Foundations

Course of Machine Learning
Master Degree in Computer Science
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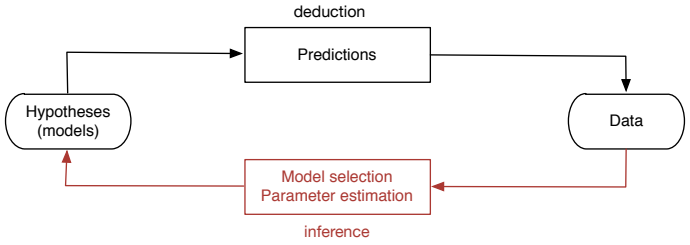
Objectives

Machine learning: inductive approach
Learning of commonalities through analysis of a set of examples (*training set*), which is assumed to be available.

- A training set of n items is represented as a set of input vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$, used to derive a *model*.
- If the purpose is item classification with respect to a collection of predefined classes, the training set also includes a *target* vector $\mathbf{t} = \{t_1, \ldots, t_n\}$, where the class of each training set item is specified.



Types of problems

Supervised learning

- We want to predict, given the values of a set (*features*) of an item **x**, the unknown value of an additional feature *target* of the item
  - Target in **R**: *regression*. Target in $\{1, \ldots, K\}$: *classification*.
- General approach: defined (by means of learning from a set of examples) a *model* of the relation between feature and target values.
- The training set $\mathbf{X}, \mathbf{t}$ includes a feature vector $\mathbf{x}_i = \{x_{i1}, \ldots, x_{im}\}$ and the corresponding target t_i for each item.
- The model could be:
  1. a function $y()$ which, for any item **x**, returns a value $y(\mathbf{x})$ as an estimate of t

2. a probability distribution which associates to each possible value $\overline{y}$ in the target domain, the corresponding probability $p(y = \overline{y}|\mathbf{x})$

Types of problems

Unsupervised learning

- We wish to extract, from a given collection of items *dataset*) $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$, with no target associated, some synthetic information, such as:
  - subsets of similar items *clustering*)
  - the distribution of items in their domain (*density estimation*)
  - the projection, as informative as possible, of items on lower dimensional subspaces, that is, their characterization by means of a smaller set of features *feature selection*, *feature extraction*)
- A suitable *model*, of just the data features, is usually defined and applied also in the case of unsupervised learning.

Reinforcement learning

- We want to identify, in a given framework, a sequence of actions to be performed in order to maximize a certain profit
- As in supervised learning, no examples are given, but an environment is available which returns a profit in correspondance to the execution of any action

Machine learning framework: domains

Domain set $\mathcal{X}$: Set of objects we may wish to label. Each object is modeled as a vector of *features*. The number of features is the *dimensionality* of the problem

Label set $\mathcal{Y}$: Set of possible label values associated to objects in $\mathcal{X}$.

- $\mathcal{Y}$ continuous: *regression*
- $\mathcal{Y}$ discrete: *classification*

Machine learning framework: learner input

Training set $\mathcal{T}$: A set of object-label pairs: $\mathcal{T} = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_n, t_n)\}$. We shall usually denote as $\mathbf{X}$ the matrix of objects (*feature matrix*), that is

$$\mathbf{X} = \begin{pmatrix} - & \mathbf{x}_1 & - \\ & \vdots & \\ - & \mathbf{x}_n & - \end{pmatrix}$$

and as $\mathbf{t}$ the vector of labels (*target vector*), that is

$$\mathbf{t} = \begin{pmatrix} t_1 \\ \vdots \\ t_n \end{pmatrix}$$

Machine learning framework: learner output

Learner output: The learner (an algorithm A) is requested to return, for a given training set $\mathcal{T}$, a *prediction rule* (*classifier*, *regressor*) $A(\mathcal{T}) = h : \mathcal{X} \mapsto \mathcal{Y}$

Machine learning framework: learner evaluation

Training objects generation model: We assume that the objects observed in the training set are sampled from $\mathcal{X}$ according to some probability distribution $\mathcal{D}_1$. That is, for any $\mathbf{x} \in \mathcal{X}$, $p_{\mathcal{D}_1}(\mathbf{x})$ is the probability that $\mathbf{x}$ is the next object sampled in the training set

Training targets generation model: In the general case, we assume the labels associated to the objects in the training set are generated according to a probability distribution $\mathcal{D}_2$ conditional on $\mathcal{X}$. That is, for any $t \in \mathcal{Y}$, $p_{\mathcal{D}_2}(t|\mathbf{x})$ is the probability that the observed label of object $\mathbf{x}$ in the training set is t. For the moment, we shall assume that the relation between object and label is deterministic, that is it exists an unknown function f such that $t_i = f(\mathbf{x}_i)$

Machine learning framework: prediction risk

Given any element $\mathbf{x} \in \mathcal{X}$:

Error: The error of a predictor h derives from the comparison of its prediction $h(\mathbf{x})$ and the correct target label y.

