Probabilistic learning

Course of Machine Learning
Master Degree in Computer Science
University of Rome "Tor Vergata"
a.a. 2021-2022

Giorgio Gambosi

Probabilistic approaches

As done before, we assume that the observed dataset (features and target) has been derived by randomly sampling:

- $\mathcal{X}$ according to the probability distribution $p_{\mathcal{D}_1}(x)$ (usually the uniform distribution)
- $\mathcal{Y}$ according to the conditional distribution $p_{\mathcal{D}_2}(y|x)$

1. we may then consider a class of possible conditional distributions $\mathcal{P}$ and
2. select (infer) the "best" conditional distribution $p^* \in \mathcal{P}$ from the available knowledge (that is, the dataset), according to some measure q
3. given any new item x, apply $p^*(y|\mathbf{x})$ to assign probabilities for each possible value of the corresponding target
4. an independent *decision strategy* must be applied to $p^*(y|\mathbf{x})$ to return a specific prediction $h(\mathbf{x})$

Inferring a best distribution

- how to define the class of possible conditional distributions $p(y|\mathbf{x})$?
  - usually, parametric approach: distributions defined by a common (arbitrary) structure and a set of parameters
- what is a measure $q(p, \mathcal{T})$ of the quality of the distribution (given the dataset $\mathcal{T} = (\mathbf{X}, \mathbf{t})$)?
  - this is related to how a dataset generated by randomly sampling from $\mathcal{D}_1$ (usually uniform) and $\mathcal{D}_2$ could be similar to the available dataset $\mathcal{T}$

A different approach

Instead of finding a best distribution $p^* \in \mathcal{P}$ and use it to predict target probabilities as $p^*(y|\mathbf{x})$ for any element $\mathbf{x}$, we could

- consider for each possible conditional distribution $p \in \mathcal{P}$ its quality $q(p, \mathcal{T})$
- compose all conditional distributions $p(y|\mathbf{x})$ each weighted by its quality $q(p, \mathcal{T})$ (for example by means of a weighted averaging)
- apply the resulting distribution

Different strategies

Assume q takes the form of a probability distribution (of probability distribution)

- first approach: take the modal value (the distribution of maximum quality) and apply it to perform predictions
- second approach: compute the expectation of the distributions, wrt the probability distribution q

Inference of predictive distribution

Dataset
We assume elements in $\mathcal{T}$ correspond to a set of n samples, independently drawn from the same probability distribution (that is, they are *independent and identically distributed*, i.i.d): they can be seen as n realizations of a single random variable.

We are interested in learning, starting from $\mathcal{T}$, a *predictive distribution* $p(\mathbf{x}|\mathbf{X})$ (or $p(\mathbf{x}, t|\mathbf{X}, \mathbf{t})$) for any new element (or element-target pair). We may interpret this as the probability that, in a random sampling, the element actually returned is indeed $\mathbf{x}$ (or $\mathbf{x}, t$).

- in the case that $\mathcal{T} = \mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$, we are interested in deriving the probability distribution $p(\mathbf{x}|\mathbf{X})$ of a new element, given the knowledge of the set $\mathbf{X}$
- in the case that $\mathcal{T} = (\mathbf{X}, \mathbf{t}) = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_n, t_n)\}$, we are interested in deriving the joint probability distribution $p(\mathbf{x}, t|\mathbf{X}, \mathbf{t})$ or, assuming $p(\mathbf{x}|\mathbf{X}, \mathbf{t})$ uniform and thus also independent from $\mathbf{X}, \mathbf{t}$, the conditional distribution $p(t|\mathbf{x}, \mathbf{X}, \mathbf{t})$, given the knowledge of the set of pairs $\mathbf{X}, \mathbf{t}$

Probabilistic models

A *probabilistic model* is a collection of probability distributions with the same structure, defined over the data domain. Probability distribution are instances of the probabilistic model and are characterized by the values assumed by a set of *parameters*.

Example 1. In a bivariate gaussian probabilistic model, distributions are characterized by the values assumed by:

1. the mean $\boldsymbol{\mu} = (\mu_1, \mu_2)$
2. the covariance matrix $\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix}$

where $\sigma_{12} = \sigma_{21}$

A probabilistic model could be

Parametric if the set of parameters is given, finite, and independent from the data

Non parametric if the set of parameters is not given in advance, but derives from the data

Bayesian learning at the model level

- Given a model space $\mathcal{M}$, let $m \in \mathcal{M}$ be a probabilistic model with parameters $\boldsymbol{\theta}$ ranging on a *parameter space* $\boldsymbol{\Theta}$.
- then, $p(\mathbf{x}|\boldsymbol{\theta}, m)$ is the predictive distribution from probabilistic model m instantiated on parameter values $\boldsymbol{\theta}$
- Assume a *prior parameter distribution* $p(\boldsymbol{\theta}|m)$ is defined for the model.
- The corresponding *prior predictive distribution* is then

$$p(\mathbf{x}|m) = \int_{\boldsymbol{\Theta}} p(\mathbf{x}|\boldsymbol{\theta}, m) p(\boldsymbol{\theta}|m) d\boldsymbol{\theta}$$

Bayesian learning at the model level

- Bayes' formula makes it possible to infer the posterior distribution of parameters, given the dataset $\mathcal{T}$

$$p(\boldsymbol{\theta}|\mathcal{T}, m) = \frac{p(\boldsymbol{\theta}|m)p(\mathcal{T}|\boldsymbol{\theta}, m)}{p(\mathcal{T}|m)} = \frac{p(\boldsymbol{\theta}|m)p(\mathcal{T}|\boldsymbol{\theta}, m)}{\int_{\boldsymbol{\Theta}} p(\boldsymbol{\theta}'|m)p(\mathcal{T}|\boldsymbol{\theta}', m)d\boldsymbol{\theta}'}$$

- The posterior predictive distribution, given the model, is then

$$p(\mathbf{x}|\mathcal{T}, m) = \int_{\boldsymbol{\Theta}} p(\mathbf{x}|\boldsymbol{\theta}, m)p(\boldsymbol{\theta}|\mathcal{T}, m)d\boldsymbol{\theta}$$

This is usually very hard, if not impossible, to be done efficiently: two high-dimensional integrations to deal with.

