theta_d) \sim \text{Categorical}(\theta_d).$$

ii. Draw a word from the topic

$$P(w_{d,n} | z_{d,n}, \beta) = \prod_{v=1}^V \beta_{z_{d,n},v}^{\mathbb{I}[w_{d,n}=v]} \implies (W_{d,n} | Z_{d,n}, \beta) \sim \text{Categorical}(\beta_{Z_{d,n}})$$

The joint probability distribution is then

$$\begin{aligned} P(\theta, z, w, \beta) &= P(\beta) \prod_{d=1}^D P(\theta_d | \alpha) \prod_{n=1}^{N_d} P(z_{d,n} | \theta_d) P(w_{d,n} | z_{d,n}, \beta) \\ &= \left(\prod_{k=1}^K P(\beta_k) \right) \prod_{d=1}^D P(\theta_d) \prod_{n=1}^{N_d} P(z_{d,n} | \theta_d) P(w_{d,n} | z_{d,n}, \beta) \end{aligned}$$

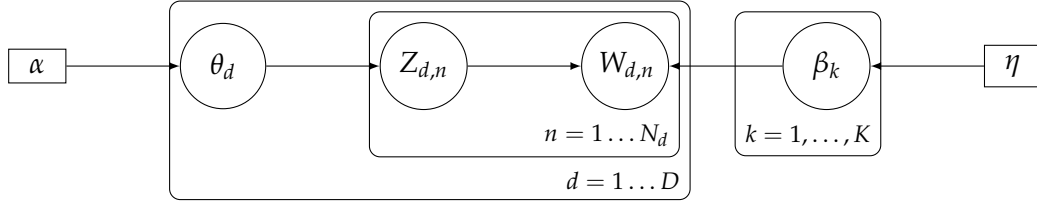


Figure 13: Latent Dirichlet Allocation model. Squares represent hyper-parameters

We start setting the complete conditional distribution of the local hidden variables. They only depend on other variables in the local context (same document) and the global variables

$$\begin{aligned} P(z_{d,n} | w_{d,n}, \theta_d, \beta) &= \frac{P(z_{d,n}, w_{d,n}, \theta_d, \beta)}{\int_{z_{d,n}} P(z_{d,n}, w_{d,n}, \theta_d, \beta)} = \frac{P(z_{d,n} | \theta_d) P(w_{d,n} | z_{d,n}, \beta)}{\int_{z_{d,n}} P(z_{d,n} | \theta_d) P(w_{d,n} | z_{d,n}, \beta)} \\ &= \frac{\prod_{k=1}^K \theta_{d,k}^{\mathbb{I}[z_{d,n}=k]} \prod_{v=1}^V \beta_{z_{d,n},v}^{\mathbb{I}[w_{d,n}=v]}}{\int_{z_{d,n}} \prod_{k=1}^K \theta_{d,k}^{\mathbb{I}[z_{d,n}=k]} \prod_{v=1}^V \beta_{z_{d,n},v}^{\mathbb{I}[w_{d,n}=v]}} = \frac{\theta_{d,z_{d,n}} \beta_{z_{d,n},w_{d,n}}}{\sum_{k=1}^K \theta_{d,k} \beta_{k,w_{d,n}}} \end{aligned}$$

Naming $\gamma_{d,n} = \theta_{d,z_{d,n}} \beta_{z_{d,n},w_{d,n}}$ and $\gamma = \{\gamma_{d,n}\}_{d=1,\dots,D}^{n=1,\dots,N_d}$, we get

$$(Z_{d,n} | w_{d,n}, \theta_d, \beta) \sim \text{Categorical}(\gamma).$$

On the other hand, the complete conditional of the topic proportions θ_d is only affected by the topic appearances, since $z_{d,n}$ is an indicator vector, the k^{th} element of the parameter to this Dirichlet is the sum of the hyperparameter α and the number of words assigned to topic k in document d :

$$\begin{aligned} P(\theta_d | z_d, w_d, \beta) &= \frac{P(\theta_d, z_d, w_d, \beta)}{\int_{\theta_d} P(\theta_d, z_d, w_d, \beta)} = \frac{P(\theta_d) \prod_{n=1}^{N_d} P(z_{d,n} | \theta_d)}{\int_{\theta_d} P(\theta_d) \prod_{n=1}^{N_d} P(z_{d,n} | \theta_d)} \\ &\propto \prod_{k=1}^K \theta_{d,k}^{\alpha-1} \prod_{n=1}^{N_d} \theta_{d,k}^{\mathbb{I}[z_{d,n}=k]} = \prod_{k=1}^K \theta_{d,k}^{\alpha-1+\sum_{n=1}^{N_d} \mathbb{I}[z_{d,n}=k]}. \end{aligned}$$

The complete conditional depends only on the topic assignments

$$(\theta_d | z_d) \sim \text{Dirichlet}_K\left(\alpha + \sum_{n=1}^{N_d} \mathbb{I}[z_{d,n} = 1], \dots, \alpha + \sum_{n=1}^{N_d} \mathbb{I}[z_{d,n} = K]\right).$$

In words, the probability of a topic in document d is updated with the number of times that topic appears in the document. The complete conditional of a topic depends on the words and topics assignments of the entire collection

Using a similar reasoning, the words distribution in a topic k , β_k , is updated with the number of appearances in all documents of the given topic.

$$(\beta_k | \mathbf{w}, \mathbf{z}) \sim \text{Dirichlet}_V \left(\eta + \sum_{d=1}^D \sum_{n=1}^{N_d} \mathbb{I}[z_{d,n} = k] \mathbb{I}[w_{d,n} = 1], \dots, \eta + \sum_{d=1}^D \sum_{n=1}^{N_d} \mathbb{I}[z_{d,n} = k] \mathbb{I}[w_{d,n} = V] \right).$$

9.3 FROM PCA TO VARIATIONAL AUTO-ENCODERS

LVMs have usually been restricted to the exponential family because, in this case, inference is feasible. But recent advances in variational inference have enabled LVMs to be extended with neural networks. For example, *Variational Auto-encoders* or VAE (Kingma & Welling (2013)) are the most influential models combining both concepts.

VAEs extent the classical technique of *principal components analysis* for data representation in lower-dimensional spaces. Suppose we have a D -dimensional representation of a data point x and z is its latent K -dimensional representation ($K < D$). PCA computes an affine transformation \mathbf{W} , represented by a $K \times D$ matrix.

A probabilistic view of PCA can be modeled with an LVM (Tipping & Bishop (1999)), with the following elements:

- $\mathbf{X} = \{X_1, \dots, X_N\}$ i.i.d \mathbb{R}^D -valued random variables and the corresponding observations $\mathbf{x} = \{x_1, \dots, x_N\}$.
- $\mathbf{Z} = \{Z_1, \dots, Z_N\}$ i.i.d latent \mathbb{R}^K -valued random variables, where Z_n models the K -dimensional representation of x_n .
- A global latent $K \times D$ -dimensional random variable \mathbf{W} .
- A noise hyper-parameter σ^2

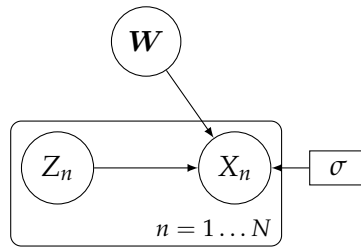


Figure 14: Probabilistic PCA model

We assume the priors are normally distributed:

$$Z_n \sim N_K(0, I) \quad \forall n = 1, \dots, N \quad \text{and} \quad \mathbf{W} \sim N_{K \times D}(0, I).$$

The data points are considered generated via a projection,

$$(X_n | Z_n, \mathbf{W}) \sim N(\mathbf{W}^T Z_n, \sigma^2 I) \quad \forall n = 1, \dots, N.$$

The probabilistic model extends the classical one in the way that the latter assumes the noise is infinitesimally small, i.e, $\sigma^2 \rightarrow 0$. The *expectation-maximization algorithm* (Section 14.1) is commonly used to solve this variational inference problem.

9.3.1 Artificial Neural networks

An *artificial neural network* or ANN with L hidden layers can be seen as a deterministic non-linear function f parameterized by a set of matrix $\mathbf{W} = \{\mathbf{W}_0, \dots, \mathbf{W}_L\}$ and non-linear activation functions $\{r_0, \dots, r_L\}$. Given an input x the output y is calculated as

$$h_0 = r_0(\mathbf{W}_0^T x), \quad \dots, \quad h_l = r_l(\mathbf{W}_l^T h_{l-1}) \quad \dots \quad y = r_L(\mathbf{W}_L^T h_{L-1}).$$

Deep neural networks or DNNs are ANNs where the number of hidden layers is higher. Commonly, any neural network with more than 2 hidden layers is considered deep. Given a dataset $\{(x_1, y_1), \dots, (x_N, y_N)\}$ and a loss function $l(y, y^*)$ that defines how well the output $y^* = f_{\mathbf{W}}(x)$ returned by the model matches the real output y , learning reduces to the optimization problem

$$\mathbf{W}^{opt} = \arg \min_{\mathbf{W}} \sum_{n=1}^N l(y_n, f_{\mathbf{W}}(x_n)).$$

This problem is usually solved by applying a variant of the stochastic gradient descent method, which involves the computation of the gradient of the loss function with respect to the parameters of the network. The algorithm for computing this gradient is known as *back-propagation*, which is based on a recursive application of the chain-rule of derivatives. This can be implemented using the computational graph on the network.

