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**Machine Learning Construction: implications to cybersecurity**

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Abstract Statistical learning is the process of estimating an unknown probabilistic input-output relationship of a system using a limited number of observations. A statistical learning machine (SLM) is the algorithm, function, model, or rule, that learns such a process; and machine learning (ML) is the conventional name of this field. ML and its applications are ubiquitous in the modern world. Systems such as Automatic target recognition (ATR) in military applications, computer aided diagnosis (CAD) in medical imaging, DNA microarrays in genomics, optical character recognition (OCR), speech recognition (SR), spam email filtering, stock market prediction, etc., are few examples and applications for ML; diverse fields but one theory. In particular, ML has gained a lot of attention in the field of cyberphysical security, especially in the last decade. It is of great importance to this field to design detection algorithms that have the capability of learning from security data to be able to hunt threats, achieve better monitoring, master the complexity of the threat intelligence feeds, and achieve timely remediation of security incidents. The field of ML can be decomposed into two basic subfields: construction and assessment. We mean by construction designing or inventing an appropriate algorithm that learns from the input data and achieves a good performance according to some optimality criterion. We mean by assessment attributing some performance measures to the constructed ML algorithm, along with their estimators, to objectively assess this algorithm. Construction and assessment of a ML algorithm require familiarity with different other fields: probability, statistics, matrix theory, optimization, algorithms, and programming, among others. To help practitioners, specially those of cyberphysical security, to understand the theoretical foundations of ML, before they delve into whole books, we compile the very basics of the first of these two subfields (construction) in this chapter. In addition to explaining the mathematical foundations of the field, we emphasize the intuitive explanation and concepts.

1 Introduction

1.1 Motivation

Consider a sample consisting of a number of cases (observations), where each case is composed of a set of inputs and the corresponding output, all of which will be given to a learning algorithm. Such a sample provides the means for the algorithm to learn during its so-called training (or learning) stage. The goal of this training or learning stage is to understand as much as possible how the output is related to the inputs in these observations, so that when a new set of inputs is given, in the future, the algorithm will have some means of predicting the corresponding output. The above terminology has been borrowed from the field of ML. However, the roots of this problem exists originally in the field of statistical decision theory, where the terminology is somewhat different. In the latter field, the inputs are called the predictors and the output is called the response. When the output is quantitative the learning algorithm is called regression; when the output is categorical or ordered categorical the learning algorithm is called classification. In other communities, the terms input features and output class are used, respectively. The learning process can be defined as follows.

Definition 1. Learning is the process of estimating an unknown input-output dependency or structure of a system using a limited number of observations (Cherkassky and Muller, 1998). □

Statistical learning is crucial to many applications. For example, In cyberphysical security, a network activity must be classified as normal or malicious to avoid any potential threat (Yousef et al, 2021b). This is an example of prediction, regardless of whether it
is done by a network analyst or by a ML algorithm. In either case, the prediction is done based on learning from previous network traffic. The features, i.e., predictors, in this case may be the activity’s IP address, number of scanned ports, duration of connection, etc. The output in this case, i.e., response, is categorical and belongs to the set: \( \mathcal{Y} = \{ \text{normal, malicious} \} \). There are so many such examples, including email filtering and spam detection, fraud detection in financial transactions, etc. All of these examples involve a prediction step based on previous learning.

This chapter reviews some of the regression and classification methods used for predicting a quantitative or categorical response variable, respectively. In addition, the chapter explains basic concepts related to the performance of these methods. The purpose is not to present a survey as much as to introduce the field in an approach that combines both mathematics and intuition, and to explain how the different ingredients relate to each other. We hope this chapter helps practitioners realize the importance of being equipped with the minimum amount of theory before diving deeply into practice.

### 1.2 Notation

Some basic concepts and terminology, necessary for the sequel, must be formally introduced. The world of variables can be categorized into two categories: deterministic variables and random variables. A deterministic variable takes a definite value; the same value will be the outcome if the experiment that yielded this value is rerun. On contrary, a random variable is a variable that takes a non-definite value with a probability value.

**Definition 2.** A random variable \( X \) is a function from a sample space \( S \) into the real numbers \( \mathbb{R} \), that associates a real number, \( x = X(s) \), with each possible outcome \( s \in S \). \( \square \)

Details on the topic can be found in (Casella and Berger, 2002, Ch. 1). For more rigorous treatment of random variables based on measure theoretic approach see Billingsley (1995). Variables can be categorized well, based on value, into: quantitative (or metric), qualitative (or categorical), and ordered categorical. A quantitative variable takes a value on \( \mathbb{R} \), and it can be discrete or continuous. A categorical variable does not necessarily take a numerical value; rather it takes a value from a finite set. E.g., the set \( \mathcal{G} = \{ \text{red, green, blue} \} \) is a set of possible qualitative values that can be assigned to a color. An ordered categorical variable is a categorical variable with relative algebraic relations among the values. E.g., the set \( \mathcal{G} = \{ \text{small, medium, large} \} \) includes ordered categorical values.

Variables in a particular process are related to each other in a certain manner. When variables are random the process is said to be stochastic, i.e., when the inputs of this process have some specified values there is no deterministic value for the output, rather a probabilistic one. The output in this case is a random variable.

Before delving into mathematical details, it is convenient to introduce some commonly used notation. A random variable—or a random vector—is referred to by an upper-case letter, e.g., \( X \). An instance, case, or observation, of that variable is referred to by a lower-case letter, e.g., \( x \). A collection of \( n \) observations for the \( p \)-dimensional random vector \( X \) is collected into an \( n \times p \)-dimensional matrix \( X \) and represented by a bold upper-case \( \mathbf{X} \). A lower-case bold letter \( \mathbf{x} \) is reserved for describing a vector of any \( n \)-observations of a variable, even a tuple consisting of non-homogeneous types. The main notation in the sequel will be as follows: \( \mathbf{tr} : \{ t_i = (x_i, y_i), \ i = 1, \ldots, n \} \) represents an \( n \)-case training dataset, i.e., one on which the learning mechanism will execute to train, or learn. Every observation \( t_i \) of this set represents a tuple of the predictors \( x_i \), represented in a \( p \)-dimensional vector, and the corresponding response variable \( y_i \). All the \( n \) observations \( x_i \)'s may be written in a single \( n \times p \) matrix \( \mathbf{X} \), while all the observations \( y_i \) may be written in a vector \( \mathbf{y} \). Some terminologies may arise from diverse scientific communities. To avoid confusion, the word algorithm can be used exchangeably with function, model, or rule. Using the dataset \( \mathbf{tr} \) for learning, training, or fitting, means replacing, or estimating, the algorithm’s unknown parameters with appropriate values, as will be explained throughout the chapter. Therefore, at the end of this learning process, the final algorithm, function, model, or rule, is called learned, trained, or fitted.

### 1.3 Roadmap

The remainder of this chapter is structured as follows. Sec. 2 introduces the statistical decision theory, which constitutes the foundation of ML. The chapter explains how the ideal (the best performing) ML algorithm can be constructed, either for regression or classification, if we know the probability distribution of the data. Sec. 3 introduces some important parametric models for both regression and classification, and how they are constructed. Sec. 4 introduces the nonparametric and smoothing models, and explains the connection to neural network. These three sections will follow Hastie et al (2009), an excellent comprehensive source for regression and classification methods with practical approaches and illustrative examples. Sec. 5 introduces mathematical optimization and how it is strongly connected to the construction of ML algorithms. This section will follow Boyd and Vandenberghe
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Conditional Distribution of $Y \mid X$

Fig. 1: Conditional expectation of a r.v. $Y$, conditional on a r.v. $X$, is the best regression function under the squared-error loss.

(2004). Sec. 6 discusses, in more detail, the performance of classification rules. It provides the link between the present and the next chapter. Sec. 7 concludes the chapter and provides a general advice for practitioners.