Loss: The comparison is performed by applying a predefined *loss function* $L : \mathcal{Y} \times \mathcal{Y} \mapsto \mathbf{R}$.

Risk of prediction: The error of a prediction $\hat{y}$ is defined in terms of *prediction risk* as given by applying the loss

$$\mathcal{R}(\hat{y}, y) = L(h(\mathbf{x}), y)$$

In the general case when only a probabilistic relation $p_{\mathcal{D}_2}(y|\mathbf{x})$ is assumed between label and target, this corresponds to

$$\mathcal{R}(\hat{y}, \mathbf{x}) = E_{\mathcal{D}_2}[L(\hat{y}, y)] = \int_{\mathcal{Y}} L(\hat{y}, y) \cdot p_{\mathcal{D}_2}(y|\mathbf{x}) dy$$

or, in the case of classification

$$\mathcal{R}(\hat{y}, \mathbf{x}) = E_{\mathcal{D}_2}[L(\hat{y}, y)] = \sum_{y \in \mathcal{Y}} L(\hat{y}, y) \cdot p_{\mathcal{D}_2}(y|\mathbf{x})$$

Bayes estimator

In this framework, the optimal prediction is the one which minimizes the risk,

$$y^*(\mathbf{x}) = \operatorname*{argmin}_{\hat{y}} \mathcal{R}(\hat{y}, \mathbf{x}) = \operatorname*{argmin}_{\hat{y}} E_{\mathcal{D}_2}[L(\hat{y}, y)]$$

that is,

$$y^*(\mathbf{x}) = \operatorname*{argmin}_{\hat{y}} L(\hat{y}, f(\mathbf{x})) \qquad \text{in the simpler case}$$

$$y^*(\mathbf{x}) = \operatorname*{argmin}_{\hat{y}} E_{\mathcal{D}_2}[L(\hat{y}, y)] = \operatorname*{argmin}_{\hat{y}} \int_{\mathcal{Y}} L(\hat{y}, y) \cdot p_{\mathcal{D}_2}(y|\mathbf{x}) dy \qquad \text{in the general case}$$

in the general case, this is denoted as *Bayes estimator*.

However, observe that this approach cannot be applied since both the function f and the distribution $\mathcal{D}_2$ of $p(y|\mathbf{x})$ are assumed unknown.

Machine learning framework: predictor risk

The error of a predictor h is defined in terms of *risk* expected loss on all objects in $\mathcal{X}$

$$\mathcal{R}(h) = E_{\mathcal{D}_1, f}[L(h(\mathbf{x}), f(\mathbf{x}))] = \int_{\mathcal{X}} L(h(\mathbf{x}), f(\mathbf{x})) \cdot p_{\mathcal{D}_1}(\mathbf{x}) d\mathbf{x}$$

In the general case,

$$\mathcal{R}(h) = E_{\mathcal{D}_1,\mathcal{D}_2}[L(h(\mathbf{x}), y)] = \int_{\mathcal{X}} \int_{\mathcal{Y}} L(h(\mathbf{x}), y) \cdot p_{\mathcal{D}_1}(\mathbf{x}) \cdot p_{\mathcal{D}_2}(y|\mathbf{x}) d\mathbf{x} dy$$

Machine learning framework: learner evaluation

Since $\mathcal{D}_1$ and $\mathcal{D}_2$ (or f) are not known, the risk can only be estimated from the data available (the training set $\mathcal{T}$).

Empirical risk: The risk can be estimated from the training set by estimating the expectation of the loss function as the average loss on the set.

$$\overline{\mathcal{R}}_{\mathcal{T}}(h) = \frac{1}{|\mathcal{T}|} \sum_{(x,t)\in\mathcal{T}} L(h(x), t)$$

Machine learning framework: from learning to optimization

The fundamental approach in machine learning is deriving a predictor h which (at least approximately) minimizes the empirical risk computed on the available training set.