The main idea of a computational graph is to express a deterministic function, as is the case of a neural network, using an acyclic directed graph. It is composed of input, output and operation nodes, where model data and parameters are shown as input nodes.

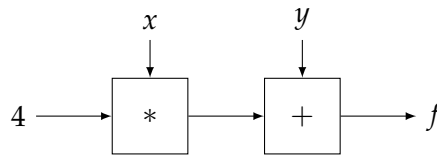


Figure 15: Computational graph example of function $f(x, y) = 4x + y$

9.3.2 Variational Auto Encoders

Variational auto encoders extend the classical PCA where the relation between the low dimensional space and the observed data is governed by a DNN instead of a linear transformation. It can be seen as a non-linear probabilistic PCA model.

The model is quite similar to the one presented for the PCA, the difference comes from the conditional distribution of X , that depends on Z through a fully-connected ANN with a single hidden layer.

The prior of the latent variable is a centered Gaussian

$$Z_n \mid N(0, I) \quad \forall n \in 1, \dots, N$$

Using four hyper-parameters $\alpha_0, \alpha_1, \beta_0$ and β_1 , we define the ANN with

$$h(z) = \text{relu}(\beta_0^T z + \alpha_0) \quad \mu(z_n) = \beta_1^T h(z) + \alpha_1.$$

The data-points are then generated as

$$(X_n \mid Z_n) \sim N(\mu_n, \sigma^2 I) \quad \forall n \in 1, \dots, N$$

Part IV

BAYESIAN NETWORKS LEARNING

INTRODUCTION

In Machine Learning and related fields, the distributions are not fully specified and need to be learned from the data.

From now on, \mathcal{V} will denote the known data and θ the set of parameters of the data distributions. The main task is to determine this set of parameters using the information given by the data. No latent or hidden variables are being considered right now.

The goal now is to determine the posterior $P(\theta \mid \mathcal{V})$ using a prior belief $P(\theta)$ and the likelihood function $P(\mathcal{V} \mid \theta)$.

$$P(\theta \mid \mathcal{V}) = \frac{P(\mathcal{V} \mid \theta)P(\theta)}{P(\mathcal{V})}$$

We are using the following example to illustrate the situation, in it we will try to learn the bias of a coin, given a set of tossing results.

Example 3. Let $\mathcal{V} = \{v_n\}_{n=0,\dots,N}$ be the results of tossing a coin $N \in \mathbb{N}$ times, let 1 symbolize *heads* and 0 *tails*.

Our objective is to estimate the probability θ that the coin will be head $P(v_n = 1 \mid \theta)$, for this we have the i.i.d random variables v_1, \dots, v_n and θ , and we require a model $P(v_1, \dots, v_n, \theta)$. We have a Belief Network shown in figure 16

$$P(\mathcal{V}, \theta) = P(\theta) \prod_{n=1}^N P(v_n \mid \theta)$$

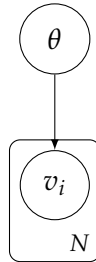


Figure 16: Belief network for coin tossing

We want to calculate

$$P(\theta \mid \mathcal{V}) = \frac{P(\mathcal{V} \mid \theta)P(\theta)}{P(\mathcal{V})}$$

to do so, we need to specify the prior $P(\theta)$, we are using a discrete model where

$$P(\theta = 0.2) = 0.1 \quad P(\theta = 0.5) = 0.7 \quad P(\theta = 0.8) = 0.2$$

This means that we have a 70% belief that the coin is fair, a 10% belief that is biased to tails and 20% that is biased to heads. Notice that $P(v_n = 1 \mid \theta) = \theta$ and $P(v_n = 0 \mid \theta) = 1 - \theta$.

Let n_h be the number of heads in our observed data and n_t the number of tails

$$n_h = \#\{v = 1\} \quad n_t = \#\{v = 0\}$$

then the posterior has the form

$$P(\theta \mid \mathcal{V}) = \frac{P(\theta)}{P(\mathcal{V})} \theta^{n_h} (1 - \theta)^{n_t}$$

Suppose now that $n_h = 2$ and $n_t = 8$, then

$$\begin{aligned} P(\theta = 0.2 \mid \mathcal{V}) &= \frac{1}{P(\mathcal{V})} \times 0.1 \times 0.2^2 \times 0.8^8 = \frac{1}{P(\mathcal{V})} \times 6.71 \times 10^{-4} \\ P(\theta = 0.5 \mid \mathcal{V}) &= \frac{1}{P(\mathcal{V})} \times 0.7 \times 0.5^2 \times 0.5^8 = \frac{1}{P(\mathcal{V})} \times 6.83 \times 10^{-4} \\ P(\theta = 0.8 \mid \mathcal{V}) &= \frac{1}{P(\mathcal{V})} \times 0.2 \times 0.2^2 \times 0.8^8 = \frac{1}{P(\mathcal{V})} \times 3.27 \times 10^{-7} \end{aligned}$$

Now, we can compute

$$\frac{1}{P(\mathcal{V})} = 6.71 \times 10^{-4} + 6.83 \times 10^{-4} + 3.27 \times 10^{-7} = 0.00135$$

So,

$$\begin{aligned} P(\theta = 0.2 \mid \mathcal{V}) &= 0.4979 \\ P(\theta = 0.5 \mid \mathcal{V}) &= 0.5059 \\ P(\theta = 0.8 \mid \mathcal{V}) &= 0.00024 \end{aligned}$$

These are the posterior parameter beliefs of our experiment. Given this, if we were to choose a single value for the posterior it would be $\theta = 0.5$. This result is intuitive, we had a strong belief of the coin being fair and even though the number of tails was quite bigger than heads, it was not enough to make the difference. Obviously the posterior of the coin being biased to tails is now bigger than the prior.

Suppose an uniform prior distribution so that $P(\theta) = k \implies \int_0^1 P(\theta) d\theta = k = 1$ due to normalization.

Using the previous calculations we have

$$P(\theta \mid \mathcal{V}) = \frac{1}{P(\mathcal{V})} \theta^{n_h} (1 - \theta)^{n_t}$$

where

$$P(\mathcal{V}) = \int_0^1 \theta^{n_h} (1 - \theta)^{n_t} d\theta$$

this implies that

$$P(\theta | \mathcal{V}) = \frac{\theta^{n_h} (1 - \theta)^{n_t}}{\int_0^1 u^{n_h} (1 - u)^{n_t} du} \implies \theta | \mathcal{V} \sim \text{Beta}(n_h + 1, n_t + 1)$$

Let's use a Beta distribution as the prior in the last example

$$\theta \sim \text{Beta}(\alpha, \beta) \implies P(\theta) = \frac{1}{B(\alpha, \beta)} \theta^{\alpha-1} (1 - \theta)^{\beta-1}$$

then, repeating the same as before we get that

$$P(\theta, \mathcal{V}) = \frac{1}{B(\alpha + n_h, \beta + n_t)} \theta^{\alpha+n_h-1} (1 - \theta)^{\beta+n_t-1} \implies (\theta, \mathcal{V}) \sim \text{Beta}(\alpha + n_h, \beta + n_t)$$

So both the prior and posterior are Beta distributions, then the Beta distribution is called “conjugate” of the Binomial distribution.

10.1 UTILITY

The Bayesian posterior says nothing about how to benefit from the beliefs it represents, in order to do this we need to specify the utility of each decision.

With this idea we define an utility function over the parameters

$$U(\theta, \theta_{true}) = \alpha \mathbb{I}[\theta = \theta_{true}] - \beta \mathbb{I}[\theta \neq \theta_{true}]$$

where $\alpha, \beta \in \mathbb{R}$. This symbolizes the gains or losses of choosing the parameter θ , when the true value of the parameter is supposed to be θ_{true} . Then the expected utility of a parameter θ_0 is calculated as

$$U(\theta = \theta_0) = \sum_{\theta_{true}} U(\theta = \theta_0, \theta_{true}) P(\theta = \theta_{true} | \mathcal{V})$$

Using the last example, we may define our utility function as

$$U(\theta, \theta_{true}) = 10 \mathbb{I}[\theta = \theta_{true}] - 20 \mathbb{I}[\theta \neq \theta_{true}]$$

Where we interpret that the loss of choosing the wrong parameter is twice as important as the gains from doing it right.

The expected utility of the decision that the parameter is $\theta = 0.2$ in our discrete example would be

$$\begin{aligned}
 U(\theta = 0.2) &= U(\theta = 0.2, \theta_{true} = 0.2)P(\theta_{true} = 0.2 \mid \mathcal{V}) \\
 &\quad + U(\theta = 0.2, \theta_{true} = 0.5)P(\theta_{true} = 0.5 \mid \mathcal{V}) \\
 &\quad + U(\theta = 0.2, \theta_{true} = 0.8)P(\theta_{true} = 0.8 \mid \mathcal{V}) \\
 &= 10 \times 0.4979 - 20 \times 0.5059 - 20 \times 0.00024 \\
 &= -5.1438 \\
 U(\theta = 0.5) &= -4.9038 \\
 U(\theta = 0.8) &= -20.0736
 \end{aligned}$$

This illustrates how an utility function can affect the results of the inference. The most probable value for θ was 0.2, but, using this utility function, 0.5 is the one with which we expect minor losses.