- no analytical solutions, in general
- numerical solutions can be computationally expensive
- approximate solutions when possible

Bayesian learning at the model level

- $p(\mathbf{x}|\boldsymbol{\theta}, m)$ is a specific predictive distribution in the collection defined by model m
- $p(\boldsymbol{\theta}|\mathcal{T}, m)$ is the probability of its parameter values given the observed dataset, it can be seen as a quality measure q of the distribution wrt $\mathcal{T}$
- the predictive probability of an element $\mathbf{x}$ corresponds to the average of the distributions $p(\mathbf{x}|\boldsymbol{\theta}, m)$, weighted by the quality measure $p(\boldsymbol{\theta}|\mathcal{T}, m)$

Bayesian learning of predictive distribution

Let $p(m)$ be any *prior distribution* of probabilistic models on model space $\mathcal{M}$

$$\sum_{m\in\mathcal{M}} p(m) = 1$$

In a bayesian framework, we may consider the posterior probability of each model

$$p(m|\mathcal{T}) = \frac{p(\mathcal{T}|m)p(m)}{p(\mathcal{T})}$$

Bayesian learning of predictive distribution

The analytical expression of the predictive distribution turns out to be quite complex

$$\begin{aligned}
p(\mathbf{x}|\mathcal{T}) &= \sum_{m\in\mathcal{M}} p(m|\mathcal{T})p(\mathbf{x}|\mathcal{T}, m) = \sum_{m\in\mathcal{M}} p(m|\mathcal{T}) \int_{\boldsymbol{\Theta}} p(\mathbf{x}|\boldsymbol{\theta}, m)p(\boldsymbol{\theta}|\mathcal{T}, m)d\boldsymbol{\theta} \\
&= \sum_{m\in\mathcal{M}} p(m|\mathcal{T}) \int_{\boldsymbol{\Theta}} p(\mathbf{x}|\boldsymbol{\theta}, m) \frac{p(\boldsymbol{\theta}|m)p(\mathcal{T}|\boldsymbol{\theta}, m)}{\int_{\boldsymbol{\Theta}} p(\boldsymbol{\theta}'|m)p(\mathcal{T}|\boldsymbol{\theta}', m)d\boldsymbol{\theta}'} d\boldsymbol{\theta} \\
&= \sum_{m\in\mathcal{M}} \frac{p(\mathcal{T}|m)p(m)}{p(\mathcal{T})} \int_{\boldsymbol{\Theta}} p(\mathbf{x}|\boldsymbol{\theta}, m) \frac{p(\boldsymbol{\theta}|m)p(\mathcal{T}|\boldsymbol{\theta}, m)}{\int_{\boldsymbol{\Theta}} p(\boldsymbol{\theta}'|m)p(\mathcal{T}|\boldsymbol{\theta}', m)d\boldsymbol{\theta}'} d\boldsymbol{\theta} \\
&= \sum_{m\in\mathcal{M}} \frac{p(m)}{p(\mathcal{T})} \int_{\boldsymbol{\Theta}} p(\mathcal{T}|\boldsymbol{\theta}, m)p(\boldsymbol{\theta}|m)d\boldsymbol{\theta} \cdot \int_{\boldsymbol{\Theta}} p(\mathbf{x}|\boldsymbol{\theta}, m) \frac{p(\boldsymbol{\theta}|m)p(\mathcal{T}|\boldsymbol{\theta}, m)}{\int_{\boldsymbol{\Theta}} p(\boldsymbol{\theta}'|m)p(\mathcal{T}|\boldsymbol{\theta}', m)d\boldsymbol{\theta}'} d\boldsymbol{\theta}
\end{aligned}$$

Evaluating this expression seems unfeasible: how to make things simpler?

1. apply model inference

Model inference

Model inference is the task of deriving, given a dataset $\mathcal{T}$ the "best" probability distribution defined on the same data domain, according to some quality measure

Two phases

Model selection From a collection of possible probabilistic models select the probabilistic model $\mathcal{M}$ best suited for $\mathcal{T}$

Estimation Given a probabilistic model m with parameters $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_D)$ derive the probability distribution (that is the assignment of values to $\boldsymbol{\theta}$) best suited for $\mathcal{T}$

Model comparison

Instead of composing the predictions of all probabilistic models, select and apply the one which best suit wrt $\mathcal{T}$.