2 Statistical Decision Theory

This section provides an introduction to statistical decision theory, which serves as the foundation of ML. If a random vector $X$ and a random variable $Y$ have a joint probability density function (PDF) $f_{X,Y}(x,y)$ the problem is defined as follows: how to predict the variable $Y$ from an observed value for the variable $X$. In this section we assume having a full knowledge of the joint density $f_{X,Y}$; therefore, there is no learning yet (Definition 1). The prediction function $\eta(X)$ is required to have minimum average prediction error. The prediction error should be defined in terms of some loss function $L(Y, \eta(X))$ that penalizes for any deviation in the predicted value of the response from the correct value. Define the predicted value by:

$$\hat{Y} = \eta(X).$$

(1)

The risk of this prediction function is defined by the average loss, according to the defined loss function:

$$R(\eta) = E L(Y, \hat{Y}).$$

(2)

2.1 Regression

Suppose that the response $Y$ is a quantitative variable. This is the starting point of the statistical branch of regression, where (1) is the regression function. A form should be assumed for the loss function. A mathematically convenient and widely used form is the squared-error loss function:

$$L(Y, \eta(X)) = (Y - \eta(X))^2.$$

(3)

In this case (2) becomes:

$$R(\eta) = \int (Y - \eta(X))^2 dF_{X,Y}(X,Y)$$

$$= E_X E_{Y|X} [(Y - \eta(X))^2 | X].$$

(4a)

(4b)

Hence, (4b) is minimized by minimizing the inner expectation over every possible value for the variable $X$; and the best regression function is then given by:

$$\eta^*(X) = \arg \min_{\eta(X)} \left[ E_{Y|X} [(Y - \eta(X))^2 | X] \right]$$

$$= E_Y [Y | X].$$

(5a)

(5b)
This means that if the joint distribution for the response and predictor is known the best regression function, in the sense of minimizing the risk, is the expectation of the response conditional on the predictor (Fig. 1). In that case the risk of regression in (4b) will be:

\[ R_{\text{min}}(\eta) = R(\eta^*) = E_X \text{Var}[Y|X]. \] (6)

### 2.2 Classification

Recalling (2), and supposing that the response is a qualitative (or categorical) variable, give rise to the classification problem. Now the loss function cannot be the squared-error loss function defined in (3), because this has no meaning for categorical variables. Because \( Y \) may take now a qualitative value from a set of size \( K \) (Sec. 1), the loss function can be defined by the matrix

\[ L(Y, \eta(X)) = \left( c_{ij} \right), \quad 1 \leq i, j < K, \] (7)

where the non-negative element \( c_{ij} \) is the cost, the penalty, or the price, paid for classifying an observation as \( y_j \) when it belongs to \( y_i \). Under this assumption, the risk defined by (2) can be rewritten for the categorical variables to be:

\[ R(\eta) = E_X E_{Y|X} L(Y, \eta(X)) \] (8a)

\[ = E_X \sum_{i=1}^{K} c_{ij} \Pr[Y = y_i|X], \] (8b)

where \( \Pr[Y|X] \) is the probability mass function for \( Y \) conditional on \( X \). Then, the conditional risk for the decision \( y_j \),

\[ R(j, \eta) = \sum_{i=1}^{K} c_{ij} \Pr[Y = y_i|X], \] (9)

is the expected loss when classifying an observation as belonging to \( y_j \), where the expectation is taken over all the possible values of the response. Again, (8b) can be minimized by minimizing the inner expectation to give:

\[ \eta^*(X) = \arg\min_{j} \left[ \sum_{i=1}^{K} c_{ij} \Pr[Y = y_i|X] \right]. \] (10)

Expressing the conditional probability of the response in terms of Bayes law, and substituting in (10) gives:

\[ \eta^*(X) = \arg\min_{j} \left[ \sum_{i=1}^{K} c_{ij} f_X(X|Y = y_i) \Pr[y_i] \right]. \] (11)

The probability \( \Pr[y_i] \) is the prior probability for \( y_i \), while \( \Pr[y_i|X] \) is the posterior probability, i.e., the probability that the observed case belongs to \( y_i \), given the value of \( X \). This is what is called Bayes classification, Bayes decision rule, or alternatively, the Bayes classifier.

Some special cases here may be of interest. The first case is when equal costs are assigned to all misclassifications and there is no cost for correct classification, i.e., \( c_{11} = c_{22} = 0 \) and \( c_{12} = c_{21} = 1 \), which is called the 0-1 cost, or loss function. This reduces (10) to:

\[ \eta^*(X) = \arg\min_{j} \left[ 1 - \Pr[Y = y_j|X] \right] \] (12a)

\[ = \arg\max_{j} \Pr[Y = y_j|X]. \] (12b)

The rule thus is to classify the observed case to the class having maximum posterior probability, which is very intuitive.

Another special case of great interest is binary classification, i.e., the case of \( K = 2 \). In this case (10) reduces to:

\[ \frac{\Pr[y_1|X]}{\Pr[y_2|X]} \begin{cases} \frac{c_{22}}{c_{21}} & y_1 \leq y_2 \\ \frac{c_{11}}{c_{12}} & y_2 < y_1 \end{cases}. \] (13)

Alternatively, this can be expressed as:
The decision taken in (10) has the minimum risk, which can be calculated by substituting back in (8b) to give:

$$R_{\text{min}}(\eta) = \sum_{i=1}^{K} \int_{X} c_{ij} \Pr[y_i] dF_X(X|y_i),$$

(15)

where $j = \eta(X)$, which is the class decision prediction.

For the case where $K = 2$ and $c_{ii} = 0$, $i = 1, 2$, Eq. (15) reduces further to:

$$R_{\text{min}}(\eta) = c_{12} \Pr[y_1] \int_{R_2} dF_X(X|y_1) + c_{21} \Pr[y_2] \int_{R_1} dF_X(X|y_2),$$

(16)

where each of $R_1$ and $R_2$ is the predictor hyperspace over which the optimum decision (13) predicts as class 1 or class 2, respectively. Later, the response variable $Y$ may be referred to $\Omega$ in case of classification; and to follow the notation of Sec. 1, the response of an observation is assigned a value $\omega_i$, $i = 1, \ldots, K$, to express a certain class.

Example 1. Fig. 2 illustrates an example of a binary classification problem, where each class has a two dimensional predictor, with a binormal distribution, with two different mean vectors $\mu_1$, $\mu_2$, and two different covariance matrices $\Sigma_1$, $\Sigma_2$. The best decision surface appears as the intersection of the two PDFs (left). The observations sampled from these two classes, along with this best decision surface, are drawn in the 2D space of the predictors (right). It is interesting, and may be counter-intuitive for some practitioners, to know that although the two distributions are normally distributed, the likelihood ratio (14) is not necessarily normally distributed (Yousef, 2020). For an early development of the theory of binary classification under the multinormal assumption of the class distribution, Fukunaga (1990) is an indispensable resource.

\[ \tag{14} \]

\[ \tag{15} \]

\[ \tag{16} \]

\[ \tag{17a} \]

\[ \tag{17b} \]

2.3 Where Is Learning?

To recap, this section emphasized the fact that there is no distinction between regression and classification from the conceptual point of view. Each minimizes the risk of predicting the response variable for an observation, i.e., a sample case with known predictor(s). If the joint PDF for the response and predictors is known, it is just a matter of direct substitution in the above results, which produces the best regression or classification function that minimizes the risk. If the joint distribution is known but its parameters are not known, e.g., multinormal distribution with unknown mean vector and covariance matrix, a learning process in this case is nothing but estimating those parameters from the dataset $\mathbf{tr}$ by well known methods of statistical inference. However, if the joint distribution is unknown, this gives rise to two different branches of prediction: (1) parametric regression (or classification), where the regression or classification function is modeled and a training sample is used to build that model, (2) and nonparametric regression (or classification), where no particular parametric model is assumed. Subsequent sections in this chapter briefly review some of these techniques, and explain the interesting connections among them.

3 Parametric Regression and Classification

The prediction method introduced in Sec. 2 assumes, as indicated, that the joint PDF of the response and the predictor is known. If such knowledge does not exist all the methods revolve around modeling the regression function (1) in the case of regression or the posterior probabilities in (10) in the case of classification.

3.1 Linear Models (LM)

In LM theory, it is assumed that $Y$ is in the form:

$$Y = EY + e$$

$$= \alpha + X'\beta + e,$$

(17a)\hspace{1cm}(17b)
where the randomness of $Y$ comes only from $e$, the conditional expectation of $Y$ is linear in the predictors $X$, and the random error component $e$ has a zero mean and a constant variance with $X$. The regression function (1) is then written as:

$$\eta(X) = \alpha + X'\beta. \tag{18}$$

More generally, still a LM, it can be rewritten as:

$$\eta(X) = X'_{\text{new}}\beta, \tag{19a}$$

$$X'_{\text{new}} = (f_1(X), \ldots, f_d(X)), \tag{19b}$$

where the predictor $X$ is replaced by a new $d$-dimensional vector, $X_{\text{new}}$, whose elements are scalar functions of the original random vector $X$. The intercept $\alpha$ in (18) may be absorbed in terms of (19a) by setting $f_1(X) = 1$. Eq. (19a) can be seen as equivalent to (18), where $X$ has been transformed to $X_{\text{new}}$, which became the new predictor, on which $Y$ will be regressed.

Now $\beta$ must be estimated, and this point estimation is done for some observed values of the predictor; this is merely the learning process of the LM. Writing the equations for $n$ observed values gives:

$$y = X\beta + e. \tag{20}$$

Eq. (20) can be solved for $\beta$ to give the least sum-of-squares for the components of error vector $e$, which is quite known as the least-squares (LS) problem (Sec. 5). Said differently, it can be solved to minimize the residual sum-of-squares (RSS) between the predicted and the true response:

$$\text{RSS} = e'e$$
$$= (y - X\beta)'(y - X\beta) \tag{21a}$$
$$= \sum (y_i - x'_i\beta)^2, \tag{21b}$$

to give:

$$\hat{\beta} = (XX')^{-1}X'y. \tag{22}$$

Then the prediction $\hat{Y}$ of $Y$ is done by estimating its expectation, which is given by:

$$\hat{Y} = \hat{\eta}(X) = \hat{E}Y = X'\hat{\beta}. \tag{23}$$
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For short notation we always write \( \hat{Y} \) instead of \( \hat{E}[Y] \). The rational behind minimizing the RSS is that \( \frac{\text{RSS}}{n} \) is a good estimate of the mean squared error (MSE), or the expected squared-loss \( E(Y - X'\beta)^2 \). In addition, the latter is differentiable, which leads to the closed-form solution (22).