MAXIMUM LIKELIHOOD TRAINING

In this section we will introduce two concepts, Maximum Likelihood and Maximum a Posteriori, showing that *training* a model's parameter to maximize the Maximum Likelihood equals to take the empirical distribution as it.

Let $\{X_1, \dots, X_N\}$ be a set of real i.i.d random variables and $\mathcal{V} = \{x_1, \dots, x_N\}$ be the set of observations and θ the considered parameters of the model.

Definition 42. Maximum Likelihood is calculated as

$$\theta^{ML} = \arg \max_{\theta} P(\mathcal{V} \mid \theta)$$

it refers to the value of the parameter θ for which the observed data better fits the model.

Definition 43. Maximum A Posteriori refers to

$$\theta^{MAP} = \arg \max_{\theta} P(\mathcal{V} \mid \theta)P(\theta)$$

The decision of taking the Maximum A Posteriori can be motivated using an utility that equals zero for all but the correct parameter

$$U(\theta, \theta_{true}) = \mathbb{I}[\theta = \theta_{true}]$$

using this, the expected utility of a parameter $\theta = \theta_0$ is

$$U(\theta = \theta_0) = \sum_{\theta_{true}} \mathbb{I}[\theta_{true} = \theta_0]P(\theta = \theta_{true} \mid \mathcal{V}) = P(\theta_0 \mid \mathcal{V})$$

This means that the maximum utility decision is to take the value θ_0 with the highest posterior value.

Remark 4. When using a flat prior, i.e, $P(\theta)$ is constant, $\theta^{ML} = \theta^{MAP}$.

11.1 ML AND KL DIVERGENCE

Now, we are going to show the relation between the Maximum Likelihood and the Kullback-Leibler divergence of the empirical distribution and our model. Firstly, we define the empirical distribution as a distribution whose probability mass function Q is

$$Q(x) = \frac{1}{N} \sum_{i=1}^N \mathbb{I}[x = x_i]$$

We may calculate the Kullback-Leibler divergence between the empirical and our considered model $P(x | \theta)$ and study their functional independence.

$$KL(Q | P) = \mathbb{E}_Q[\log(Q(x))] - \mathbb{E}_Q[\log(P(x | \theta))]$$

Notice the term $\mathbb{E}_Q[\log(Q(x))]$ is a constant and the log likelihood under Q takes the form

$$\mathbb{E}_Q[\log(P(x | \theta))] = \frac{1}{N} \int_x \sum_{i=1}^N \mathbb{I}[x = x_i] \log P(x | \theta) = \frac{1}{N} \sum_{i=1}^N \log P(x_i | \theta)$$

As the logarithm is a strictly increasing function, maximizing the log likelihood equals to maximize the likelihood itself, and we can see here how it is equivalent to minimize the Kullback-Leibler divergence between the empirical distribution and our distribution.

$$\begin{aligned} \arg \min_{\theta} KL(Q | P) &= \arg \min_{\theta} -\mathbb{E}_Q[\log(P(x | \theta))] = \arg \max_{\theta} \mathbb{E}_Q[\log(P(x | \theta))] \\ \arg \max_{\theta} \frac{1}{N} \sum_{i=1}^N \log P(x_i | \theta) &= \arg \max_{\theta} \frac{1}{N} \sum_{i=1}^N P(x_i | \theta) = \arg \max_{\theta} \sum_{i=1}^N P(x_i | \theta) = \theta^{ML} \end{aligned}$$

In case $P(x | \theta)$ is unconstrained, the optimal choice is $P(x | \theta) = Q(x)$, that is, the **maximum likelihood distribution corresponds to the empirical distribution**.

For a Belief Network we know there is the following constraint

$$P(x_1, \dots, x_m | \theta) = \prod_{i=1}^K P(x_i | pa(x_i), \theta)$$

We now want to minimize the Kullback-Leibler divergence between the empirical distribution $Q(x)$ and $P(x | \theta)$ in order to get the Maximum Likelihood.

$$\begin{aligned} KL(Q | P) &= -\mathbb{E}_Q\left[\sum_{i=1}^K \log P(x_i | pa(x_i), \theta)\right] + \mathbb{E}_Q\left[\sum_{i=1}^K \log Q(x_i | pa(x_i))\right] \\ &= -\sum_{i=1}^K \mathbb{E}_Q\left[\log P(x_i | pa(x_i), \theta)\right] + \sum_{i=1}^K \mathbb{E}_Q\left[\log Q(x_i | pa(x_i))\right] \end{aligned}$$

Notice the expectation is over the full distribution $Q(x_1, \dots, x_k)$, we can use proposition 1 on $\log P(x_i | pa(x_i), \theta)$ and $Q(x_i, pa(x_i))$.

$$\begin{aligned}
KL(Q \mid P) &= \sum_{i=1}^K \mathbb{E}_{Q(x_i, pa(x_i))} [\log Q(x_i \mid pa(x_i))] - \mathbb{E}_{Q(x_i, pa(x_i))} [\log P(x_i \mid pa(x_i), \theta)] \\
&= \sum_{i=1}^K \mathbb{E}_{Q(x_i, pa(x_i))} [KL(Q(x_i \mid pa(x_i)) \mid P(x_i \mid pa(x_i), \theta))]
\end{aligned}$$

The minimal setting is then

$$P(x_i \mid pa(x_i), \theta) = Q(x_i \mid pa(x_i))$$

in terms of the initial data it is to set $P(x_i \mid pa(x_i))$ to the number of times the state appears in it.

BAYESIAN TRAINING

A Bayesian approach where we set a distribution over the parameters is an alternative to Maximum Likelihood training of a Bayesian Network, as we did in the coin tossing example.

We go deep into it using the following scenario, consider a disease D and two habits A and B . Let $N = 7$ be the number of observations of the variables as shown in the table below, that means we are considering the following i.i.d variables $\{A_1, \dots, A_N\}$, $\{B_1, \dots, b_N\}$ and $\{D_1, \dots, D_N\}$ governed by the parameters θ_A, θ_B and θ_D as shown in the following Bayesian Network.

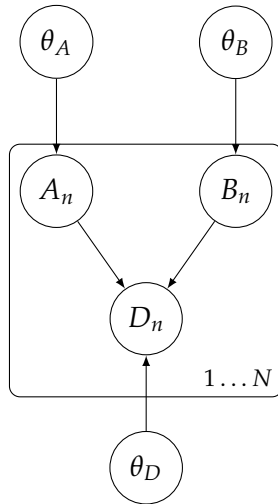


Figure 17: Bayesian parameter model for the relation between A, B, D

A	B	D
1	1	1
1	0	0
0	1	1
0	1	0
1	1	1
0	0	0
1	0	1

Table 1: Observations

The graph gives the following joint probability distribution over A, B and D

$$P(a, b, d) = P(d | a, b)P(a)P(b)$$

Let $\mathcal{V} = \{(a_n, b_n, d_n), n = 1, \dots, N\}$ be the set of observations.

We need a notation for the parameters, as all the variables are binary we are going to use

$$P(A = 1 | \theta_A) = \theta_A, \quad P(B = 1 | \theta_B) = \theta_B, \quad P(D = 1 | A = 0, B = 1, \theta_D) = \theta_1$$

$$\theta_D = (\theta_0, \theta_1, \theta_2, \theta_3)$$

Where we are using a binary to decimal transformation between the states of A and B and the sub-index of θ .

We need to specify a prior and since dealing with multidimensional continuous distributions is computationally problematic it is normal to use uni-variate distributions.

12.1 GLOBAL AND LOCAL PARAMETER INDEPENDENCE

A convenient assumption is that the prior factorizes, this is usually called *global parameter independence*.

$$P(\theta_A, \theta_B, \theta_D) = P(\theta_A)P(\theta_B)P(\theta_D)$$

Using this

$$P(\theta_A, \theta_B, \theta_D, \mathcal{V}) = P(\theta_A)P(\theta_B)P(\theta_D) \prod_n P(a_n | \theta_A)P(b_n | \theta_B)P(d_n | a_n, b_n, \theta_D)$$

Learning then corresponds to inference

$$\begin{aligned} P(\theta_A, \theta_B, \theta_D | \mathcal{V}) &= \frac{P(\mathcal{V} | \theta_A, \theta_B, \theta_D)P(\theta_A, \theta_B, \theta_D)}{P(\mathcal{V})} = \frac{P(\mathcal{V} | \theta_A, \theta_B, \theta_D)P(\theta_A)P(\theta_B)P(\theta_D)}{P(\mathcal{V})} \\ &= \frac{1}{P(\mathcal{V})}P(\theta_A)P(\theta_B)P(\theta_D) \prod_n P(a_n | \theta_A)P(b_n | \theta_B)P(d_n | a_n, b_n, \theta_D) \\ &= P(\theta_A | \mathcal{V}_A)P(\theta_B | \mathcal{V}_B)P(\theta_D | \mathcal{V}) \end{aligned}$$

If we further assume that $P(\theta_D)$ factorizes as $P(\theta_D) = P(\theta_0)P(\theta_1)P(\theta_2)P(\theta_3)$, this is called *local parameter independence*, then it follows that

$$P(\theta_D | \mathcal{V}) = P(\theta_0 | \mathcal{V})P(\theta_1 | \mathcal{V})P(\theta_2 | \mathcal{V})P(\theta_3 | \mathcal{V})$$

12.2 LEARNING BINARY VARIABLES

The simplest cases to continue are $P(a | \theta_A)$ and $P(b | \theta_B)$ since they require only a uni-variate prior distribution $P(\theta_A)$ or $P(\theta_B)$. We use $P(\theta_A)$ as the other case is analogous.