How to compare models? Use the posterior probability of each model, given the dataset

$$p(m|\mathcal{T}) = \frac{p(\mathcal{T}|m)p(m)}{p(\mathcal{T})}$$

Observe that:

- If we assume that no specific knowledge on probabilistic models is initially available, then the prior distribution is uniform.
- The evidence $p(\mathcal{T})$ is a constant with respect to m

As a consequence, $p(m|\mathcal{T}) \propto p(\mathcal{T}|m)$ and we may refer to the likelihood $p(\mathcal{T}|m)$ in order to compare models

Model selection in practice

Validation

Test set Dataset is split into Training set (used for learning parameters) and Test set (used for measuring effectiveness). Good for large datasets: otherwise, small resulting training and test set (few data for fitting and validation)

Cross validation Dataset partitioned into K equal-sized sets. Iteratively, in K phases, use one set as test set and the union of the other $K-1$ ones as training set (K-fold cross validation). Average validation measures.

As a particular case, iteratively leave one element out and use all other points as training set (Leave-one-out cross validation).

Time consuming for large datasets and for models which are costly to fit.

Model selection in practice

Information measures

Faster methods to compare model effectiveness, based on computing measures which take into account data fitting and model complexity.

Akaike Information Criterion (AIC) Let $\boldsymbol{\theta}$ be the set of parameters of the model and let $\boldsymbol{\theta}_{ML}$ be their maximum likelihood estimate on the dataset $\mathbf{X}$. Then,

$$AIC = 2|\boldsymbol{\theta}| - 2\log p(\mathbf{X}|\boldsymbol{\theta}_{ML}) = 2|\boldsymbol{\theta}| - 2\max_{\boldsymbol{\theta}} l(\boldsymbol{\theta}|\mathbf{X})$$

lower values correspond to models to be preferred.

Bayesian Information Criterion (BIC) A variant of the above, defined as

$$BIC = |\boldsymbol{\theta}| - \log|\mathbf{X}|2\log p(\mathbf{X}|\boldsymbol{\theta}_{ML})$$
$$= |\boldsymbol{\theta}|\log|\mathbf{X}| - 2\max_{\boldsymbol{\theta}} l(\boldsymbol{\theta}|\mathbf{X})$$

Bayesian learning of predictive distribution

Given a probabilistic model m^*, selected according to some approach, the predictive distribution turns out to be quite complex

$$p(\mathbf{x}|\mathcal{T}) \approx p(\mathbf{x}|\mathcal{T}, m^*) = \int_{\boldsymbol{\Theta}} p(\mathbf{x}|\boldsymbol{\theta}, m^*)p(\boldsymbol{\theta}|\mathcal{T}, m^*)d\boldsymbol{\theta}$$
$$= \int_{\boldsymbol{\Theta}} p(\mathbf{x}|\boldsymbol{\theta}, m^*)\frac{p(\boldsymbol{\theta}|m^*)p(\mathcal{T}|\boldsymbol{\theta}, m^*)}{\int_{\boldsymbol{\Theta}} p(\boldsymbol{\theta}'|m^*)p(\mathcal{T}|\boldsymbol{\theta}', m^*)d\boldsymbol{\theta}'}d\boldsymbol{\theta}$$

Point estimate of parameters

- As noticed above, computing $p(\boldsymbol{\theta}|\mathcal{T}, m^*)$ and, from it, $p(\mathbf{x}|\mathcal{T}, m^*)$ can be quite hard if not impossible
- This leads to the idea of only estimating model inference that is the task of deriving, given $\mathcal{T}$ and m^*, the "best" probability distribution defined on the same data domain, according to some quality measure
- Only an estimate of the "best" value $\boldsymbol{\theta}^*$ in $\boldsymbol{\Theta}$ (according to some measure) is performed.
- The posterior predictive distribution can then be approximated as follows

$$p(\mathbf{x}|\mathcal{T}) \approx p(\mathbf{x}|\mathcal{T}, m^*) = \int_{\boldsymbol{\Theta}} p(\mathbf{x}|\boldsymbol{\theta}, m^*)p(\boldsymbol{\theta}|\mathcal{T}, m^*)d\boldsymbol{\theta} \approx \int_{\boldsymbol{\Theta}} p(\mathbf{x}|\boldsymbol{\theta}^*, m^*)p(\boldsymbol{\theta}|\mathcal{T}, m^*)d\boldsymbol{\theta}$$
$$= p(\mathbf{x}|\boldsymbol{\theta}^*, m^*)\int_{\boldsymbol{\Theta}} p(\boldsymbol{\theta}|\mathcal{T})d\boldsymbol{\theta} = p(\mathbf{x}|\boldsymbol{\theta}^*, m^*)$$

Likelihood

Given a dataset $\mathcal{T}$ and a probability distribution p of parameters $\boldsymbol{\theta}$ defined on the same data domain,

- the *likelihood* of $\boldsymbol{\theta}$ wrt $\mathcal{T}$ is defined as

  $$L(\boldsymbol{\theta}|\mathcal{T}) = p(\mathcal{T}|\boldsymbol{\theta})$$

  the probability of the dataset (that the dataset is generated) under distribution p with parameters $\boldsymbol{\theta}$
- while the probability $p(\mathcal{T}|\boldsymbol{\theta})$ is considered as a function of $p(\mathcal{T}|\boldsymbol{\theta})$ with $\boldsymbol{\theta}$ fixed, the likelihood $L(\boldsymbol{\theta}|\mathcal{T})$ is a function of $\boldsymbol{\theta}$ with $\mathcal{T}$ fixed
- parameters $\boldsymbol{\theta}$ are considered as (independent) variables (*frequentist interpretation* of probability)