Nothing up to this point involves statistical inference. This is just fitting a mathematical model using the squared-error loss function. Statistical inference starts when considering the random error vector \( e \) and the effect of that on the confidence interval for \( \hat{\beta} \), and the confidence in predicted values of the response for particular predictor variable, or any other needed inference. All of these important questions are answered by the theory of LMs. *Bowerman and O’Connell (1990)* is a very good reference for an applied approach to LMs, without any mathematical proofs. For a theoretical approach and derivations, the reader is referred to *Christensen (2002)*, *Graybill (1976)*, and *Rencher (2000)*.

It is remarkable that if the joint distribution of the response and the predictor is multinormal, the LM assumption (17b) is an exact expression of the random variable \( Y \). This result arises from the fact that the conditional expectation of the multinormal distribution is linear in the conditional variable. That is, by assuming the joint PDF is multinormal with mean vector \( \mu \) and covariance matrix \( \Sigma \), and given by:

\[
\begin{pmatrix}
Y \\
X
\end{pmatrix} \sim N(\mu, \Sigma), \quad \mu = \begin{pmatrix}
\mu_Y \\
\mu_X
\end{pmatrix}, \quad \Sigma = \begin{pmatrix}
\Sigma_{11} & \Sigma_{12} \\
\Sigma_{21} & \Sigma_{22}
\end{pmatrix},
\]

(24)

then the conditional expectation of \( Y \) on \( X \) is given by:

\[
E[Y|X = x] = \mu_Y + \Sigma_{12}\Sigma_{22}^{-1}(x - \mu_X).
\]

(25)

For more details on the multinormal properties see *Anderson (2003)*.

In the case of classification, the classes are categorical variables but a dummy variable can be used as coding for the class labels. Then a linear regression is carried out for this dummy variable on the predictors. A drawback of this approach is what is called class masking, i.e., if more than two classes are used, one or more can be masked by others and they may not be assigned to any of the observations in prediction. For a clear example of masking see *(Hastie et al, 2009, Sec. 4.2)*.

### 3.2 Generalized Linear Models (GLM)

In a LM, the response variable is directly related to the regression function by a linear expression of the form (17b). In many cases a model can be improved by indirectly relating the response to the predictor through a LM—some times it is necessary, as well, for the classification problem, as will be shown. This is done through a transformation or a *link* function \( g \), by assuming:

\[
g(EY) = X'\beta.
\]

(26)

Now it is the transformed expectation that is modeled linearly. Hence, LMs are merely a special case of the GLM when the link function is the identity function \( g(EY) = EY \).

A very useful link function is the *logit* function defined by:

\[
g(\mu) = \log \frac{\mu}{1 - \mu}, \quad 0 < \mu < 1.
\]

(27)

Through this function the regression function is modeled in terms of the predictor as:

\[
E[Y] = \frac{\exp(X'\beta)}{1 + \exp(X'\beta)},
\]

(28)

which is known as logistic regression (LR). Eq. (28) implies a constraint on the response \( Y \), i.e., it must satisfy \( 0 < E[Y] < 1 \), a feature that makes LR an ideal approach for modeling the posterior probabilities in (10) for the classification problem. Eq. (27) models the two-class problem, i.e., binary classification, by considering the new responses \( Y_1 \) and \( Y_2 \) to be defined in terms of the old responses \( \omega_1 \) and \( \omega_2 \), the classes, as:

\[
Y_1 = \Pr[\omega_1|X],
\]

(29a)

\[
Y_2 = \Pr[\omega_2|X] = 1 - \Pr[\omega_1|X].
\]

(29b)

The general case of the \( K \)-class problem can be modeled using \( K - 1 \) equations, because of the constraint \( \sum_k \Pr[\omega_k|X] = 1 \), as:
\[
\log \frac{\Pr[\omega_k|X = x]}{\Pr[\omega_K|X = x]} = x'\beta_k, \quad k = 1, \ldots, K - 1.
\] (30)

Alternatively, (30) can be rewritten as:

\[
\Pr[\omega_k|X = x] = \frac{\exp(x'\beta_k)}{1 + \sum_{k' = 1}^{K-1} \exp(x'\beta_{k'})}, \quad 1 \leq k \leq K - 1,
\] (31)

\[
\Pr[\omega_K|X = x] = \frac{1}{1 + \sum_{k' = 1}^{K-1} \exp(x'\beta_{k'})}.
\] (32)

The question now is how to estimate \(\beta_k\) \(\forall\ k\). The multinomial distribution for modeling observations is appropriate here. For illustration, consider the case of binary classification; the log-likelihood for the \(n\)-observations can then be written as:

\[
l(\beta) = \sum_{i=1}^{n} \left[ y_i \log \Pr[\omega_1|X_i, \beta] + (1 - y_i) \log(1 - \Pr[\omega_1|X_i, \beta]) \right]
\] (33a)

\[
= \sum_{i=1}^{n} \left[ y_i x_i' \beta - \log(1 + e^{x_i' \beta}) \right].
\] (33b)

To maximize this likelihood, the first derivative is set to zero to obtain:

\[
\frac{\partial l(\beta)}{\partial \beta} = \sum_{i=1}^{n} x_i \left( y_i - \frac{e^{x_i' \beta}}{1 + e^{x_i' \beta}} \right) \text{ set} = 0.
\] (34)

This is a set of \(p\), or \(d\), nonlinear equations, because the vector \(X\) can be either the original predictor \((x_1, \ldots, x_p)'\) or any transformation \((f_1(X), \ldots, f_d(X))'\) as in (19b). These equations can be solved by iterative numerical methods like the Newton-Raphson algorithm. Finding the optimal values of these parameters is one of the optimization problems (Sec. 5), whose solution exists in many software packages. For more details with numerical examples see (Hastie et al, 2009, Sec. 4.4) or (Casella and Berger, 2002, Sec. 12.3).

It can be noted that (33a) is valid under the assumption of the following general distribution:

\[
f(X) = \phi(\theta, \gamma) h(X, \gamma) \exp(\theta'_i X),
\] (35)

with probability \(p_i, i = 1, 2, p_1 + p_2 = 1\), which is the exponential family. So LR is no longer an approximation for the posterior class probability if the distribution belongs to the exponential family. For insightful comparison between LR and the Bayes classifier under the multinormal assumption see Efron (1975).

It is very important to mention that LR, and all subsequent classification methods, assume equal a priori probabilities. Then the ratio between the posterior probabilities will be the same as the ratio between the densities that appear in (11). Hence, the estimated posterior probabilities from any classification method are used in (11) as if they are the estimated densities.

### 3.3 Nonlinear Models

The link function in the GLM is modeled linearly in the predictors (26). Consequently, the response variable is modeled as a nonlinear function. In contrast to the LMs described in Sec. 3.1, in nonlinear models the response can be modeled nonlinearly right from the beginning, without the need for a link function.

### 4 Nonparametric Regression and Classification

In contrast to parametric regression, the regression function (1) is not modeled parametrically; i.e., there is no particular parametric form to be imposed on the function. Nonparametric regression is a versatile and flexible method of exploring the relationship of two variables. It may appear that this technique is more efficient than the LMs, but this is not the case. LMs and nonparametric models can be thought of as two different techniques in the analyst’s toolbox. If there is an a priori reason to believe that the data
follow a parametric form, then LMs or parametric regression in general may provide an argument for an optimal choice. If there is no prior knowledge about the parametric form the data may follow, or no prior information about the physical phenomenon that generated the data, there may be no choice other than nonparametric regression. There are many nonparametric techniques proposed in the statistical literature. What was said above, when comparing parametric and nonparametric methods, can also be said when comparing nonparametric methods to each other. None can be preferred across all situations (Sec. 7).

4.1 Smoothing Techniques

Smoothing is a tool for summarizing, in a nonparametric way, a trend between a response and a predictor such that the resulting relationship is less variable than the original response, hence the name smoothing. When the predictor is uni-dimensional, the smoothing is called scatter-plot smoothing. In this section, some methods used in scatter-plot smoothing are considered. These smoothing methods do not succeed in higher dimensionality. This is one bad aspect of what is called the curse of dimensionality (Sec. 6.5).

4.1.1 $K$-Nearest Neighbor (KNN)

The regression function (1) is estimated in the KNN approach by:

$$\eta(x) = \frac{1}{n} \sum_{i=1}^{n} y_i W_i(x),$$  \hspace{1cm} (36)

$$W_i(x) = \begin{cases} n/K & i \in J_x = \{i : x_i \in N_K(x)\} \\ 0 & \text{otherwise} \end{cases},$$  \hspace{1cm} (37)

where $N_K(x)$ is the set consisting of the nearest $K$ points to the point $x$. In words, this technique approximates the conditional mean, i.e., the regression function that gives minimum risk, by local averaging the response $Y$.