The posterior is

$$P(\theta_A | \mathcal{V}_A) = \frac{1}{P(\mathcal{V}_A)}P(\theta_A)\theta_A^{\#(a=1)}(1 - \theta_A)^{\#(a=0)}$$

The most convenient choice for the prior is a Beta distribution as conjugacy will hold.

$$\theta_A \sim \text{Beta}(\alpha_A, \beta_A) \implies P(\theta_A) = \frac{1}{B(\alpha_A, \beta_A)}\theta_A^{\alpha_A-1}(1 - \theta_A)^{\beta_A-1}$$

So it follows that

$$(\theta_A | \mathcal{V}_A) \sim \text{Beta}(\alpha_A + \#(A = 1), \beta_A + \#(A = 0))$$

The marginal is then

$$\begin{aligned}
 P(A = 1 \mid \mathcal{V}_A) &= \frac{P(A = 1, \mathcal{V}_A)}{P(\mathcal{V}_A)} = \int_{\theta_A} \frac{P(A = 1, \mathcal{V}_A, \theta_A)}{P(\mathcal{V}_A)} = \int_{\theta_A} \frac{P(A = 1 \mid \mathcal{V}_A, \theta_A) P(\mathcal{V}_A, \theta_A)}{P(\mathcal{V}_A)} \\
 &= \int_{\theta_A} \frac{P(A = 1 \mid \mathcal{V}_A, \theta_A) P(\theta_A \mid \mathcal{V}_A) P(\mathcal{V}_A)}{P(\mathcal{V}_A)} = \int_{\theta_A} P(\theta_A \mid \mathcal{V}_A) \theta_A = \mathbb{E}[\theta_A \mid \mathcal{V}_A] \\
 &= \frac{\alpha_A + \#(A = 1)}{\alpha_A + \#(A = 1) + \beta_A + \#(A = 0)}
 \end{aligned}$$

Where the last equality is the expected value of a Beta distribution.

For $P(d \mid a, b)$ the situation is more complex, the simplest approach to specify a Beta prior for each of the components of θ_D . Focus on θ_2 , notice the parameters α and β we used before are now dependent from A and B , these are called *hyperparameters*.

$$\theta_2 \sim \text{Beta}(\alpha_D(1, 0) + \#(D = 1, A = 1, B = 0), \beta_D(1, 0) + \#(D = 0, A = 1, B = 0))$$

Repeating the procedure we used with A we get that

$$P(D = 1 \mid A = 1, B = 0, \mathcal{V}) = \frac{\alpha_D(1, 0) + \#(D = 1, A = 1, B = 0)}{\alpha_D(1, 0) + \beta_D(1, 0) + \#(A = 1, B = 0)}$$

In case we had no preference, we could set all hyperparameters to the same value, where a complete ignorance prior would correspond to set them to 1.

Once we get to this situation there are two limit possibilities depending on the amount of data we got.

- **No data.** The marginal probability corresponds to the prior which in the last case is

$$P(D = 1 \mid A = 1, B = 0, \mathcal{V}) = \frac{\alpha_D(1, 0)}{\alpha_D(1, 0) + \beta_D(1, 0)}$$

Note that equal hyperparameters would give a result of 0.5.

- **Infinite data.** When infinite data is available, the marginal is generally dominated by it, this corresponds to the Maximum Likelihood solution.

$$P(D = 1 \mid A = 1, B = 0, \mathcal{V}) = \frac{\#(D = 1, A = 1, B = 0)}{\#(A = 1, B = 0)}$$

This happens unless the prior has a pathologically strong effect.

Consider the data given in the table in figure 17, and equal parameters and hyperparameters 1. Then we can compute the differences between this and using the Maximum Likelihood technique.

$$P(A = 1 \mid \mathcal{V}) = \frac{1 + \#(A = 1)}{2 + N} = \frac{5}{9} \approx 0.556$$

By comparison, the Maximum Likelihood result is $4/7 = 0.571$, the Bayesian result is more prudent than this one, which fits in with our belief that any setting is equally probable i.e 0.5.

12.3 LEARNING DISCRETE VARIABLES

The natural generalization to more than two states is using a Dirichlet distribution as prior, assuming i.i.d data, local and global prior independence. We are considering two different scenarios, firstly one where the variable has no parents, as the case for A and B in the previous example. Secondly, we will consider a variable with a non void set of parents.

12.3.1 No parents

Consider a variable $X \sim \text{Categorical}(\theta)$ with $\text{Dom}(X) = \{1, \dots, I\}$ and $\theta = (\theta_1, \dots, \theta_I)$ so that

$$P(x) = \prod_{i=1}^I \theta_i^{\mathbb{I}[x=i]} \text{ with } \sum_{i=1}^I \theta_i = 1$$

So that the posterior (considering N observations of the variable $\mathcal{V} = (x_1, \dots, x_N)$) is

$$P(\theta \mid \mathcal{V}) = \frac{1}{P(\mathcal{V})} P(\theta) \prod_{n=1}^N \prod_{i=1}^I \theta_i^{\mathbb{I}[x_n=i]} = \frac{1}{P(\mathcal{V})} P(\theta) \prod_{i=1}^I \theta_i^{\sum_n \mathbb{I}[x_n=i]}$$

Then assuming a prior $\theta \sim \text{Dirichlet}(\mathbf{u})$ with $\mathbf{u} = (u_1, \dots, u_I)$

$$P(\theta) = \frac{1}{B(\mathbf{u})} \prod_{i=1}^I \theta_i^{u_i-1} \implies P(\theta \mid \mathcal{V}) = \frac{1}{B(\mathbf{u})P(\mathcal{V})} \prod_{i=1}^I \theta_i^{u_i-1+\sum_n \mathbb{I}[x_n=i]}$$

Which means that, defining $\mathbf{c} = (\sum_{n=1}^N \mathbb{I}[x_n = i])_{i=1, \dots, I}$

$$(\theta \mid \mathcal{V}) \sim \text{Dirichlet}(\mathbf{u} + \mathbf{c})$$

It may not be easy to decompose $B(\mathbf{u} + \mathbf{c})$ as $B(\mathbf{u})P(\mathcal{V})$, but using that it ensures normalization of the Beta distribution we may use that

$$\int_{\theta} P(\theta \mid \mathcal{V}) = 1 \implies \int_{\theta} \prod_{i=1}^I \theta_i^{u_i+c_i-1} = B(\mathbf{u} + \mathbf{c}) = B(\mathbf{u})P(\mathcal{V})$$

Remark 5. Summarizing the above information, we just proved that the Dirichlet distribution is the conjugate prior of the Categorical Distribution.

The marginal is then given by

$$\begin{aligned} P(X = i \mid \mathcal{V}) &= \int_{\theta} P(X = i \mid \theta) P(\theta \mid \mathcal{V}) = \int_{\theta} \theta_i P(\theta \mid \mathcal{V}) \\ &= \int_{\theta_i} \theta_i P(\theta_i \mid \mathcal{V}) = \mathbb{E}[\theta_i \mid \mathcal{V}] \end{aligned}$$

Where we used that

$$\int_{\theta_j \neq i} \theta_i P(\theta \mid \mathcal{V}) = \theta_i \prod_{k \neq j} P(\theta_k \mid \mathcal{V}) \int_{\theta_j} P(\theta_j \mid \mathcal{V}) = \theta_i \prod_{k \neq j} P(\theta_k \mid \mathcal{V})$$

As we already know from Proposition 2, the uni-variate marginal of a Dirichlet distribution is a Beta Distribution of parameters

$$(\theta_i \mid \mathcal{V}) \sim \text{Beta}(u_i + c_i, \sum_{j \neq i} u_j + c_j)$$

Using the expectation of a Beta distribution we get that

$$P(X = i \mid \mathcal{V}) = \frac{u_i + c_i}{\sum_j u_j + c_j}$$

12.3.2 Parents

Consider now that X has a set of parent variables $pa(X)$, in this case, we want to compute the marginal given a state of its parents and the data

$$P(X = i \mid pa(X) = \mathbf{j}, \mathcal{V})$$

We are using the following notation for the parameters

$$P(X = i \mid pa(X) = \mathbf{j}, \theta) = \theta_{i,j} \quad \theta_j = (\theta_{1,j}, \dots, \theta_{L,j})$$