Likelihood

- By assuming that elements in $\mathcal{T}$ are i.i.d.,

$$L(\boldsymbol{\theta}|\mathcal{T}) = p(\mathbf{X}|\boldsymbol{\theta}) = \prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta}) \qquad \text{in the first case}$$
$$L(\boldsymbol{\theta}|\mathcal{T}) = p(\mathbf{X}, \mathbf{t}|\boldsymbol{\theta}) = \prod_{i=1}^{n} p(\mathbf{x}_i, t_i|\boldsymbol{\theta}) = \prod_{i=1}^{n} p(t_i|\mathbf{x}_i, \boldsymbol{\theta})p(\mathbf{x}_i|\boldsymbol{\theta}) = p(\mathbf{x}|\boldsymbol{\theta})\prod_{i=1}^{n} p(t_i|\mathbf{x}_i, \boldsymbol{\theta})$$
$$= p(\mathbf{x})\prod_{i=1}^{n} p(t_i|\mathbf{x}_i, \boldsymbol{\theta}) \propto \prod_{i=1}^{n} p(t_i|\mathbf{x}_i, \boldsymbol{\theta}) \qquad \text{in the second case, assuming } p(\mathbf{x}|\boldsymbol{\theta}) \text{ uniform}$$

Maximum likelihood estimate

Approach

Frequentist point of view: parameters are deterministic variables, whose value is unknown and must be estimated.

Determine the parameter value that maximize the likelihood

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\text{argmax}}\, L(\boldsymbol{\theta}|\mathcal{T}) = \underset{\boldsymbol{\theta}}{\text{argmax}}\, p(\mathbf{X}|\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}}{\text{argmax}} \prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta})$$

or

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\text{argmax}}\, L(\boldsymbol{\theta}|\mathcal{T}) = \underset{\boldsymbol{\theta}}{\text{argmax}}\, p(\mathbf{X}, \mathbf{t}|\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}}{\text{argmax}}\, p(\mathbf{x}) \prod_{i=1}^{n} p(t_i|\mathbf{x}_i, \boldsymbol{\theta}) = \underset{\boldsymbol{\theta}}{\text{argmax}} \prod_{i=1}^{n} p(t_i|\mathbf{x}_i, \boldsymbol{\theta})$$

Maximum likelihood estimate

Log-likelihood

$l(\boldsymbol{\theta}|\mathcal{T}) = \ln L(\boldsymbol{\theta}|\mathcal{T})$

is usually preferrable, since products are turned into sums, while $\boldsymbol{\theta}^*$ remains the same (since log is a monotonic function), that is

$$\underset{\boldsymbol{\theta}}{\text{argmax}}\, l(\boldsymbol{\theta}|\mathcal{T}) = \underset{\boldsymbol{\theta}}{\text{argmax}}\, L(\boldsymbol{\theta}|\mathcal{T})$$

Estimate

$$\boldsymbol{\theta}^*_{ML} = \underset{\boldsymbol{\theta}}{\text{argmax}}\, p(\mathbf{X}|\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}}{\text{argmax}} \sum_{i=1}^{n} \ln p(\mathbf{x}_i|\boldsymbol{\theta})$$

or

$$\boldsymbol{\theta}^*_{ML} = \underset{\boldsymbol{\theta}}{\text{argmax}}\, p(\mathbf{X}, \mathbf{t}|\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}}{\text{argmax}} \sum_{i=1}^{n} \ln p(t_i|\mathbf{x}_i, \boldsymbol{\theta})$$

Maximum likelihood estimate

Solution

Solve the system

$$\frac{\partial l(\boldsymbol{\theta}|\mathcal{T})}{\partial \theta_i} = 0 \qquad\qquad i = 1, \ldots, d$$

more concisely,

$$\nabla_{\boldsymbol{\theta}} l(\boldsymbol{\theta}|\mathcal{T}) = \mathbf{0}$$

Prediction

Probability of a new observation $\mathbf{x}$:

$$p(\mathbf{x}|\mathbf{X}) = \int_{\boldsymbol{\theta}} p(\mathbf{x}|\boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathbf{X}) d\boldsymbol{\theta} \approx \int_{\boldsymbol{\theta}} p(\mathbf{x}|\boldsymbol{\theta}^*_{ML}) p(\boldsymbol{\theta}|\mathbf{X}) d\boldsymbol{\theta} = p(\mathbf{x}|\boldsymbol{\theta}^*_{ML}) \int_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathbf{X}) d\boldsymbol{\theta} = p(\mathbf{x}|\boldsymbol{\theta}^*_{ML})$$

Predictive distribution $t|\mathbf{x}$:

$$p(t|\mathbf{x},\mathbf{X},\mathbf{t}) = \int_{\boldsymbol{\theta}} p(t|\mathbf{x},\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X},\mathbf{t})d\boldsymbol{\theta} \approx \int_{\boldsymbol{\theta}} p(t|\mathbf{x},\boldsymbol{\theta}^*_{ML})p(\boldsymbol{\theta}|\mathbf{X})d\boldsymbol{\theta} = p(\mathbf{x}|\boldsymbol{\theta}^*_{ML}) \int_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathbf{X},\mathbf{t})d\boldsymbol{\theta} = p(t|\mathbf{x},\boldsymbol{\theta}^*_{ML})$$