In the case of classification, the posterior probability is estimated by:

$$\Pr[\omega_j|x] = \frac{1}{n} \sum_{i=1}^{n} I_{\omega_i=\omega_j} W_i(x),$$  \hspace{1cm} (38)

and $I$ is the indicator function defined by:

$$I_{\text{cond}} = \begin{cases} 1 & \text{cond = True} \\ 0 & \text{cond = False} \end{cases}.$$  \hspace{1cm} (39a)

That is, replacing the continuous response in (36) by an indicator function for each class given each observation. So, the posterior probability is approximated by a frequency of occurrence in a $K$-point neighborhood.

A single-nearest-neighbor method (1-NN) is a special case of the KNN method, where $K = 1$. It can be thought of as narrowing the window $W$ on which regression are carried out. In effect, this makes the regression function or the classifier more complex because it is trying to estimate the distribution at each point, which results in decreasing the bias and increasing the variance (Sec. 6.4).

4.1.2 Kernel Smoothing

In this approach, a kernel smoothing function $\kappa$ is assumed. This means that a weighting and convolution (or mathematical smoothing) is carried out for the points in the neighborhood of the predicted point according to the chosen kernel function. Formally this is expressed as:

$$\eta(x) = \sum_{i=1}^{n} y_i \kappa \left( \frac{x-x_i}{h_x} \right) / \sum_{i=1}^{n} \kappa \left( \frac{x-x_i}{h_x} \right).$$  \hspace{1cm} (40)

Choosing the bandwidth $h_x$ of the kernel function is not an easy task. Usually, it is done numerically by cross validation (as explained in the next chapter). It is worth remarking that KNN smoothing is nothing but a kernel smoothing for which the kernel function is an unsymmetrical flat window spanning the range of the $K$-nearest neighbors of the point $x$. The kernel (40) is called Nadaraya-Watson kernel. Historically, and interestingly, Parzen (1962) first introduced the window method density function estimation; his work was pioneered later by Nadaraya (1964) and Watson (1964) in regression.
4.2 Additive Models (AM)

Recalling (19), and noticing that the function $f_i(X)$ is a scalar parametric function of the whole predictor, show that LMs are parametric AMs. By dropping the parametric assumption and letting each scalar function be a function of just one element of the predictor, i.e., $X_i$, allows defining a new nonparametric regression method, namely AMs, as:

$$\eta(x) = \alpha + \sum_{i=1}^{p} f_i(X_i),$$

where the predictor is of $p$ dimensions. The response variable itself, $Y$, is modeled as in (17a) by assuming zero mean and constant variance for the random component $\epsilon$. Then, $f_i(X_i)$ is fit by any smoothing method defined in Sec. 4.1. Every function $f_i(X_i)$ fits the value of the response minus the contribution of the other $p-1$ functions from the previous iteration. This is called the back-fitting algorithm (Hastie and Tibshirani, 1990, Sec. 4.3)

4.3 Generalized Additive Models (GAM)

GAMs can be developed in a way analogous to how GLMs were developed above, i.e., by working with a transformation of the response variable, hence the name generalized additive models. Eq. (41) describes the regression function as an AM; alternatively it can be described through another link function:

$$g(\eta(x)) = \alpha + \sum_{i=1}^{p} f_i(X_i).$$

Again, if a logit function is used the model can be used for classification exactly as was done in the case of GLMs. Rewriting the score equations (34) for the GAM, using the posterior probabilities as the response variable, produces the nonparametric classification method using the GAM. Details of fitting the model can be found in (Hastie and Tibshirani, 1990, Sec. 4.5 and Ch. 6).

4.4 Projection Pursuit Regression (PPR)

PPR, introduced by Friedman and Stuetzle (1981), is a direct attack on the dimensionality problem, since it considers the regression function as a summation of terms, each of which is a function of a projection of the whole predictor onto a direction (specified by some unit vector). Formally it is expressed as:

$$\eta(x) = \sum_{i=1}^{M} g_i(\alpha' x).$$

The function $g_i$, for every selection of the direction $\alpha_i$, is to be fit by a smoother in the new single variable $\alpha_i' x$. It should be noted that (43) assumes that the function $g_i(\alpha'_ix)$, named the ridge function, is constant along any direction perpendicular to $\alpha_i$. Fitting the model is done by iteratively finding the best directions $\alpha_i$’s that minimize(s) the RSS, hence the name pursuit. Details of fitting the model and finding the best projection directions can be found in Friedman and Stuetzle (1981) and Hastie et al (2009).

In (43), by deliberately setting each unit vector $\alpha_i$ to have zero components except $\alpha_{ii} = 1$, reduces the PPR to AM. Moreover, and interestingly as well, introducing the logit link function to the regression function $\eta(x)$ in (43) suits the classification problem exactly as was done in the GAM. This turns out to be exactly the same as the single-hidden-layer NN, as will be presented in the next section.

4.5 Neural Networks (NN)

The field of NN has been evolving, since its start in the engineering community around 1950s, until we reached now the era of deep neural networks (DNN). A single-hidden-layer NN can be considered as a process for modeling the output in terms of a linear combination of the inputs. The set of $p$ input features, i.e., the predictor components $X_1, \ldots, X_p$, are weighted linearly to form a new set of $M$ arguments, $Z_1, \ldots, Z_M$, that go through the sigmoid function $\sigma$, which can have different values of steepness, or learning rate. Fig. 3 illustrates a single-hidden-layer NN with its architecture (left), and a plot of its sigmoid function with different learning rates (right). The output of the sigmoid function accounts for a hidden layer consisting of $M$ intermediate values. Then
Fig. 3 A single-hidden-layer NN. The architecture that reflects Eq. (44) (left), and the sigmoid function with different learning rates $a$ (right).

these $M$ hidden values are in turn weighted linearly to form a new set of $K$ arguments that go through the final output functions, whose output is the response variables $Y_1, \ldots, Y_K$. This can be expressed mathematically in the form:

$$Z_m = \sigma(\alpha_m + \alpha'_m X), \quad m = 1, \ldots, M,$$

$$\sigma(\mu) = \frac{1}{1 + e^{-\mu}},$$

$$Y_k = f_k \left( \beta_0 + \sum_{m=1}^{M} \beta_{mk} Z_m \right), \quad k = 1, \ldots, K. \quad (44c)$$

Eq. (44c) shows that if the function $f$ is chosen to be the identity function, i.e., $f(\mu) = \mu$, the NN is simply a special case of the PPR method defined in (43), where the sigmoid function has been explicitly imposed on the model rather than being developed by any smoothing mechanism as in PPR. This is what is done when the output of the network is quantitative. When it is categorical, i.e., the case of classification, the function $f$ can be simply modeled as:

$$f_k(\mu_k) = e^{\mu_k} / \sum_{k'=1}^{K} e^{\mu_{k'}}. \quad (45)$$

In this case each output node models the posterior probability $Pr[\omega_k | X]$, which is exactly what is done by the LR link function defined in (27). Again, the model will be an extension to the GAM as defined at the end of Sec. 4.4. Although equations (44) are indeed parametric, we list NN in this section for the strong connection to the AM, GAM, and PPR that were just explained. Excellent references for the early basics and foundations of NN are Bishop (1995) and Ripley (1996). We conclude this section by quoting the following statement from Hastie et al (2009):

"There has been a great deal of hype surrounding neural networks, making them seem magical and mysterious. As we make clear in this section, they are just nonlinear statistical models, much like the projection pursuit regression model discussed above."

5 Optimization

Optimization serves an amazing variety of practical problems: e.g., optimizing power consumption in electrical stations, optimizing overall budget in project management, and most importantly to us in this chapter optimizing ML algorithms to provide the best performance. In this section, we will provide a very basic introduction to optimization and its strong connection to the construction of ML algorithms.
5.1 Introduction

The mathematical optimization problem (MOP) is an abstraction of how to make the “best” possible choice of some vector $\beta$ under some constraints. These constraints represent a set of trim requirements, or specifications, that limits the possible choices of this vector. The objective function of this problem represents the cost, or loss, to minimize, or the utility to maximize, for each vector $\beta$, and this what makes that value of $\beta$ the “best” possible choice. This is formalized in the following definition.