A learning problem is then reduced to a minimization problem in some functional space $\mathcal{H}$, the set of all possible predictors h.

$$h^* = \operatorname*{argmin}_{h\in\mathcal{H}} \overline{\mathcal{R}}_{\mathcal{T}}(h)$$

Here, $\mathcal{H}$ is the set of *hypotheses* or *inductive bias*

Issues related to the inductive bias

The choice of the set of hypotheses is an important issue in ML:

- what is the effect of the structure and size of $\mathcal{H}$?
- how to define $\mathcal{H}$ in such a way to make it feasible to compute h^*?

Choice of $\mathcal{H}$

- The hypotheses class $\mathcal{H}$ can be viewed as reflecting some prior knowledge that the learner has about the task
  - a belief that one of the members of the class $\mathcal{H}$ is a low-error model for the task
- A trivial way of pursuing this goal would be to define a very rich class, that is assuming that many possible functions belong to $\mathcal{H}$
- As a limit, $\mathcal{H}$ could be defined just as the set of all functions $f : \mathcal{X} \mapsto \mathcal{Y}$

Choice of $\mathcal{H}$

Problem with large $\mathcal{H}$:

- Assume a binary classification problem with training set $\mathcal{T} = (\mathbf{X}, \mathbf{t})$, with $0/1$ loss

$$L(y,t) = \begin{cases} 0 & \text{if } y = t \\ 1 & \text{otherwise} \end{cases}$$

that is, the loss is 1 if the item is misclassified, 0 otherwise. As a consequence, the risk is the expected number of classification errors, while the empirical risk is the fraction of items in the training set which are misclassified.

- Assume $p(t = 1|\mathbf{x}) = \frac{1}{2}$ for $\mathbf{x} \in \mathcal{X}$, that is, the two classes have same size in the population

Choice of $\mathcal{H}$

Consider the classification function defined as:

$$h(x) = \begin{cases} 1 & \text{if } \mathbf{x} = \mathbf{x}_i \in \mathbf{X}, t_i = 1 \\ 0 & \text{otherwise} \end{cases}$$

that is, h assigns to class 1 all items labeled as 1 in the training set. All other items are classified as 0.

Clearly, the empirical risk here is 0 by definition, but the risk is $\approx \frac{1}{2}$. When applied to a dataset randomly sampled from the population, the quality of h^* is the same of a function which randomly assigns items to classes.

This is called *overfitting*: the classification method behaves well on the training set, but poorly on new data from the population.

Choice of $\mathcal{H}$

With respect to $\mathcal{H}$, the following considerations can be done:

- If $\mathcal{H}$ is too large (complex), *overfitting* may occur: a function which behaves very well on the training set may be available which however performs poorly on new data
- If $\mathcal{H}$ is too small (simple), *underfitting* may occur: no function behaving in a satisfactory way, both on the training set and on new sets of data, is available in $\mathcal{H}$

This is related to the so-called *bias variance tradeoff*

Bias vs variance

The risk associated to the h^*, the predictor which minimizes the empirical risk, can be decomposed in two parts:

$$\mathcal{R}(h^*) = \epsilon_B + \epsilon_V$$

where:

- ϵ_B is the minimum risk achievable by any $h \in \mathcal{H}$: this is only determined by the inductive bias, and independent from the training set. It is a property of the class of hypotheses considered with respect to the prediction task. This is called *bias*
- ϵ_V is the difference between the above minimum risk in $\mathcal{H}$ and the risk associated to the best predictor in $\mathcal{H}$ with respect to the training set: it is related to the fact that empirical risk minimization only provides an estimate of the best predictor achievable for the given inductive bias. It is a measure of how well the predictor computed from a particular training set approximates the best possible one. Its expectation with respect to all possible training sets is a measure of how much a predictor derived from a random training set may result in poorer performances with respect to the best possible one. This is called *variance*

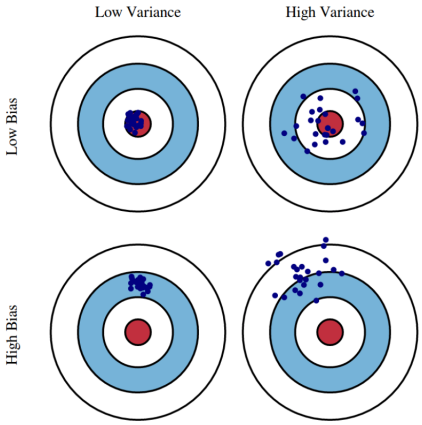
Bias vs variance

The choice of $\mathcal{H}$ is subject to a bias-variance tradeoff: higher bias tend to induce lower variance, and vice versa.