Maximum likelihood estimate

Example 2. Collection $\mathbf{X}$ of n binary events, modeled through a Bernoulli distribution with unknown parameter ϕ

$$p(x|\phi) = \phi^x(1-\phi)^{1-x}$$

Likelihood: $L(\phi|\mathbf{X}) = \prod_{i=1}^n \phi^{x_i}(1-\phi)^{1-x_i}$

Log-likelihood: $l(\phi|\mathbf{X}) = \sum_{i=1}^n (x_i \ln\phi + (1-x_i)\ln(1-\phi)) = n_1 \ln\phi + n_0 \ln(1-\phi)$

where n_0 (n_1) is the number of events $x \in \mathbf{X}$ equal to 0 (1)

$$\frac{\partial l(\phi|\mathbf{X})}{\partial\phi} = \frac{n_1}{\phi} - \frac{n_0}{1-\phi} = 0 \qquad \Longrightarrow \qquad \phi^*{}_{ML} = \frac{n_1}{n_0+n_1} = \frac{n_1}{n}$$

Maximum likelihood estimate

Example 3. Linear regression: collection $\mathbf{X}, \mathbf{t}$ of value-target pairs, modeled as $p(\mathbf{x},t) = p(\mathbf{x})p(t|\mathbf{x},\mathbf{w},\sigma^2)$, with $\mathbf{w} \in \mathbf{R}^d$, $w_0 \in \mathbf{R}$:

- $p(\mathbf{x})$ uniform
- $p(t|\mathbf{x},\mathbf{w},\sigma^2) = \mathcal{N}(\mathbf{w}^T\mathbf{x} + w_0, 1/\beta)$ (β, the inverse of the variance, is the *precision*)

Likelihood: $L(\mathbf{t}|\mathbf{X},\mathbf{w},w_0,\beta) = \prod_{i=1}^n p(t_i|\mathbf{x}_i,\mathbf{w},w_0,\beta) = \prod_{i=1}^n \mathcal{N}(\mathbf{w}^T\mathbf{x}_i + w_0, \beta)$

Log-likelihood:

$$l(\mathbf{t}|\mathbf{X},\mathbf{w},w_0,\beta) = \sum_{i=1}^n \ln p(t_i|\mathbf{x}_i,\mathbf{w},w_0,\beta) = \sum_{i=1}^n \ln\left(\sqrt{\frac{\beta}{2\pi}}e^{-\frac{\beta(\mathbf{w}^T\mathbf{x}_i+w_0-t_i)^2}{2}}\right) = \sum_{i=1}^n \left(-\frac{\beta(\mathbf{w}^T\mathbf{x}_i+w_0-t_i)^2}{2} + \frac{1}{2}\ln\beta - \frac{1}{2}\ln$$

$$= -\frac{\beta}{2}\sum_{i=1}^n (\mathbf{w}^T\mathbf{x}_i + w_0 - t_i)^2 + \frac{n}{2}\ln\beta - \frac{n}{2}\ln(2\pi)$$

Maximum likelihood estimate

Example 4.

$$\frac{\partial}{\partial w_k} l(\mathbf{t}|\mathbf{X},\mathbf{w},w_0,\beta) = -\frac{\beta}{2}\sum_{i=1}^n (\mathbf{w}^T\mathbf{x}_i + w_0 - t_i)x_{ik} \qquad k = 1,\dots,d$$

$$\frac{\partial}{\partial w_0} l(\mathbf{t}|\mathbf{X},\mathbf{w},w_0,\beta) = -\frac{\beta}{2}\sum_{i=1}^n (\mathbf{w}^T\mathbf{x}_i + w_0 - t_i)$$

$$\frac{\partial}{\partial \beta} l(\mathbf{t}|\mathbf{X},\mathbf{w},w_0,\beta) = -\frac{1}{2}\sum_{i=1}^n (\mathbf{w}^T\mathbf{x}_i + w_0 - t_i)^2 + \frac{n}{2\beta}$$

The ML estimation for $\mathbf{w}, w_0$ (linear regression coefficients) is obtained as the solution of the $(d+1, d+1)$ linear system

$$\sum_{i=1}^n (\mathbf{w}^T\mathbf{x}_i + w_0 - t_i)x_{ik} = 0 \qquad k = 1,\dots,d$$

$$\sum_{i=1}^n (\mathbf{w}^T\mathbf{x}_i + w_0 - t_i) = 0$$

The ML estimation for β is obtained by

$$-\frac{1}{2}\sum_{i=1}^{n}(\mathbf{w}^T\mathbf{x}_i + w_0 - t_i)^2 + \frac{n}{2\beta} = 0 \qquad \Longrightarrow \qquad \beta_{ML} = \left(\frac{1}{n}\sum_{i=1}^{n}(\mathbf{w}^T\mathbf{x}_i + w_0 - t_i)^2\right)^{-1}$$

ML and overfitting

Overfitting
Maximizing the likelihood of the observed dataset tends to result into an estimate too sensitive to the dataset values, hence into *overfitting*. The obtained estimates are suitable to model observed data, but may be too specialized to be used to model different datasets.

Penalty functions
An additional function $P(\boldsymbol{\theta})$ can be introduced with the aim to limit overfitting and the overall complexity of the model. This results in the following function to maximize

$$C(\boldsymbol{\theta}|\mathbf{X}) = l(\boldsymbol{\theta}|\mathbf{X}) - P(\boldsymbol{\theta})$$

as a common case, $P(\boldsymbol{\theta}) = \frac{\gamma}{2}\|\boldsymbol{\theta}\|^2$, with γ a *tuning* parameter.