**Definition 3.** A mathematical optimization problem has the form:

$$
\begin{align*}
\text{minimize} & \quad f_0(\beta) \\
\text{subject to:} & \quad f_i(\beta) \leq 0, \quad i = 1, \ldots, m, \\
& \quad h_i(\beta) = 0, \quad i = 1, \ldots, l,
\end{align*}
$$

where

- $\beta = (\beta_1, \ldots, \beta_p) \in \mathbb{R}^p$, (optimization variable)
- $f_0 : \mathbb{R}^p \mapsto \mathbb{R}$, (objective (cost) function)
- $f_i : \mathbb{R}^p \mapsto \mathbb{R}$, (inequality constraints (functions))
- $h_i : \mathbb{R}^p \mapsto \mathbb{R}$, (equality constraints (functions))

$$
D = \bigcap_{i=1}^m \text{dom} f_i \cap \bigcap_{i=1}^l \text{dom} h_i
$$

(domain of constraints: feasible set)

$$
\beta^* : \{ \beta \mid \beta \in \mathbb{R}^p \land f_i(\beta) \leq 0 \land h_i(\beta) = 0 \}
$$

(solution)

where the solution $\beta^*$ is called the optimizer (or minimizer). $\square$

The problem aims at minimizing a mathematical function, under some constraints. From definition 3, it is clear that minimizing $f_0$ is the same problem as maximizing $-f_0$; the constraints $f_i \leq 0$ are equivalent to $-f_i \geq 0$; the constraints $f_i \leq 0$ are equivalent to $f_i \leq b_i$, where $b_i$ can be simply absorbed into $f_i$; and, finally, $m = l = 0$ is the case of unconstrained problem with global minimization.

**Example 2.** The is a very basic example of an MOP in a single dimension, with a single constraint:

$$
\begin{align*}
\text{minimize} & \quad f_0(\beta) = \beta^2 \\
\text{subject to:} & \quad \beta \leq 2, \\
& \quad 1 \leq \beta.
\end{align*}
$$

It is clear that the minimizer is $\beta^* = 1$; however, the minimizer for the unconstrained problem is $\beta^* = 0$ (Fig. 4). $\square$

**Example 3.** (Chong and Zak, 2013, Ex. 20.1, P. 454): This example shows how the MOP may not be as simple as finding the derivatives:
Fig. 5 A simple objective function in two dimensions (the colored surface, shown along with its contours drawn in black), with two constraints (the red lines). Although the surface has no global minimum, the constrained problem does have.

![Graph of a simple objective function in two dimensions with constraints.]

Fig. 6 ML and MOP. A training dataset of three observations, for a regression problem with a single feature, to be fitted by a linear model having only two parameters $\beta_0$ and $\beta_1$ (left). The RSS of this model is the objective function, of these two parameters, to be minimized (right). The red point on the surface is the value (not the minimum yet), at some initial values of $\beta_0$ and $\beta_1$ that corresponds to the intercept and slope of the line on the left.

\[
\begin{align*}
\minimize_{\beta} & \quad f_0(\beta_1, \beta_2) = (\beta_1 - 1)^2 + \beta_2 - 2 \\
\text{subject to:} & \quad \beta_2 - \beta_1 = 1, \\
& \quad \beta_1 + \beta_2 \leq 2.
\end{align*}
\]

This 2D objective function, along with the constraints, are illustrated in Fig. 5. It is obvious that the function has no global minimizer ($\partial f_0 / \partial \beta_2 = 1 \neq 0$). After setting the constraints, it is quite easy to see that $f_0(\beta_2 = \beta_1 = 1) = (\beta_1 - 1)^2 + (\beta_1 - 1)$ attains a minima at $\beta_1 = 1/2$, and hence, the minimizer is $\beta^* = (1/2, 3/2)^t$.

5.2 Connection to Machine Learning

As explained earlier in this chapter, all parametric ML algorithms, e.g., LM, LR, SVM, NN, DNN, etc., include parameters that need to be replaced by numerical values. This is performed with the help of a dataset that is called a training dataset. The following simple example illustrates the connection between ML and MOP, and relates both to the title of the present chapter.
Fig. 7 100 pairs of true AUC vs. true MSE. Each pair is obtained from training the same NN, to minimize the RSS, on a new training datasets, then testing on a very large testing dataset to mimic the population. Although there is an obvious trend of getting a high AUC with low MSE, it is not a guaranteed behaviour for each training dataset.

Example 4 (Machine Learning: construction). Suppose that we have a strong belief that the best regression function for a particular problem is the LM $Y = \beta_0 + \beta_1 X$. Then, for a given training dataset $\text{tr} : \{t_i = (x_i, y_i), i = 1, \ldots, n\}$, we need to minimize the RSS of this model on this dataset. This is a typical MOP, which can be formalized as:

$$\min_{\beta_0, \beta_1} \sum_{i=1}^{n} (\beta_0 + \beta_1 x_i - y_i)^2, \ (x_i, y_i) \in \text{tr}.$$

Fig. 6 illustrates a dataset of only three observations ($n = 3$), along with a straight line of initial values of the parameters $\beta_0, \beta_1$, all drawn in the feature space (left). The objective function to be minimized (the RSS) is drawn as a function of the two parameters $\beta_0, \beta_1$ (right). Each pair of values of $\beta_0, \beta_1$ results in a new line (fitted model) in the feature space, and a new point on the surface of the objective function in the parameter space. The solution of this MOP is the vector $\beta^* = (\beta_0, \beta_1)$ that minimizes the objective function, which fortunately for linear models has a closed-form solution given earlier in Eq. (22).

Departing from the previous example, in the following few paragraphs we will emphasize important concepts. The example demonstrated the relationship between: (1) the ML model, along with the training dataset, in the feature space, and (2) the objective function, which should be minimized, in the parameter space. All other ML models, whether for regression or classification, have parameters that should be replaced, tuned, or estimated, to optimize (minimize or maximize) some objective function. Ideally, this objective function should be a good estimator for the same intended performance measure of the model, not for any other performance measure. However, some mathematical difficulties may preclude this ideal practice, as will be seen next.

In Example 4, the objective function to be minimized was the RSS, which minimizes $\text{RSS}/n$, an estimator of the MSE. However, in some circumstances it is very difficult mathematically to optimize the targeted performance measure. In such cases, another performance measure is optimized, because of the tractability of its mathematical formalization, hoping that the solution optimizes, as well, the targeted performance measure. Figure 7 illustrates this fact for a very simple four-neuron single-layer NN, trained on a simulated two-class univariate normal dataset. The NN is required to achieve a high AUC (a performance measure that will be explained in Sec. 6); however, because its estimator is non differentiable, and therefore is very hard to maximize using conventional mathematical approaches, the NN is trained to minimize the RSS, instead. For illustration, the NN is trained on 100 different training datasets, and tested after each training on a very large testing dataset to provide a good estimate of the true AUC and MSE. The figure shows the 100 pairs of values of these two performance measures, with a general trend of exhibiting a high AUC with a low MSE. However, some instances exhibited a low MSE (good performance) associated with a low AUC (bad performance).

Another important fact to emphasize is that all of the model’s parameters that are estimated during the learning process are functions of the training dataset. Hence, the following facts hold: these parameters are random variables, the model is a random model, the objective function is a random function, and the minimum value of this objective function, which is the model optimal performance, is a random variable (as will be detailed in Sec. 6); all will vary if the training dataset varies.

To recap, example 4 demonstrated how LM, one of the ML models explained in this chapter, represents an MOP whose solution fortunately can be found in closed form. Other ML models belong to a class of MOP that is difficult to solve; DNN is an example.
In the next section, we will provide a very short account of the taxonomy of the MOP to show its different types and the connection of each of these types to ML.

5.3 Types of MOP

According to the nature of the objective function and its constraints, the MOP can be classified into one of these nested classes:

Linear ⊂ Quadratic ⊂ Convex ⊂ Nonlinear.

For each of these classes, several questions arise: (1) is there a closed-form solution? (2) if not, is there a numerical solution? (3) if yes, is it guaranteed? (4) what are the ML models that belong to this class? In the following subsections, we discuss very briefly each of these classes, and provide some answers to these questions. It is important to emphasize that although these classes are mathematically nested—in the very strict sense that any linear is quadratic, any quadratic is convex, and any convex is nonlinear—the solution techniques for each class are quite different from others. The solution techniques for these classes vary between: closed-form, numerical (e.g., Newton’s methods, gradient descent, etc.), or even intelligent-based methods (e.g. genetic algorithms, particle swarm, etc.).

5.3.1 Linear Programming

Definition 4. A linear programming problem is an MOP with an objective and all constraints are linear:

\[
\begin{align*}
\text{minimize} & \quad f_0(\beta) = c' \beta \\
\text{subject to:} & \quad a_i' \beta \leq b_i, \quad i = 1, \ldots, m, \\
& \quad h_i' \beta = g_i, \quad i = 1, \ldots, l.
\end{align*}
\]

Example 5 (Chebyshev minimization). The MOP:

\[
\begin{align*}
\text{minimize} \quad f_0(\beta) = \max_{i = 1, \ldots, n} |y_i - x_i' \beta|,
\end{align*}
\]

can be understood in terms of ML terminology as minimizing the maximum possible error, measured in absolute deviance between the true response value \( y_i \) and the predicted value \( x_i' \beta \). This should be contrasted with the least-squares MOP of the LM (as illustrated in example 4 and will be more detailed in Sec. 5.3.2 below) in two important aspects: (1) the error is measured in terms of absolute deviance rather than squared difference. (2) the objective function here focuses only on the single observation that achieves the maximum error rather than summing over all observations. After little manipulations, the problem can be reduced, and found to be equivalent, to the following:

\[
\begin{align*}
\text{minimize} & \quad t \\
\text{subject to:} & \quad x_i' \beta - t \leq y_i, \quad i = 1, \ldots, n, \\
& \quad -x_i' \beta - t \leq -y_i, \quad i = 1, \ldots, n,
\end{align*}
\]

which is a typical linear programming problem, per definition 4.