Local independence means that

$$P(\theta) = \prod_j P(\theta_j)$$

As we did before, we consider a Dirichlet prior

$$\theta_j \sim \text{Dirichlet}(\mathbf{u}_j)$$

The posterior is then

$$\begin{aligned} P(\theta \mid \mathcal{V}) &= \frac{P(\theta)P(\mathcal{V} \mid \theta)}{P(\mathcal{V})} = \frac{1}{P(\mathcal{V})} \left(\prod_j P(\theta_j) \right) P(\mathcal{V} \mid \theta) \\ &= \frac{1}{P(\mathcal{V})} \left(\prod_j \frac{1}{B(\mathbf{u}_j)} \prod_i \theta_{i,j}^{u_{i,j}-1} \right) P(\mathcal{V} \mid \theta) \\ &= \frac{1}{P(\mathcal{V})} \left(\prod_j \frac{1}{B(\mathbf{u}_j)} \prod_i \theta_{i,j}^{u_{i,j}-1} \right) \left(\prod_n \prod_j \prod_i \theta_{i,j}^{\mathbb{I}[x_n=i, pa(x_n)=j]} \right) \\ &= \frac{1}{P(\mathcal{V})} \prod_j \frac{1}{B(\mathbf{u}_j)} \prod_i \theta_{i,j}^{u_{i,j}-1+\#(X=i, pa(X)=j)} \end{aligned}$$

Naming $\mathbf{v}_j = \mathbf{u}_j + \#(X = i, pa(X) = \mathbf{j})$ and using the same argument as we did in the *no parents* case with the normalization constants, the posterior then follows

$$(\theta \mid \mathcal{V}) \sim \prod_j \text{Dirichlet}(\mathbf{v}_j)$$

Noting $v_{i,j}$ the components of \mathbf{v}_j , the marginal is then

$$P(X = i, pa(X) = \mathbf{j}, \mathcal{V}) = \frac{v_{i,j}}{\sum_i v_{i,j}}$$

Notice all the above has been done using a fixed variable X , so that all the parameters depend on that variable.

We can define the data likelihood under a model, usually called the *model likelihood* using the same calculations as we did with $P(\theta \mid \mathcal{V})$ but applied to all the variables of the model

$$\begin{aligned} P(\mathcal{V} \mid \mathcal{M}) &= \int_{\theta} P(\theta) P(\mathcal{V} \mid \theta, \mathcal{M}) = \prod_x \prod_j \frac{1}{B(\mathbf{u}_j)} \int_{\theta} \prod_i \theta_{i,j}^{u_{i,j}-1+\#(x=i, pa(x)=j)} \\ &= \prod_x \prod_j \frac{B(\mathbf{v}_j)}{B(\mathbf{u}_j)} \end{aligned}$$

STRUCTURE LEARNING

So far, we have assumed the Bayesian Network was an hypothesis of the problem, however, this structure is not always given and may be learned also from the data.

Even considering complete data (no missing observations), there are some problems that need to be taken into account.

- The number of Belief networks is exponential over the number of variables so a brute force algorithm would not be viable.
- Testing dependencies requires a large amount of data. So a threshold must be set to measure when a dependence is significant.
- A Belief Network or a Markov Network may not be enough to represent the data due to the existence of unobserved variables.

13.1 PC ALGORITHM

An approach to learn the structure is the PC algorithm, it begins with a complete graph G and tries to remove as many links as possible studying the independence of the variables.

The algorithm [2](#) iterates over neighborhoods, from smaller to bigger ones. It chooses a linked pair of variables $(X, Y) \in E$ and a subset $S_{XY} \subset ne(X)$, verifying $Y \notin S_{XY}$. If $X \perp\!\!\!\perp Y \mid S$, then the link is removed and S_{XY} is stored.

The main idea behind this is that a set of independencies is faithful to a graph if there is no link between two nodes X and Y if and only if there exists a subset of $ne(X)$ such that they are independent given this subset.

This gives the skeleton of the Bayesian Network, no more edges will be removed or added. The directed graph may be constructed following two rules rule:

1. For any undirected link $X - Y - Z$, if $Y \notin S_{XZ}$ then set $X \rightarrow Y \leftarrow Z$ (we are creating a collider for that path).
2. The rest of links may oriented arbitrarily not creating cycles or colliders.

The reasoning behind this is the d-separation theorem [2](#), if $Y \notin S_{XZ}$ then $X \not\perp\!\!\!\perp Z \mid Y$ so Y must d-connect them, to get this we set it as a collider. On the other hand, if $Y \in S_{XZ}$ and $X \perp\!\!\!\perp Z \mid S_{XZ}$ then we want S_{XZ} to d-separate them, that is, using any configuration that doesn't create a collider in S_{XZ} .

Algorithm 2: PC Algorithm

Data: Complete undirected graph G , with vertices \mathcal{V} **Result:** G with removed links $i = 0;$ **while** all nodes have $\leq i$ neighbors **do** **for** $X \in \mathcal{V}$ **do** **for** $Y \in ne(x)$ **do** **if** $\exists S \subset ne(X) \setminus Y$ such that $\#S = i$ and $X \perp\!\!\!\perp Y \mid S$ **then** Remove $X - Y$ from G ; $S_{XY} = S$; **end** **end** **end** $i = i + 1$;**end**

13.2 INDEPENDENCE LEARNING

Our main concern now is given three variables X, Y, Z to measure $X \perp\!\!\!\perp Y \mid Z$. One approach is to measure the empirical *conditional mutual information* of the variables.

Definition 44. Given two random variables X, Y , we define their *mutual information* as the Kullback-Leibler divergence of their joint distribution and the product of their marginals and

$$MI(X; Y) = KL(P_{X,Y} \mid P_X P_Y)$$

Definition 45. Given three random variables X, Y, Z we define the *conditional mutual information* of X and Y over Z as

$$MI(X; Y \mid Z) = \mathbb{E}_Z \left[KL(P_{X,Y|Z} \mid P_{X|Z} P_{Y|Z}) \right]$$

Where $MI(X; Y \mid Z) \geq 0$ and $MI(X; Y \mid Z) = 0 \iff P_{X,Y|Z} = P_{X|Z} P_{Y|Z} \iff X \perp\!\!\!\perp Y \mid Z$. We can estimate this using the empirical distributions, however, this *empirical* mutual information will be typically greater than 0 even when $X \perp\!\!\!\perp Y \mid Z$, therefore a threshold must be established.

A Bayesian approach would be comparing the model likelihood under independence and dependence hypothesis. That is computing the model likelihood for the below joint distributions assuming local and global parameter independence

$$P_{indep}(x, y, z) = P(x \mid z, \theta_1) P(y \mid z, \theta_2) P(z \mid \theta_3) P(\theta_1) P(\theta_2) P(\theta_3)$$

$$P_{dep}(x, y, z) = P(x, y, z \mid \theta) P(\theta)$$

VARIATIONAL INFERENCE IN BAYESIAN NETWORKS

Until this moment we have assume that the data we are given is completed but in practice this data is not in two different ways. There may be unobserved or *hidden* variables that affect the visible ones, and there may be *missing* information, that is, states of visible variables that are missing.

Think about the example with the disease and the two habits we used in the last section, missing data would be a row in the table where some entry is missing, for example $x_3 = \{D = 1, A = 1\}$, where we know that this person got the disease and had habit A but we have no information about habit B , this is an example of *missing* data.

One approach to handle this situation would be marginalizing over that variable

$$P(x_3 | \theta) = \int_b P(d_3, a_3, b | \theta) = P(a_3 | \theta_A) \int_b P(b | \theta_B) P(d_3 | b, a_3, \theta_D)$$

This leads to a non-factorized form of the posterior which is computationally difficult to handle, notice the problem is not conceptual but computational. Using the marginal to handle missing information does not always lead to this situation, in fact, marginalizing over a collider (D in our example) would mean loosing that variable as the integral simply equals 1.

$$P(x_3 | \theta) = \int_d P(d, a_3, b_3 | \theta) = P(a_3 | \theta_A) P(b_3 | \theta_B) \int_d P(d | b_3, a_3, \theta_D) = P(a_3 | \theta_A) P(b_3 | \theta_B)$$

There are three main types of missing data:

- **Missing completely at random (MCAR).** If the events that lead to any particular data to be missing is independent from both the observed and the unobserved variables, and occur at random.
- **Missing at random (MAR).** When the absence is not random but can be explained with the observed variables.
- **Missing not at random (MNAR).** The missing data is related with the reason why it is missing. For example, skipping a question in a survey for being ashamed of the answer.

To express this mathematically, split the variables \mathcal{X} into visible \mathcal{X}_{vis} and hidden \mathcal{X}_{hid} , let M be a variable denoting that the state of the hidden variables is known (0) or unknown (1). So the difference between the three types resides on how $P(M = 1 | x_{vis}, x_{hid}, \theta)$ simplifies.