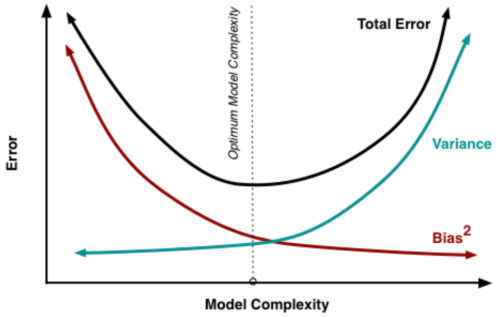
- High bias and low variance implies that all predictors which can be obtained from different training sets tend to behave similarly, with a similar risk (low variance). However, all of them then to behave poorly (high bias), since $\mathcal{H}$ is too poor to include a satisfactory predictor for the task considered. This results into underfitting

- Low bias and high variance implies that lot of predictors are available in $\mathcal{H}$, and among them a good one is usually avaliable (low bias). However, quite different predictors can be obtained from different training sets, which implies that it may easily happen that, while a very good performance can be obtained on the training set, the resulting predictor can behave quite differently and more poorly that the best possible one, which implies overfitting

Bias vs variance



Bias vs variance



Computing h^*

- The optimization required to derive h^* can be complex in the general case, when a function must be derived in a function space.
- Usually, the situation is made easier by considering $\mathcal{H}$ as a space of functions parameterized by a suitable set of coefficients (for example, all polynomials of degree at most d, for a given d): this results in a minimization to be performed over a set of d-dimensional points.
- That is, $\mathcal{H} = \{h_\theta | \theta \in \Theta\}$, where Θ is the coefficients domain and h is a function template, parameterized by elements in Θ
- Minimizing the Empirical risk results into computing

$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmin}} \overline{\mathcal{R}}_{\mathcal{T}}(h_\theta)$$

Computing h^*

- In most cases, $\Theta = \mathbf{R}^d$ for some $d > 0$: in this case, the minimization of $\overline{\mathcal{R}}_{\mathcal{T}}(h_\theta)$ is unconstrained and a (at least local) minimum could be computed setting all partial derivatives to 0

  $$\frac{\partial}{\partial \theta_i}\overline{\mathcal{R}}_{\mathcal{T}}(h_\theta) = 0$$

  that is, setting to zero the gradient of the empirical risk with respect to the vector of parameters θ

  $$\nabla_\theta \overline{\mathcal{R}}_{\mathcal{T}}(h_\theta) = \mathbf{0}$$

- The analytical solution of this set of equations is usually quite hard
- Numerical methods can be applied

Gradient descent

- Gradient descent performs minimization of a function $J(\theta)$ through iterative updates of the current value of θ (starting from an initial value $\theta^{(0)}$) in the opposite direction to the one specified by the current value of the gradient $J'(\theta) = \nabla_\theta J(\theta)$

  $$\theta^{(k+1)} = \theta^{(k)} - \eta \nabla_\theta J(\theta)\ |_{\theta=\theta^{(k)}}$$

  that is, for each parameter θ_i

  $$\theta^{(k+1)} = \theta^{(k)} - \eta \frac{\partial J(\theta)}{\partial \theta_i}\Big|_{\theta=\theta^{(k)}}$$

- η is a tunable parameter, which controls the amount of update performed at each step

Gradient descent and ERM

In Machine learning, minimization of the Empirical Risk is performed, hence gradient descent takes the form

$$\begin{aligned}\theta_i^{(k+1)} &= \theta_i^{(k)} - \eta \frac{\partial}{\partial \theta_i}\frac{1}{|\mathcal{T}|}\sum_{(x,t)\in\mathcal{T}} L(h_\theta(x), t)|_{\theta=\theta^{(k)}} \\ &= \theta_i^{(k)} - \frac{\eta}{|\mathcal{T}|}\sum_{(x,t)\in\mathcal{T}} \frac{\partial}{\partial \theta_i} L(h_\theta(x), t)|_{\theta=\theta^{(k)}}\end{aligned}$$

This is called *batch gradient descent*: observe that, at each step, all items in the training set must be considered

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