In general, there is no closed-form solution to the linear programming problems. However, there exists a set of very robust, reliable, and computationally effective methods of numerical solutions: e.g., Dantzig’s simplex and interior point that can solve problems with several thousands of variables.

5.3.2 Least-Squares (LS) Problems

Definition 5. A LS problem is an MOP with no constraints (i.e., \( m = l = 0 \)), and an objective in the form:

\[
\begin{align*}
\text{minimize} f_0(\beta) = \sum_{i=1}^{n} (x_i' \beta - y_i)^2 = \|X_{n \times p} \beta_{p \times 1} - y_{n \times 1}\|^2.
\end{align*}
\]
Example 6 (LM). The linear models for regression, discussed in Sec. 3.1 and Example 4, is a typical example for the LS problem, where the solution is given in the closed form by \( \beta = (X'X)^{-1}X'y \). □

The algorithms for finding the matrix inversion and matrix multiplication in this closed-form solution exist in many scientific computing software, and this technology is quite mature even for thousands of variables.

There is a more elaborate version of the LS problem that is called weighted LS. This type of problem appears in ML, e.g., when more emphasis is required on some observations than others:

\[
\min_{\beta} f_0(\beta) = \sum_{i=1}^{n} w_i (x_i' \beta - y_i)^2,
\]

or when it is required to penalize for using extra parameters to guard against overfitting (Sec. 6.4), an approach known as regularization:

\[
\min_{\beta} f_0(\beta) = \sum_{i=1}^{n} (x_i' \beta - y_i)^2 + \rho \sum_{j=1}^{p} \beta_j^2.
\]

It is quite easy to show that both problems can be solved as LS problem, per definition 5.

5.3.3 Convex Optimization

Definition 6. A convex optimization problem is an MOP with an objective and all constraints are convex:

\[
\begin{align*}
\min_{\beta} & \quad f_0(\beta) \\
\text{subject to:} & \quad f_i(\beta) \leq 0, \quad i = 1, \ldots, m, \\
& \quad h_i(\beta) = 0, \quad i = 1, \ldots, l, \\
& \quad f_i(a\alpha + b\beta) \leq af_i(\alpha) + bf_i(\beta), \quad a + b = 1, \quad 0 \leq a, b, \quad 0 \leq i \leq m, \\
& \quad h_i(\beta) = \epsilon_i \beta + d_i, \quad 0 \leq i \leq p.
\end{align*}
\]

Example 7 (Lasso Regression). Similar to the penalized LS problem, lasso regression minimizes the RSS; however, it does so with an \( L_1 \) penalty rather than the \( L_2 \) of the LS problem. The problem is formalized as:

\[
\begin{align*}
\min_{\beta} & \quad \sum_{i=1}^{n} (y_i - x_i' \beta)^2 \\
\text{subject to:} & \quad \sum_{j=1}^{p} |\beta_j| \leq t,
\end{align*}
\]

which can be shown to be equivalent to the MOP:

\[
\min_{\beta} f_0(\beta) = \sum_{i=1}^{n} (y_i - x_i' \beta)^2 + \rho \sum_{j=1}^{p} |\beta_j|,
\]

The latter, in contrast to the LS penalization, has no closed-form solution because of the difficulty introduced by the non-differentiable term \(|\beta_j|\). However, the numerical solution is quite feasible and reliable as all convex optimization problems are. □

The numerical solution of a convex optimization problem is well established through the methods of interior point, although no closed-form solution exists. Problems with thousands of variables can be solved robustly as in linear programming problems. In addition, many problems are initially formulated, then with some mathematical manipulation they can be transformed to a solvable convex problem.

5.3.4 Nonlinear Optimization

Definition 7. A nonlinear optimization problem is an MOP with objective and constraint functions are nonlinear □
Fig. 8 A plot of a 3D function (Chong and Zak, 2013, Ex. 14.3, P.290): $f(\beta_0, \beta_1) = 3(1 - \beta_0)^2 e^{-\beta_0^2} - (\beta_1 + 1)^2 - 10e^{-\beta_0^2} - \beta_1^2 \left(-\beta_0^3 + \frac{2\beta_0}{3} - \beta_1^2\right) - \frac{1}{5} e^{-\beta_0^2 - \beta_1^2}$ that shows several minima, maxima, and saddle points.

Example 8. A nonlinear objective function, just in two dimensions, with several minima, maxima, and saddle points, is illustrated in Fig. 8. A NN, or in its more complex form, a DNN with several layers, can have hundreds of millions of parameters, not only two as illustrated in the figure! □

The nonlinear optimization problems can be very hard to solve, even for simple-looking problems in few parameters (variables). Several approaches exist for solving the problem; these approaches can be divided into two main categories: numerical methods and computational intelligence, as briefly explained in the following two paragraphs, respectively.

Finding the minima or the maxima of a function numerically is a well known topic in mathematics and numerical analysis. However, the challenge of nonlinear optimization, especially for problems like DNN, remains in the computational complexity that grows exponentially with the dimensions of the objective function, the matter that makes it almost impossible to find a global minimum. Alternatively, finding a local minimum is a practical compromise, although it does not guarantee converging to the global one. Local minimization starts at a point in the parameter space (usually is selected randomly, or by other criteria determined by the numerical algorithm) then the space is navigated, and guided by the multi-dimensional derivatives (with respect to the parameters) of the objective function. All the well known methods, starting form Newton’s method to the most recent approaches used for DNN, e.g., stochastic gradient descent (SGD), belong to this category. It is obvious that the initial starting point in the parameter space heavily affects the convergence process and the final solution.

The term computational intelligence was first coined early by Bezdek (1992, 1994):

“A system is computationally intelligent when it: deals only with numerical (low-level) data, has a pattern recognition component, and does not use knowledge in the AI (Artificial Intelligence) sense; and additionally, when it (begins to) exhibit (i) computational adaptivity; (ii) computational fault tolerance; (iii) speed approaching human-like turnaround, and (iv) error rates that approximate human performance.”

Since that time, the term computational intelligence (CI) has been accepted as a generic term to the field that combines NNs, fuzzy logic, and evolutionary algorithms (Schwefel et al., 2003; Zimmermann et al., 2002). Later, the area of swarm detection was considered as a peer paradigm to the other three mentioned above Engelbrecht (2002).

6 Performance

From what has been early discussed at the beginning of this chapter, there is not any conceptual difference between regression and classification for the problem of supervised learning. Abstractly, both aim to achieve the minimum risk (2) under a certain loss function, for predicting a response, from a particular predictor. Although risk is a very obvious performance measure for assessing ML algorithms, we will elaborate in this section and show how we can depart and define other important performance measures, e.g., the individual error components, ROC, and AUC. It is must be noted that what will be defined in this section is the parametric form (also known as the true performance or the population performance), which can only be calculated if the posterior probabilities are known. On the contrary, if the posterior probabilities are not known all performance measures can be estimated from a given dataset, called the testing dataset, using appropriate estimators. If the testing dataset is infinitely large, i.e. testing on the population, the estimated performance will converge to the true performance. Performance estimation and different estimators are discussed in the next chapter.
6.1 Error Components

We will elaborate on the special case of binary classification, with no cost on correct classification ($c_{ii} = 0$, $i = 1, 2$), which is of great interest in many applications. In this case, the risk of each classifier is reduced to (16), which can be rewritten as:

$$R_{\min} = c_{12}P_1e_1 + c_{21}P_2e_2,$$  \hspace{1cm} (46)

where $e_1$ is the probability of classifying a case as belonging to class 2 when it belongs to class 1, and $e_2$ is vice versa.

In the feature space, the regions of classification have the dimensionality $p$, and it is very difficult to calculate the error components from multi-dimensional integration. It is easier to look at (14) as:

$$h(x) \overset{\omega_1}{\geq} th,$$  \hspace{1cm} (47a)

$$h(x) = \log \frac{f_X(X = x|\omega_1)}{f_X(X = x|\omega_2)},$$  \hspace{1cm} (47b)

$$th = \log \frac{Pr[\omega_1]c_{21}}{Pr[\omega_2]c_{12}},$$  \hspace{1cm} (47c)

where the log is taken just as a convention to simplify the analysis for the case of multinormal distribution (because it has an exponent); however, it has no other significance. The function $h(X)$ is called the log-likelihood ratio (LLR), which is obviously a random variable, whose variability comes from the feature vector $X$. The LLR has a PDF conditional on each of the two classes, as indicated in Fig. 9; (it can be easily shown that the two curves in this figure cross at $h(X) = 0$, when the threshold is zero.)