When data is *missing at random*, we assume that we can explain the missing information with the visible one, so the probability of being missing only depends on the visible data, that is

$$P(M = 1 \mid x_{vis}, x_{hid}, \theta) = P(M = 1 \mid x_{vis})$$

so that,

$$P(x_{vis}, M = 1 \mid \theta) = P(M = 1 \mid x_{vis})P(x_{vis} \mid \theta)$$

Assuming the data is *missing completely at random* is stronger, as we are supposing that there is no reason behind the missing data, so that it being missing is independent from the visible and hidden data.

$$P(M = 1 \mid x_{vis}, x_{hid}, \theta) = P(M = 1)$$

so now

$$P(x_{vis}, M = 1 \mid \theta) = P(M = 1)P(x_{vis} \mid \theta)$$

In both cases we may simply use the marginal $P(x_{vis} \mid \theta)$ to assess parameters as $P(x_{vis}, M = 1 \mid \theta)$ does not depend on the missing variables.

In case data is *missing not at random* then no independence assumption is made over the probability of the data being unknown, meaning it depends on both the visible and the hidden information. From now on, we will assume missing information is either MAR or MCAR, even though this could lead to a misunderstanding of the problem as in the following example.

Example 4. Consider a situation where data is obtained from a survey where people are asked to choose between 3 options A, B and C . Assume that no one chose option C because they are ashamed of the answer, and the answers are uniform between A, B and not answering.

Normalizing the missing information would lead to setting $P(A \mid \mathcal{V}) = 0.5 = P(B \mid \mathcal{V})$ and $P(C \mid \mathcal{V}) = 0$ when the reasonable result is that not answering equals to choosing C so that $P(A \mid \mathcal{V}) = P(B \mid \mathcal{V}) = P(C \mid \mathcal{V}) = \frac{1}{3}$

14.1 EXPECTATION MAXIMIZATION

The *expectation maximization* algorithm is an iterative method to find maximum likelihood or maximum a posteriori estimates of parameters in statistical models, where the model depends on hidden variables. The main idea is to set a lower bound to the marginal likelihood, then using an iterative method to increase this lower bound, and the marginal likelihood with it.

14.1.1 General case

Consider we have only two variables, one visible V and one hidden H . Consider also the Kullback-Leibler divergence between a ‘variational’ distribution $Q(h \mid v)$ (where variational

means that this distribution is the object of an optimization problem) and a parametric one $P(h \mid v, \theta)$.

$$\begin{aligned} KL(Q(h \mid v) \mid P(h \mid v, \theta)) &= \mathbb{E}_Q \left[\log Q(h \mid v) - \log P(h \mid v, \theta) \right] \\ &= \mathbb{E}_Q \left[\log Q(h \mid v) \right] - \mathbb{E}_Q \left[\log P(h, v \mid \theta) \right] + \mathbb{E}_Q \left[\log P(v \mid \theta) \right] \\ &= \mathbb{E}_Q \left[\log Q(h \mid v) \right] - \mathbb{E}_Q \left[\log P(h, v \mid \theta) \right] + \log P(v \mid \theta) \geq 0 \end{aligned}$$

We got then a lower bound for $\log P(v \mid \theta)$

$$\log P(v \mid \theta) \geq \underbrace{-\mathbb{E}_Q \left[\log Q(h \mid v) \right]}_{\text{Entropy}} + \underbrace{\mathbb{E}_Q \left[\log P(h, v \mid \theta) \right]}_{\text{Energy}} \quad ^1$$

Assume a set of observations, $\mathcal{V} = \{x_1, \dots, x_N\}$ where each $x_n = (v_n, h_n)$ where v_n is the visible or the visible variables and h_n denotes a state of the hidden ones, that is, it is not fixed for each data-point. Then, has the variables of the observations are i.i.d we got that

$$\log P(v_1, \dots, v_N \mid \theta) = \sum_{n=1}^N \log P(v_n \mid \theta) \geq \sum_{n=1}^N -\mathbb{E}_Q \left[\log Q(h_n \mid v_n) \right] + \mathbb{E}_Q \left[\log P(h_n, v_n \mid \theta) \right]$$

And we know equality holds if and only if $Q(h_n \mid v_n) = P(h_n \mid v_n, \theta) \forall n = 1, \dots, N$.

This suggest the following iterative procedure to optimize the parameter θ consisted in two steps.

- **E-step.** For a fixed θ , find the distributions that maximize the above bound, i.e, choose $Q(h_n \mid v_n) = P(h_n \mid v_n, \theta)$.
- **M-step.** For a fixed distribution Q , find the parameter θ that maximizes the bound. Since Q does not depend on the parameter, this is equivalent to maximize the energy term.

Example 5. Consider a single variable V with $\text{Dom}(V) = \mathbb{R}$ and a single hidden variable H with $\text{dom}(H) = \{1, 2\}$. Consider the model

$$P(v \mid h, \theta) = \frac{1}{\sqrt{\pi}} e^{-(v-\theta h)^2}$$

and $P(H = 1) = P(H = 2) = 0.5$. Suppose an observation $v = 2.75$ we want to optimize the parameter θ in the marginal

$$P(V = 2.75 \mid \theta) = \int_h P(V = 2.75 \mid h, \theta) P(h) = \frac{1}{2\sqrt{\pi}} (e^{-(2.75-\theta)^2} + e^{-(2.75-2\theta)^2})$$

Then using a distribution $Q(h \mid v)$, the lower bound given to the log likelihood is

$$\log P(v \mid \theta) \geq -Q(1 \mid 2.75) \log Q(1 \mid 2.75) - Q(2 \mid 2.75) \log Q(2 \mid 2.75) - \mathbb{E}_Q \left[(v - \theta h)^2 \right] + \text{const.}$$

¹ Energy and Entropy terms come from a statistical physics terminology

Algorithm 3: Expectation Maximization Algorithm

Data: A distribution $P(x \mid \theta)$ and a dataset \mathcal{V} . Where X splits in visible variables V and hidden variables H

Result: Parameter θ that maximizes the likelihood

while *Convergence stop criteria* **do**

for $n \in 1, \dots, N$ **do**

$Q(h \mid v_n) = P(h \mid v_n, \theta);$

end

$\theta = \arg \max_{\theta} \sum_{n=1}^N \mathbb{E}_{Q(h|v_n)} [\log P(h, v_n \mid \theta)];$

end

return $\theta;$

The M-step can be done analytically, noticing that due to the negative sign we want to minimize $\mathbb{E}_Q[(v - \theta h)^2]$

$$\frac{d}{d\theta} \mathbb{E}_Q[(v - \theta h)^2] = \mathbb{E}_Q[2vh + 2\theta h^2] = 2v\mathbb{E}_Q[h] + 2\theta\mathbb{E}_Q[h^2] = 0 \iff \theta = \frac{v\mathbb{E}_Q[h]}{\mathbb{E}_Q[h^2]}$$

$$\frac{d^2}{d^2\theta} \mathbb{E}_Q[(v - \theta h)^2] = 2\mathbb{E}_Q[h^2] \geq 0$$

so the new parameter optimal parameter is

$$\theta_{new} = v \frac{\mathbb{E}_Q[H]}{\mathbb{E}_Q[H^2]}$$

The E-step would set $Q_{new}(h \mid v) = P(h \mid v, \theta)$, in this case

$$Q_{new}(h) = \frac{P(V = 2.75 \mid h, \theta)P(H = 2)}{P(V = 2.75)} = \frac{e^{-(2.75-h\theta)}}{e^{-(2.75-\theta)} + e^{-(2.75-2\theta)}}$$

14.1.2 EM increases the marginal likelihood

It is clear that the EM algorithm does increase the lower bound in each iteration but we would like it to increase not only the bound but also the marginal likelihood. We will be using a single data point as it easy holds by summation when using the full dataset.

Let θ^{new} be the value of the parameter after one iteration, we assume that Q is set to

$$Q(h \mid v) = P(h \mid v, \theta)$$

So the lower bound in terms of θ and θ^{new} is

$$LB(\theta^{new} \mid \theta) = \underbrace{-\mathbb{E}_{P(h|v,\theta)} [\log P(h \mid v, \theta)]}_{\text{Entropy}} + \underbrace{\mathbb{E}_{P(h|v,\theta)} [\log P(h, v \mid \theta^{new})]}_{\text{Energy}}$$

From the definition of the Kullback-Leibler we get that

$$\log P(v | \theta^{new}) = LB(\theta^{new} | \theta) + KL(P(h | v, \theta) | P(h | v, \theta^{new}))$$

We could use θ in the above formula getting

$$\log P(v | \theta) = LB(\theta | \theta) + KL(P(h | v, \theta) | P(h | v, \theta)) = LB(\theta | \theta)$$

So we can compute the difference between the log likelihood between two consecutive iterations as

$$\log P(v | \theta^{new}) - \log P(v | \theta) = LB(\theta^{new} | \theta) - LB(\theta | \theta) + KL(P(h | v, \theta) | P(h | v, \theta^{new}))$$

Where we know the last term is always positive, about the difference of bounds, the M-step ensures the new parameter makes the lower bound higher or equal to the current one, so that difference is also positive.

$$\log P(v | \theta^{new}) - \log P(v | \theta) \geq 0$$

14.1.3 Bayesian Networks case

As we did before let $\mathcal{X} = (\mathcal{V}, \mathcal{H}) = \{X_1, \dots, X_M\}$ be the set of variables partitioned in visible and hidden. Let $\mathcal{D} = \{(v^1, h^1), \dots, (v^N, h^N)\}$ be the set of observations.