Maximum a posteriori estimate

Idea
Inference through maximum a posteriori (MAP) is similar to ML, but $\boldsymbol{\theta}$ is now considered as a random variable (bayesian approach), whose distribution has to be derived from observations, also taking into account previous knowledge (prior distribution). The parameter value maximizing

$$p(\boldsymbol{\theta}|\mathcal{T}) = \frac{p(\mathcal{T}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathcal{T})}$$

is computed.

Maximum a posteriori estimate

Estimate

$$\begin{aligned}\boldsymbol{\theta}^*_{MAP} &= \operatorname*{argmax}_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathcal{T}) = \operatorname*{argmax}_{\boldsymbol{\theta}} p(\mathcal{T}|\boldsymbol{\theta})p(\boldsymbol{\theta}) \\ &= \operatorname*{argmax}_{\boldsymbol{\theta}} L(\boldsymbol{\theta}|\mathcal{T})p(\boldsymbol{\theta}) = \operatorname*{argmax}_{\boldsymbol{\theta}} \left(l(\boldsymbol{\theta}|\mathcal{T}) + \ln p(\boldsymbol{\theta})\right)\end{aligned}$$

which results into

$$\boldsymbol{\theta}^*_{MAP} = \operatorname*{argmax}_{\boldsymbol{\theta}} \left(\sum_{i=1}^{n} \ln p(\mathbf{x}_i|\boldsymbol{\theta}) + \ln p(\boldsymbol{\theta})\right)$$

or

$$\boldsymbol{\theta}^*_{MAP} = \operatorname*{argmax}_{\boldsymbol{\theta}} \left(\sum_{i=1}^{n} \ln p(t_i|\mathbf{x}_i, \boldsymbol{\theta}) + \ln p(\boldsymbol{\theta})\right)$$

MAP and gaussian prior

Hypothesis

Assume $\boldsymbol{\theta}$ is distributed around the origin as a multivariate gaussian with uniform variance and null covariance.That is,

$$p(\boldsymbol{\theta}) \sim \mathcal{N}(\boldsymbol{\theta}|\mathbf{0}, \sigma^2) = \frac{1}{(2\pi)^{d/2}\sigma^d} e^{-\frac{\|\boldsymbol{\theta}\|^2}{2\sigma^2}} \propto e^{-\frac{\|\boldsymbol{\theta}\|^2}{2\sigma^2}}$$

Inference
From the hypothesis,

$$\boldsymbol{\theta}^*_{MAP} = \underset{\boldsymbol{\theta}}{\text{argmax}}\, p(\boldsymbol{\theta}|\mathcal{T}) = \underset{\boldsymbol{\theta}}{\text{argmax}}\ (l(\boldsymbol{\theta}|\mathcal{T}) + \ln p(\boldsymbol{\theta}))$$
$$= \underset{\boldsymbol{\theta}}{\text{argmax}} \left(l(\boldsymbol{\theta}|\mathcal{T}) + \ln e^{-\frac{\|\boldsymbol{\theta}\|^2}{2\sigma^2}} \right) = \underset{\boldsymbol{\theta}}{\text{argmax}} \left(l(\boldsymbol{\theta}|\mathcal{T}) - \frac{\|\boldsymbol{\theta}\|^2}{2\sigma^2} \right)$$

which is equal to the penalty function introduced before, if $\gamma = \frac{1}{\sigma^2}$

MAP estimate

Example 5. Collection $\mathbf{X}$ of n binary events, modeled as a Bernoulli distribution with unknown parameter ϕ. Initial knowledge of ϕ is modeled as a Beta distribution:

$$p(\phi|\alpha, \beta) = \text{Beta}(\phi|\alpha, \beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \phi^{\alpha-1}(1-\phi)^{\beta-1}$$

Log-likelihood

$$l(\phi|\mathbf{X}) = \sum_{i=1}^{n} (x_i \ln \phi + (1-x_i) \ln(1-\phi)) = n_1 \ln \phi + n_0 \ln(1-\phi)$$

$$\frac{\partial}{\partial \phi} \big(l(\phi|\mathbf{X}) + \ln \text{Beta}(\phi|\alpha, \beta) \big) = \frac{n_1}{\phi} - \frac{n_0}{1-\phi} + \frac{\alpha-1}{\phi} - \frac{\beta-1}{1-\phi} = 0 \qquad \Longrightarrow$$

$$\phi^*_{MAP} = \frac{N_1 + \alpha - 1}{n_0 + n_1 + \alpha + \beta - 2} = \frac{n_1 + \alpha - 1}{n + \alpha + \beta - 2}$$

Note

Gamma function
The function

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

is an extension of the factorial to the real numbers field: in fact, for any integer x,

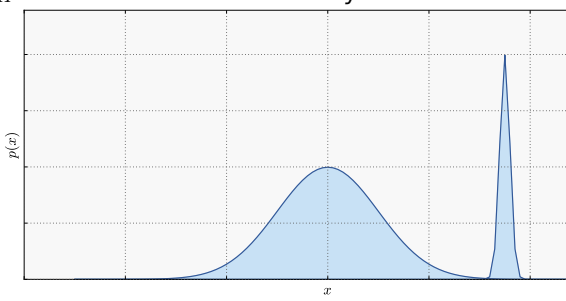
$$\Gamma(x) = (x-1)!$$

Applying bayesian inference

Mode and mean
Once the posterior distribution

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{X})} = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) d\boldsymbol{\theta}}$$

is available, MAP estimate computes the most probable value (mode) $\boldsymbol{\theta}_{MAP}$ of the distribution. This may lead



to inaccurate estimates, as in the figure below:

Applying bayesian inference

Mode and mean
A better estimation can be obtained by applying a fully bayesian approach and referring to the whole posterior distribution, for example by deriving the expectation of $\boldsymbol{\theta}$ w.r.t. $p(\boldsymbol{\theta}|\mathbf{X})$,

$$\boldsymbol{\theta}^* = E_{p(\boldsymbol{\theta}|\mathbf{X})}[\boldsymbol{\theta}] = \int_{\boldsymbol{\theta}} \boldsymbol{\theta} p(\boldsymbol{\theta}|\mathbf{X}) d\boldsymbol{\theta}$$

Bayesian estimate

Example 6. Collection $\mathbf{X}$ of n binary events, modeled as a Bernoulli distribution with unknown parameter ϕ. Initial knowledge of ϕ is modeled as a Beta distribution:

$$p(\phi|\alpha,\beta) = \text{Beta}(\phi|\alpha,\beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\phi^{\alpha-1}(1-\phi)^{\beta-1}$$

Posterior distribution

$$\begin{aligned} p(\phi|\mathbf{X},\alpha,\beta) &= \frac{\prod_{i=1}^{N}\phi^{x_i}(1-\phi)^{1-x_i}p(\phi|\alpha,\beta)}{p(\mathbf{X})} \\ &= \frac{\phi^{N_1}(1-\phi)^{N_0}\phi^{\alpha-1}(1-\phi)^{\beta-1}}{\frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}p(\mathbf{X})} = \frac{\phi^{N_1+\alpha-1}(1-\phi)^{N_0+\beta-1}}{Z} \end{aligned}$$

Hence,

$$p(\phi|\mathbf{X},\alpha,\beta) = \text{Beta}(\phi|\alpha+N_1,\beta+N_0)$$

1 Example: learning in the dirichlet-multinomial model

Language modeling
A *language model* is a (categorical) probability distribution on a vocabulary of terms (possibly, all words which occur in a large collection of documents).

Use
A language model can be applied to predict the next term occurring in a text. The probability of occurrence of a term is related to its information content and is at the basis of a number of information retrieval techniques.

Hypothesis
It is assumed that the probability of occurrence of a term is independent from the preceding terms in a text (*bag of words* model).

Generative model

Given a language model, it is possible to sample from the distribution to generate random documents statistically equivalent to the documents in the collection used to derive the model.

Language model

- Let $\mathcal{T} = \{t_1, \ldots, t_n\}$ be the set of terms occurring in a given collection $\mathcal{C}$ of documents, after *stop word* (common, non informative terms) removal and *stemming* (reduction of words to their basic form).
- For each $i = 1, \ldots, n$ let m_i be the multiplicity (number of occurrences) of term t_i in $\mathcal{C}$
- A language model can be derived as a categorical distribution associated to a vector $\hat{\boldsymbol{\phi}} = (\hat{\phi}_1, \ldots, \hat{\phi}_n)^T$ of probabilities: that is,

$$0 \leq \hat{\phi}_i \leq 1 \quad i = 1, \ldots, n \qquad\qquad \sum_{i=1}^{n} \hat{\phi}_i = 1$$

  where $\hat{\phi}_j = p(t_j|\mathcal{C})$

Learning a language model by ML

Applying maximum likelihood to derive term probabilities in the language model results into setting

$$\hat{\phi}_j = p(t_j|\mathcal{C}) = \frac{m_j}{\sum_{k=1}^{n} m_k} = \frac{m_j}{N}$$

where $N = \sum_{i=1}^{n} m_i$ is the overall number of occurrences in $\mathcal{C}$ after stopword removal.

Smoothing

According to this estimate, a term t which never occurred in $\mathcal{C}$ has zero probability to be observed (black swan paradox). Due to overfitting the model to the observed data, typical of ML estimation.

Solution: assign small, non zero, probability to events (terms) not observed up to now. This is called *smoothing*.

Bayesian learning of a language model

We may apply the dirichlet-multinomial model:

- this implies defining a Dirichlet prior $\text{Dir}(\boldsymbol{\phi}|\boldsymbol{\alpha})$, with $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_n)$ that is,

$$p(\phi_1, \ldots, \phi_n|\boldsymbol{\alpha}) = \frac{1}{\Delta(\alpha_1, \ldots, \alpha_n)} \prod_{i=1}^{n} \phi_i^{\alpha_i - 1}$$

- the posterior distribution of $\boldsymbol{\phi}$ after $\mathcal{C}$ has been observed is then $\text{Dir}(\boldsymbol{\phi}|\boldsymbol{\alpha}')$, where

$$\boldsymbol{\alpha}' = (\alpha_1 + m_1, \alpha_2 + m_2, \ldots, \alpha_n + m_n)$$

  that is,

$$p(\phi_1, \ldots, \phi_n|\boldsymbol{\alpha}') = \frac{1}{\Delta(\alpha_1 + m_1, \ldots, \alpha_n + m_n)} \prod_{i=1}^{n} \phi_i^{\alpha_i + m_i - 1}$$

Bayesian learning of a language model

The language model $\hat{\boldsymbol{\phi}}$ corresponds to the predictive posterior distribution

$$\begin{aligned}\hat{\phi}_j = p(t_j|\mathcal{C}, \boldsymbol{\alpha}) &= \int p(t_j|\boldsymbol{\phi}) p(\boldsymbol{\phi}|\mathcal{C}, \boldsymbol{\alpha}) d\boldsymbol{\phi} \\ &= \int \phi_j \text{Dir}(\boldsymbol{\phi}|\boldsymbol{\alpha}') d\boldsymbol{\phi} = E[\phi_j]\end{aligned}$$

where $E[\phi_j]$ is taken w.r.t. the distribution $\text{Dir}(\boldsymbol{\phi}|\boldsymbol{\alpha}')$. Then,

$$\hat{\phi}_j = \frac{\alpha'_j}{\sum_{k=1}^n \alpha'_k} = \frac{\alpha_j + m_j}{\sum_{k=1}^n (\alpha_k + m_k)} = \frac{\alpha_j + m_j}{\alpha_0 + N}$$

The α_j term makes it impossible to obtain zero probabilities (*Dirichlet smoothing*).