In general, the two error components appearing in (46) can be rewritten, equivalently to their corresponding terms in Eq. (16), using the LLR in (47), as:

$$e_1 = \int_{-\infty}^{th} f_h(h(x)|\omega_1)dh(x),$$  \hspace{1cm} (48a)

$$e_2 = \int_{th}^{\infty} f_h(h(x)|\omega_2)dh(x).$$  \hspace{1cm} (48b)

Now, it is very important to realize the generality of this error equation and the two messages it conveys. (1) It expresses the two components of error for any classifier that produces an output, or a score, of $h(x)$ for a predictor $X = x$, even if it is not the best (Bayes’) classifier. The only exception then would be that the score $h(X)$ is no longer the LLR that produces the minimum risk. (2) Whether $h(X)$ is the score of the Bayes’ classifier or not, Eq. (48) says that at each threshold value $th$ there is a pair of two components of error. Over the continuum of threshold values there is a continuum of these pairs, which define a new curve. This curve is called the ROC curve, a device that is much more rich for assessing classification rules than a single pair of errors, as will be explained next.
6.2 Receiver Operating Characteristic (ROC) Curve

Now, assume the classifier is trained under the condition of equal prevalence and cost, i.e., the threshold is zero. In other environments there will be different a priori probabilities yielding to different threshold values. The error is not a sufficient metric now, since it is a function of a single fixed threshold. A more general way to assess a classifier is provided by the ROC curve. This is a plot for the two components of error, $e_1$ and $e_2$, under different threshold values. It is conventional in many applications to refer to $e_1$ as the False Negative Fraction (FNF), and $e_2$ as the False Positive Fraction (FPF). This is because cases from the abnormal class typically are assigned higher classifier’s scores than cases from the normal class, hence the names “positive” and “negative”. For example, a network activity belonging to the abnormal class (the class of anomalous activities) whose classifier’s score is less than the chosen threshold will be called “negative”. This is obviously a false negative decision; hence the name FNF. The situation is reversed for the other error component.

Because the classification problem now can be seen, more generally, in terms of the classifier’s output score rather than the hard binary decision, it is apparent that each of the two error components is an integral over a univariate PDF. Therefore, the resulting ROC is a monotonically non-decreasing function. A convention in many fields is to plot the true positive fraction (TPF), which is given by $\text{TPF} = 1 - \text{FNF}$, vs. the FPF. In that case, the farther apart the two distributions $f_h(h|\omega_i)$, $i = 1, 2$ of the score function $h(X)$ from each other, the higher the ROC curve and the larger the area under the curve (AUC). Fig. 10 (left) shows ROC curves for two different competing classifiers. The first classifier performs better because it has a lower value of $e_2$ at each value of $e_1$. Thus, the first classifier unambiguously separates the two classes better than the second one. Therefore, the AUC for the first classifier is larger than that for the second one. The AUC can be thought of as one summary performance measure for the ROC curve. Formally, the AUC is given by:

$$\text{AUC} = \int_0^1 \text{TPF} \, d(\text{FPF}).$$  \hfill (49)

And it can be shown that it is also given by:

$$\text{AUC} = \text{Pr}[h(x)|\omega_2 < h(x)|\omega_1].$$  \hfill (50)

which expresses how the classifier scores for class $\omega_1$ are stochastically larger than those of class $\omega_2$, and hence more capable of the classification task.

If two ROC curves cross (Fig. 10, right), this means each classifier is better than the other only for a certain range of the threshold setting, and vice versa. In that case, some other performance measure can be used, such as the partial area under the ROC curve in a specified region (Yousef, 2013).
6.3 The True Performance Is A Random Variable!

As was explained in Sec. 5.2, regardless of whether the ML task is regression or classification, the model, its parameters, and its performance, all are random variables, where the randomness comes from the training dataset. In addition, this variation depends on the complexity of the model, and its capacity to learn, relative to the training dataset size.

For instance, the output scoring function \( h(X) \) of a particular classifier is indeed \( h_{\text{tr}}(X) \), which is subscripted to show the dependence on the training dataset; hence, the PDFs \( f_{h_{\text{tr}}}(h|\omega_i) \) and \( \text{ROC}_{\text{tr}} \), all should be subscripted as well. Therefore, there is a population of ROC curves that corresponds to the population of training datasets (Fig. 11). For more elaboration, consider the AUC as the performance measure of interest. Then, the fundamental quantities of interest are the following:

1. \( \text{AUC}_{\text{tr}} \): the true performance of the classifier, conditional on a particular training dataset \( \text{tr} \) of a specified size \( n \) but over the population of testing datasets (as if we trained on \( \text{tr} \) then tested on infinite number of observations),
2. \( E_{\text{tr}} \text{AUC}_{\text{tr}} \): the expectation of the true performance over the population of training datasets of the same size \( n \), and
3. \( \text{Var}_{\text{tr}} \text{AUC}_{\text{tr}} \): the variance of the true performance over the population of training datasets of the same size \( n \). This variance expresses how the classifier is sensitive to retraining, e.g. in the case of obtaining a new training dataset.

Any other performance measure, e.g., each of the error components, the risk, etc., is a r.v. as well, should be similarly subscripted \( \text{tr} \), and has a mean and a variance as explained above. For more elaboration, we explain this crucial concept in Sec. 6.4, in a more mathematical detail, for the case of regression, because it is more obvious and easier to explain.

6.4 Bias-Variance Decomposition

Over-training (or overfitting) a particular algorithm is an expression used to describe the complexity of this algorithm, and hence its capacity, to fit the current training (e.g. getting a very small value of the RSS). Although this seems a success, it is not! This is because what is required is to have the best performance on the unseen data (the population of testers, as opposed to the training dataset itself). As explained in Sec. 5.2, when a ML algorithm trains on a training dataset there are two things to realize: (1) the training dataset is taken as an example of the population, and (2) the objective function, to be minimized on this training dataset, is an estimator of the performance measure that we hope to be minimized on the population. For example, recall that we used the RSS as an objective function to estimate the MSE as a performance measure.

Overfitting an algorithm results in decreasing the bias of the performance measure and increasing its variance, and vice versa; and there is always a trade-off between this bias and variance. Before delving into any mathematics, Fig. 12 qualitatively illustrates...
Fig. 12 Two regression functions with: low bias and high variance (left); high bias and low variance (right)

this phenomenon for two different ML algorithms (left and right). The bold function $\eta^*$, in both subfigures, is the conditional expectation, which is the best regression function. Training the algorithm on a training dataset $\text{tr}$ produces a function $\eta_{\text{tr}}$ that may exist anywhere in the shaded region in the figure. The pointwise mean of these functions is plotted in light black. The algorithm of the left subfigure produces a mean model $E_{\text{tr}}\eta_{\text{tr}}(x)$ that is very close to $\eta^*$ (low bias); however, a single fitted model may exist anywhere in the wide shaded region (high variance). The algorithm of the right subfigure behaves conversely.

This can be best understood if the KNN is taken as an example. At some point $x_i$, the prediction is $\sum_{j \in N_K(x_i)} y_j / K$. The expectation of this regression function is $\sum_{j \in N_K(x_i)} E[y_j] / K$, while the variance will be $\sigma^2 / K$ (where the response is assumed to have constant variance $\sigma^2$ with the predictor). If the window size of this rule is squeezed to produce a more complex rule, i.e., $K$ is decreased, the variance will increase, but the bias will decrease since $\sum_{j \in N_K(x_i)} E[y_j] / K$ tends to approach $E[y_i]$. On the contrary, increasing $K$ obviously decreases the variance, while incorporating many data points whose expectations will be very likely to vary from $E[y_i]$, hence the bias increases. This example of KNN is provided in Hastie et al. (2009). For more elaboration, (Hastie and Tibshirani, 1990, Ch. 3) review a measure of the complexity of smoothing functions in terms of an effective number of degrees of freedom.

The bias-variance decomposition for a regression function is analyzed quantitatively in Eq. (51), and is illustrated in Fig. 13. This figure is conceptually similar to Fig. 12, but with indicating each component of Eq. (51) on the figure. For better illustration and pedagogy, the colors of the figure match the colors of the corresponding terms of the equation as follows: the light red for a trained model, the bold red for its mean over the population of training datasets, the blue circles for the training dataset (observed response), the green circles for the testing dataset (observed response), the bold green for the response conditional mean (the best regression function). The symbol $\equiv$ is used to indicate how the corresponding quantity can be estimated from a dataset, regardless whether this is a good estimator or not as will be explained in the next chapter. The symbol $M$ denotes the number of training datasets drawn through Monte Carlo (MC) trials.

We end this discussion with the following two questions that pave the road for the subfield of ML assessment, the topic of the next chapter. These questions are valid for any other performance measure, and the error rate is given just as a clear example. The subfield of ML assessment explains different methods for estimating the performance of a ML algorithm, from a given dataset (because the whole population of testers is unknown) to select among a variety of competing models and assess them, which answers the following two questions.

1. How can we minimize the mean error $E_{\text{tr}}\text{Err}_{\text{tr}}$ (51f), where the expectation is taken over the population of training datasets? As appears from the equation, this error is decomposed to three terms: the response variance, the model variance, and the model squared bias, respectively. The response variance is the natural variance in the physical phenomenon that generated the data and is model independent; hence, it is irreducible. Therefore, to minimize the mean error $E_{\text{tr}}\text{Err}_{\text{tr}}$, the model complexity should be tuned so that the summation of the bias squared and variance is minimized. Tersely speaking: too simple (complex) models produce high bias (variance) and low variance (bias); and since the variance (bias squared) cannot drop below zero, the summation of these two quantities will be high.