As we are not using a single variable anymore, the variational distribution is now over the set of hidden variables conditioned on the visible $Q(\mathcal{H} | \mathcal{V})$. As the E-step is the same as in the general case, we are focusing on the M-step, where Q_{old} is fixed.

The *energy term* in a Bayesian Network is

$$\sum_{n=1}^N \mathbb{E}_{Q_{old}(h^n | v^n)} [\log P(x^n | \theta)] = \sum_{n=1}^N \sum_{i=0}^M \mathbb{E}_{Q_{old}(h^n | v^n)} [\log P(x_i^n | pa(x_i^n), \theta)]$$

It is useful to use the following notation that defines a conditional distribution of the hidden variable when the visible one equals v^n .

$$Q^n(x) = Q^n(v, h) = Q_{old}(h^n | v^n) \mathbb{I}(v = v^n)$$

We can define the mixture distribution

$$Q(x) = \frac{1}{N} \sum_{n=1}^N Q^n(x)$$

Then we have that

$$\begin{aligned} \mathbb{E}_{Q(x)} [\log P(x | \theta)] &= \int_x Q(x) \log P(x | \theta) = \int_x \frac{1}{N} \sum_{n=1}^N Q^n(x) \log P(x | \theta) \\ &= \frac{1}{N} \int_x \sum_{n=1}^N Q_{old}(h | v^n) \mathbb{I}[v = v^n] \log P(x | \theta) \\ &= \frac{1}{N} \sum_{n=1}^N \mathbb{E}_{Q_{old}(h | v^n)} [\log P(h, v^n | \theta)] \\ &= \frac{1}{N} \sum_{n=1}^N \mathbb{E}_{Q_{old}(h | v^n)} [\log P(x^n | \theta)] \end{aligned}$$

Using the Belief Network structure

$$\begin{aligned}
 \mathbb{E}_{Q(x)} \left[\log P(x \mid \theta) \right] &= \sum_{i=1}^M \mathbb{E}_{Q(x)} \left[\log P(x_i \mid pa(x_i, \theta)) \right] \\
 &= \sum_{i=1}^M \mathbb{E}_{Q(x_i, pa(x_i))} \left[\log P(x_i \mid pa(x_i, \theta)) \right] \\
 &= \sum_{i=1}^M \mathbb{E}_{Q(pa(x_i))} \left[\mathbb{E}_{Q(x_i \mid pa(x_i))} \left[\log P(x_i \mid pa(x_i), \theta) \right] \right]
 \end{aligned}$$

We add a constant to the last term so it comes with the structure of a Kullback-Leibler Divergence (notice its sign has changed)

$$\begin{aligned}
 \sum_{i=1}^M \mathbb{E}_{Q(pa(x_i))} \left[\mathbb{E}_{Q(x_i \mid pa(x_i))} \left[\log Q(x_i \mid pa(x_i)) \right] \right] - \mathbb{E}_{Q(x_i \mid pa(x_i))} \left[\log P(x_i \mid pa(x_i), \theta) \right] &= \\
 = \sum_{i=1}^M E_{Q(pa(x_i))} \left[KL \left(Q(x_i \mid pa(x_i)) \mid P(x_i \mid pa(x_i), \theta) \right) \right]
 \end{aligned}$$

So maximizing the energy term is equivalent to minimize the above formula, that is, setting

$$P^{new}(x_i \mid pa(x_i), \theta) = Q(x_i \mid pa(x_i))$$

So the first observation is that θ is not needed in order to maximize the energy term due to the Belief Network structure.

14.2 DISTRIBUTION MIXTURE EXAMPLE WITH EM

In this section we are using a coin-flipping experiment as an example to show the difference between ML training and EM training in a *mixture distribution* (Do & Batzoglou (2008)).

Consider a simple coin-flipping experiment in which we are given a pair of coins A and B of unknown biases, θ_A and θ_B , respectively. Let 1 denote *heads* and 0 denote *tails*.

$$P(A = 1) = \theta_A \quad P(B = 1) = \theta_B$$

Our goal is to estimate $\theta = (\theta_A, \theta_B)$ by repeating the following procedure five times: randomly choose one of the two coins (with equal probability), and perform ten independent coin tosses with the selected coin.

The ML approach is setting

$$\theta_A^{opt} = \frac{\text{Heads of coin } A}{\text{Total flips of coin } A} \quad \theta_B^{opt} = \frac{\text{Heads of coin } B}{\text{Total flips of coin } B}$$

Consider now that the identity on the coin that is being flipped is unknown. Let X be the random variable modeling the number of heads in M flips and Z the coin being flipped.

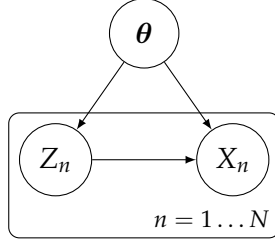


Figure 18: Bayesian Network modeling the flipping coin experiment

Consider a dataset of size N . This time, using the ML approach is not possible so the EM algorithm enters the game.

The lower bound is in this case

$$\sum_{n=1}^N \log P(x_n | \theta) \geq \sum_{n=1}^N -\mathbb{E}_Q \left[\log Q(z_n | x_n) \right] + \mathbb{E}_Q \left[\log P(z_n, x_n | \theta) \right]$$

Lets start with **E-step**, we already know it consist on setting

$$Q(z_n | x_n, \theta) = P(z_n | x_n, \theta) = \frac{P(x_n | z_n, \theta) P(z_n)}{P(x_n)} = \frac{\theta_{z_n}^{x_n} (1 - \theta_{z_n})^{M-x_n}}{\theta_A^{x_n} (1 - \theta_A)^{M-x_n} + \theta_B^{x_n} (1 - \theta_B)^{M-x_n}} \quad \forall n$$

The **M-step** consists on setting

$$\theta^{new} = \arg \max_{\theta} \sum_{n=1}^N \mathbb{E}_Q \left[P(z_n | x_n) \right]$$

Where

$$\begin{aligned} \mathbb{E}_Q \left[P(z_n | x_n) \right] &= Q(z_n = A) \left(x_n \log \theta_A + (M - x_n) \log (1 - \theta_A) \right) \\ &\quad + Q(z_n = B) \left(x_n \log \theta_B + (M - x_n) \log (1 - \theta_B) \right) \end{aligned}$$

The term affected by θ_A is

$$\sum_{n=1}^N Q(z_n = A) \left(x_n \log \theta_A + (M - x_n) \log (1 - \theta_A) \right)$$

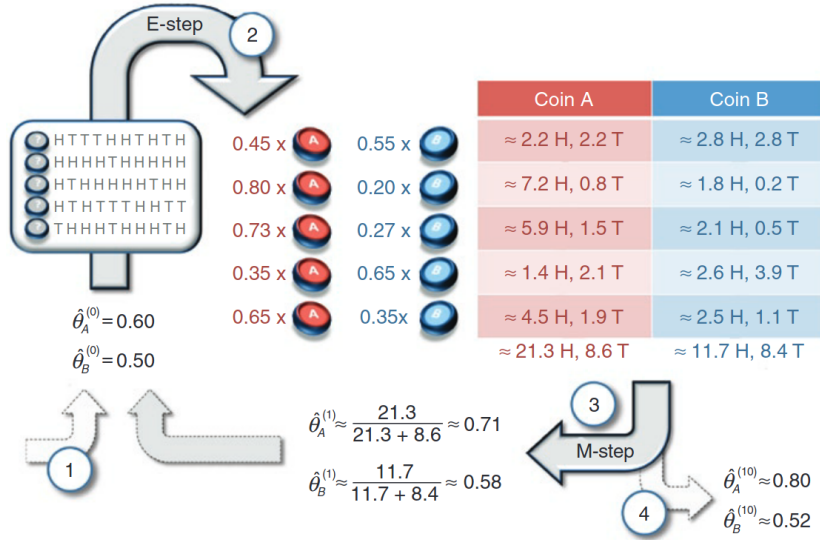
deriving and setting to 0 we get the following maxima.

$$\sum_{n=1}^N Q(z_n = A) \left(\frac{x_n}{\theta_A} - \frac{M - x_n}{1 - \theta_A} \right) = 0 \iff \theta_A = \sum_{n=1}^N Q(z_n = A) \frac{x_n}{M}$$

The same argument is valid for θ_B .

We are now using the figure 19 to set the example in a numerical context. We are following the numbers in the diagram.

1. We are considering a prior $\theta = (0.6, 0.5)$, a set of $N = 5$ samples and $M = 10$ flips per sample.

Figure 19: EM algorithm step in Mixture [Do & Batzoglou \(2008\)](#)

2. This corresponds to the **E-step**, we calculate each $Q(z_n | x_n, \theta)$.

$$Q(z_1 = A) = \frac{0.6^5 0.4^5}{0.6^5 0.4^5 + 0.5^5 0.5^5} \approx 0.45 \implies Q(z_1 = B) \approx 0.55$$

$$\vdots$$

$$Q(z_5 = A) \approx 0.65 \implies Q(z_5 = B) \approx 0.35$$

3. The **M-step** corresponds to setting

$$\theta_A = \sum_{n=1}^5 Q(z_n) \frac{x_n}{10} \approx \frac{21.3}{21.3 + 8.6} \approx 0.71$$

$$\theta_B \approx 0.58$$

4. Step 4 represents a possible solution after 10 iterations.

14.3 EM EXTENSIONS

14.3.1 Partial steps

Making a partial M-step consist on not using the optimal parameter for the energy term, but using one with just higher energy. Finding this values can be easier than finding the optimal one and convergence still follows as the only requirement to make the likelihood increase was to increase the lower bound.