Non informative prior: $\alpha_i = \alpha$ for all i, which results into

$$p(t_j|\mathcal{C}, \boldsymbol{\alpha}) = \frac{m_j + \alpha}{\alpha V + N}$$

where V is the vocabulary size.

A language model can be applied to derive document classifiers into two or more classes.

- given two classes C_1, C_2, assume that, for any document d, the probabilities $p(C_1|d)$ and $p(C_2|d)$ are known: then, d can be assigned to the class with higher probability
- how to derive $p(C_k|d)$ for any document, given a collection $\mathcal{C}_1$ of documents known to belong to C_1 and a similar collection $\mathcal{C}_2$ for C_2? Apply Bayes' rule:

  $$p(C_k|d) \propto p(d|C_k)p(C_k)$$

  the evidence $p(d)$ is the same for both classes, and can be ignored.
- we have still the problem of computing $p(C_k)$ and $p(d|C_k)$ from $\mathcal{C}_1$ and $\mathcal{C}_2$

Computing $p(C_k)$

The prior probabilities $p(C_k)$ ($k = 1, 2$) can be easily estimated from $\mathcal{C}_1, \mathcal{C}_2$: for example, by applying ML, we obtain

$$p(C_k) = \frac{|\mathcal{C}_1|}{|\mathcal{C}_1| + |\mathcal{C}_2|}$$

Computing $p(d|C_k)$

For what concerns the likelihoods $p(d|C_k)$ ($k = 1, 2$), we observe that d can be seen, according to the bag of words assumption, as a multiset of n_d terms

$$d = \{\bar{t}_1, \bar{t}_2, \ldots, \bar{t}_{n_d}\}$$

By applying the product rule, it results

$$\begin{aligned} p(d|C_k) &= p(\bar{t}_1, \ldots, \bar{t}_{n_d}|C_k) \\ &= p(\bar{t}_1|C_k)p(\bar{t}_2|\bar{t}_1, C_k) \cdots p(\bar{t}_{n_d}|\bar{t}_1, \ldots, \bar{t}_{n_d-1}, C_k) \end{aligned}$$

The naive Bayes assumption

Computing $p(d|C_k)$ is much easier if we assume that terms are pairwise conditionally independent, given the class C_k, that is, for $i, j = 1. \ldots, n_d$ and $k = 1, 2$,

$$p(\bar{t}_i, \bar{t}_j|C_k) = p(\bar{t}_i|C_k)p(\bar{t}_2|C_k)$$

as, a consequence,

$$p(d|C_k) = \prod_{j=1}^{n_d} p(\bar{t}_j|C_k)$$

Language models and NB classifiers
The probabilities $p(\bar{t}_j|C_k)$ are available for all terms if language models have been derived for C_1 and C_2, respectively from documents in $\mathcal{C}_1$ and $\mathcal{C}_2$.

Feature selection by mutual information

Feature selection
The set of probabilities in a language model can be exploited to identify the most relevant terms for classification, that is terms whose presence or absence in a document best characterizes the class of the document.

Mutual information
To measure relevance, we can apply the set of mutual informations $\{I_1, \ldots, I_n\}$

$$\begin{aligned} I_j &= \sum_{k=1,2} p(t_j, C_k) \log \frac{p(t_j, C_k)}{p(t_j)p(C_k)} \\ &= \sum_{k=1,2} p(C_k|t_j)p(t_j) \log \frac{p(C_k|t_j)}{p(C_k)} = p(t_j)KL(p(C_k|t_j)||p(C_k)) \end{aligned}$$

here, KL is a measure of the amount of information on class distributions provided by the presence of t_j. This amount is weighted by the probability of occurrence of t_j.

Feature selection by mutual information

Mutual information
Since $p(t_j, C_k) = p(C_k|t_j)p(t_j) = p(t_j|C_k)p(C_k)$, I_j can be estimated as

$$\begin{aligned} I_j &= p(t_j|C_1)p(C_1) \log \frac{p(t_j|C_1)}{p(t_j)} + p(t_j|C_2)p(C_2) \log \frac{p(t_j|C_2)}{p(t_j)} \\ &= \phi_{j1}\pi_1 \log \frac{\phi_{j1}}{\phi_{j1}\pi_1 + \phi_{j2}\pi_2} + \phi_{j2}\pi_2 \log \frac{\phi_{j2}}{\phi_{j1}\pi_1 + \phi_{j2}\pi_2} \end{aligned}$$

where ϕ_{jk} is the estimated probability of t_j in documents of class C_k and π_k is the estimated probability of a document of class C_k in the collection.

A selection of the most significant terms can be performed by selecting the set of terms with highest mutual information I_j.