On the other hand, when studying the increase on the likelihood, we supposed that the optimal E-step was being used. In general, we cannot guarantee that a partial step would increase the likelihood, even though it is guaranteed to increase the lower bound.

Another important factor is, that the EM algorithm assumes that the energy term is possible to calculate, which may not be. As an approach to solve this situation, we can set a class

of distributions \mathcal{Q} , and minimize the Kullback-Leibler divergence between $P(h | v, \theta)$ and a distribution $Q \in \mathcal{Q}$, so we pick a distribution such that

$$Q = \arg \min_{Q \in \mathcal{Q}} KL(Q(h | v) | P(h | v, \theta))$$

An extreme case is to choose \mathcal{Q} as delta functions, where the energy term is now a constant. And the optimal choice setting is

$$Q(h^n | v^n) = \delta(h^n, h_{opt}^n) \quad h_{opt}^n = \arg \max_h P(h, v^n | \theta)$$

This is called *Viterbi training* and does not guarantee that the log likelihood is being increased in each iteration.

14.4 VARIATIONAL BAYES

Another method to deal with hidden variables is using *Variational Bayes (VB)*, in contrast with the EM algorithm, this one uses a distribution that better represents the posterior than the one using a Maximum Likelihood approach.

Consider a simple datapoint $x = (v, h)$, in this situation we focus our interest on the posterior distribution.

$$P(\theta | v) = \frac{P(v | \theta)P(\theta)}{P(v)} = \frac{1}{P(v)} \int_h P(v, h | \theta)P(\theta)$$

Variational Bayes assumes the joint hidden and parameter posterior can be approximated as the product of two distributions, one over the hidden variable and one over the parameter such that

$$P(h, \theta | v) \approx Q(h)Q(\theta)^2$$

Remark 6. By doing this assumption, we are also assuming that the posterior can be approximated with $Q(\theta)$

$$P(\theta | v) = \int_h P(\theta, h | v) \approx \int_h Q(h)Q(\theta) = Q(\theta)$$

For this reason, the main goal of the algorithm is to make this approximation as tightest as possible with an iterative method that calculates both $Q(\theta)$ and $Q(h)$ distributions.

To achieve that, we minimize the Kullback-Leibler divergence between them.

$$KL(Q(h)Q(\theta) | P(h, \theta | v)) = \mathbb{E}_{Q(h)} [\log Q(h)] + \mathbb{E}_{Q(\theta)} [\log Q(\theta)] - \mathbb{E}_{Q(h)Q(\theta)} [\log P(h, \theta | v)] \geq 0$$

² We use the same letter for both distributions, as they can be differentiated from the context.

We use that $\log P(v)$ is independent from $Q(h)Q(\theta)$ to get the desired inequality.

$$\begin{aligned}
0 &\leq \mathbb{E}_{Q(h)} [\log Q(h)] + \mathbb{E}_{Q(\theta)} [\log Q(\theta)] - \mathbb{E}_{Q(h)Q(\theta)} [\log P(h, \theta | v)] \\
&= \mathbb{E}_{Q(h)} [\log Q(h)] + \mathbb{E}_{Q(\theta)} [\log Q(\theta)] - \mathbb{E}_{Q(h)Q(\theta)} \left[\log \frac{P(h, \theta, v)}{P(v)} \right] \\
&= \mathbb{E}_{Q(h)} [\log Q(h)] + \mathbb{E}_{Q(\theta)} [\log Q(\theta)] - \mathbb{E}_{Q(h)Q(\theta)} [\log P(h, \theta, v)] + \mathbb{E}_{Q(h)Q(\theta)} [\log P(v)] \\
&= \mathbb{E}_{Q(h)} [\log Q(h)] + \mathbb{E}_{Q(\theta)} [\log Q(\theta)] - \mathbb{E}_{Q(h)Q(\theta)} [\log P(h, \theta, v)] + \log P(v)
\end{aligned}$$

We got the following lower bound

$$\log P(v) \geq -\mathbb{E}_{Q(h)} [\log Q(h)] - \mathbb{E}_{Q(\theta)} [\log Q(\theta)] + \mathbb{E}_{Q(h)Q(\theta)} [\log P(h, \theta, v)]$$

So that minimizing the Kullback-Leibler divergence is equivalent to find the tightest lower bound.

The procedure is then split in two steps to keep the structure of the EM algorithm.

- **E-step.** Given a fixed $Q(\theta)$, minimize the Kullback-Leibler divergence.

$$Q^{new}(h) = \arg \min_{Q(h)} KL(Q(h)Q(\theta) | P(h, \theta | v))$$

- **M-step.** Given a fixed $Q(h)$, minimize the Kullback-Leibler divergence.

$$Q^{new}(\theta) = \arg \min_{Q(\theta)} KL(Q(h)Q(\theta) | P(h, \theta | v))$$

As in the case of the EM algorithm, each iterations guarantees an increase in the lower bound of the marginal likelihood, but increasing the marginal likelihood itself is not guaranteed.

When using an i.i.d dataset $(\mathcal{V}, \mathcal{H})$, we may assume that $Q(\mathcal{H})$ can be factorized:

$$Q(h_1, \dots, h_N) = \prod_{n=1}^N Q(h_n)$$

The lower bound to the marginal likelihood is then written as a summation of the bounds on each datapoint.

$$\log P(\mathcal{V}) \geq \sum_n -\mathbb{E}_{Q(h_n)} [\log Q(h_n)] - \mathbb{E}_{Q(\theta)} [\log Q(\theta)] + \mathbb{E}_{Q(h_n)Q(\theta)} [\log P(v_n, h_n, \theta)]$$

14.4.1 VB is a generalization of the EM algorithm

We start considering a distribution over the parameter that summarizes the information in the optimal point, let θ_{opt} be the optimal value of θ .

$$Q(\theta) = \delta(\theta - \theta_{opt})$$

The lower bound takes the form

$$\log P(v) \geq -\mathbb{E}_{Q(h)} [\log Q(h)] + \mathbb{E}_{Q(h)} [\log P(h, v, \theta_{opt})] + \text{const.}$$

The M-step is then picking the optimal parameter θ_{opt} given a fixed $Q(h)$:

$$\begin{aligned}\theta_{opt} &= \arg \max_{\theta} \left(\mathbb{E}_{Q(h)} \left[\log P(v, h, \theta) \right] \right) \\ &= \arg \max_{\theta} \left(\mathbb{E}_{Q(h)} \left[\log P(v, h | \theta) P(\theta) \right] \right) \\ &= \arg \max_{\theta} \left(\mathbb{E}_{Q(h)} \left[\log P(v, h | \theta) \right] + \log P(\theta) \right)\end{aligned}$$

If we take a flat prior ($P(\theta)$ constant), this term is equivalent to the energy one in the EM bound $\mathbb{E}_{Q(h|v)} \left[\log P(h, v | \theta) \right]$.

The VB E-step consists on minimizing $KL(Q(h) | P(h, \theta_{opt} | v))$ over $Q(h)$, as

$$\begin{aligned}KL(Q(h) | P(h, \theta_{opt}, v)) &= \mathbb{E}_{Q(h)} [Q(h)] - \mathbb{E}_{Q(h)} [P(h | \theta_{opt}, v)] \\ &= \mathbb{E}_{Q(h)} [Q(h)] - \mathbb{E}_{Q(h)} \left[\frac{P(h, \theta_{opt} | v)}{P(\theta_{opt})} \right] \\ &= \mathbb{E}_{Q(h)} [Q(h)] - \frac{1}{P(\theta_{opt})} \mathbb{E}_{Q(h)} [P(h, \theta_{opt} | v)]\end{aligned}$$

where $P(\theta_{opt})$ is a constant and

$$KL(Q(h) | P(h, \theta_{opt} | v)) = \mathbb{E}_{Q(h)} [Q(h)] - \mathbb{E}_{Q(h)} [P(h, \theta_{opt} | v)]$$

Then, as the E-step of the EM algorithm consisted on minimizing the Kullback-Leibler divergence $KL(Q(h | v) | P(h | v, \theta))$, both steps are equivalent.

Remark 7. Expectation Maximization algorithm is a special case of Variational Bayes with a flat prior and a delta function as the parameter posterior approximation.

Part V

PRACTICAL CASE WITH INFERPY

INFERPY USAGE

InferPy is a high-level API for probabilistic modeling written in Python and capable of running on top of Edward and Tensorflow. InferPy's API is strongly inspired by Keras and it has a focus on enabling flexible data processing, easy-to-code probabilistic modeling, scalable inference and robust model validation.

GAUSSIAN MIXTURE

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