2. Should we design the ML model to minimize the conditional error $\text{Err}_{\text{tr}}$ (conditional on a particular training dataset) or the mean error $E_{\text{tr}}\text{Err}_{\text{tr}}$ that involves the bias and variance components?
Fig. 13 Bias-variance decomposition. A visual illustration using the same colors of the mathematical quantities in Eq. (51). (Part of the background of the figure, namely, the bold green curve, the bold red curve, and the shaded area, is as appears in (Bishop, 2006, Figure 1.17, pp. 32)).

\[
\text{err}(x_0) = \sigma^2_{y_0|x_0} + \text{var} \hat{y}_0 + \text{Bias}(\hat{y}_0)
\]

\[
\text{Err} = \frac{1}{n_{\text{tr}}} \sum_{i \in \text{tr}} (\hat{y}_i - y_i)^2,
\] (51a)

\[
\text{Err}_{\text{tr}} = \mathbb{E}_{x_0,y_0} \left[ (\hat{y}_0 - y_0)^2 \right],
\] (51b)

\[
= \mathbb{E}_{x_0} \left[ \mathbb{E}_{y_0|x_0} (\hat{y}_0 - y_0)^2 \right] + \frac{1}{n_{\text{tr}}} \sum_{k \in \text{ks}} (\hat{y}_k - y_k)^2,
\] (51c)

\[
= \mathbb{E}_{x_0} \left[ \sigma^2_{Y|X=x_0} + \left( \hat{y}_0 - \mathbb{E}_{y_0|x_0} y_0 \right)^2 \right],
\] (51d)

\[
\text{Err} = \mathbb{E}_{\text{tr}} \text{Err}_{\text{tr}} \quad \left( \approx \frac{1}{M} \sum_{m=1}^{M} \text{Err}_{\text{tr},m} \right),
\] (51e)

\[
= \mathbb{E}_{x_0} \left[ \sigma^2_{Y|X=x_0} + \text{var_{tr}} \left( \hat{y}_0 - \mathbb{E}_{y_0|x_0} y_0 \right)^2 \right. \\
\left. + \frac{1}{n_{\text{tr}}} \sum_{i \in \text{tr}} (\hat{y}_i - y_i)^2 \right].
\] (51f)

### 6.5 Curse of Dimensionality

This expression refers to what may happen when the predictor has high dimensions, i.e., \( p \) is too large. The word “large” should be understood relatively to the size \( n \) of the available dataset. For illustration, consider smoothing in high dimensions. It will almost fail because for a fixed number of available observations (the training dataset), the volume size needed to cover a particular percentage of the total number of observations increases by a power law, and thus exponentially, with dimensionality. This makes it prohibitive to include the same sufficient number of observations within a small neighborhood, or bandwidth, to smooth the response. More quantitatively, consider a unit hyper-cube in the \( p \)-dimensional space containing uniformly distributed observations; the percentage of the points located inside a hyper-cube with side length \( l \) is \( l^p \). This means, if the suitable bandwidth for a certain smoother is \( l \), the effective number of observations in the \( p \)-dimensional problem will go as the power \( 1/p \). This deteriorates the performance dramatically for \( 3 < p \). This is why, e.g., the additive model (Sec. 4.2) and its variants are expressed as summation of functions of just one dimension. This single dimension may be just a component of the predictor or a linear combination.
Many other problems occur when \( n << p \), including increasing the model variance. In addition, the performance of the model fitted from a given dataset will not generalize on the population or a future dataset. All of these problems, and others, are indeed related and connected mathematically to each other, which is out of the scope of the present chapter.

Therefore, a very crucial topic in ML is dimensionality reduction (it is called feature selection in some other communities). Qualitatively speaking, this means selecting those predictor components that best summarize the relationship between the response and predictor. In real-life problems, some features are statistically dependent on others; this is referred to as multi-collinearity. On the other hand, there may also be some components that are statistically independent from the response. These add no additional information to the problem; thus they serve only as a source of noise.

Several existing approaches aim to reduce the dimensions of the problem. A dimensionality reduction method of course can be considered as part of the ML algorithm. Therefore, for a given problem, selecting among different methods account as selecting among different algorithms which is the main topic of the next chapter, as explained at the end of Sec. 6.4.

### 6.6 Performance of Unsupervised Learning

It should be noticed that the formal definition of the learning process, discussed thus far in the present chapter, assumed the existence of a training dataset, \( \text{tr} : \{ t_i = (x_i, y_i), \ i = 1, \ldots, n \} \). Each element \( t_i \), or sample case, in this set has an already known value for the response variable. This is what enables the learning process to develop the relationship between the predictor and the response. This is what is called supervised learning. On the contrary, in some applications the available dataset is described by \( \text{tr} : \{ t_i = x_i, \ i = 1, \ldots, n \} \), without any additional information. This situation is called unsupervised learning. It is usually required in such a situation to understand the structure of the data from the available empirical probability distribution of the points \( x_i \).

For the special case, where the data come from different classes, the data will be represented in the hyper-\( p \)-dimensional space, to some extent, as disjoint clouds of data. The task in this case is called clustering, i.e., trying to identify those classes that best describe, in some sense, the current available data. More formally, if the available dataset is \( X \), it is required to find the class vector \( \Omega = [\omega_1, \ldots, \omega_K]' \) and the clustering function \( \eta_{\text{tr}}(X) \), such that a criterion (an objective function) \( J(X, \Omega) \) is minimized:

\[
\Omega = \arg \min_{\Omega} J(X, \Omega).
\]

(52)

Different criteria give rise to different clustering algorithms. More discussion on unsupervised learning and clustering can be found in Fukunaga (1990); Duda et al (2001); Hastie et al (2009).

It is important to emphasize that although the construction of the supervised and unsupervised rules is quite distinct, the assessment procedure and the performance measures, including error rate, risk, ROC, AUC, etc., are essentially the same. This is obvious because the unsupervised rule \( \Omega_{\text{tr}}(X) \), regardless of its construction, ultimately provides the same mapping \( \eta_{\text{tr}}(X) \mapsto \{ \omega_1, \ldots, \omega_K \} \) as the supervised rule, which is assigning a class label to a predictor.

### 6.7 Classifier Calibration

As detailed throughout the chapter, the final classifier decision \( \eta_{\text{tr}}(x) \) of a classifier is obtained by comparing its output score \( h_{\text{tr}}(x) \) to a threshold \( t/h \). However, there are two important issues to consider. (1) The scores do not necessarily equal to the posterior probabilities \( \text{Pr} [\omega_i | x] \), which are much more informative than a mere numerical score; indeed, many classifiers provide score values outside the period \([0, 1] \). (2) Scores of two different classifiers cannot be compared, simply because they are not on the same scale. Classifier calibration is a remedy to these two issues, not naively by linear scaling, but by providing a one-to-one nonlinear monotonic transformation that maps the output scores to the posterior probabilities. It is important to observe that this transformation will not affect the performance of the classifier on the population or on a finite testing dataset. For a formal proof of this result, and for a full account of the calibration process including a recent comparative study among different calibrators see Yousef et al (2021a).

### 7 Discussion and Conclusion

This chapter is intended to provide a pilot view of the field of ML to illustrate how mathematics and intuition together work, which helps cyberphysical security practitioners, who apply ML in many applications, understand subtle concepts and connect scattered pieces. The importance of the theoretical aspects of ML are stressed, and demonstrating examples are provided. The mathematical
foundations of the field, along with different methods and construction, have been motivated. Important and fundamental references have been cited for readers, who are interested in more elaboration.

When it comes to real-life applications, many practitioners leverage some ML approaches, or models, without having the fundamental rigour or the enough insight, a matter that results in a lot of fallacies and pitfalls. A simple example is the use of complex models, that have high capacity, relative to the training dataset size. A second example is to perform data preprocessing or transformation without including the step into the resampling mechanism that estimates the final performance. A third example is thinking of a particular model or approach as “magical” that can consistently outperform others ubiquitously.

“No overall winner” is a statement that has been touched upon throughout previous sections. If there is no prior information for the joint distribution between the response and the predictor, and if there is no prior information about the phenomenon to which that regression or classification will be applied, there is no overall winner among regression or classification techniques. If one method is found to outperform others in some applications, this is likely to be limited to that very situation or that specific kind of problem; it may be beaten by other methods for other situations. In the engineering and computer science communities, this concept is referred to as the no-free-lunch theorem (see Duda et al, 2001, Sec. 9.2). This situation holds because each method makes different assumptions about the application or the process being modeled, and not all real-life applications are the same. If one or more of the assumptions are not satisfied in a given application, the performance will not be optimal in that setting. The only unique overall winner is the conditional expectation (for regression) or the Bayes’ classifier (for classification) when the probability distributions are known.

To recap, practitioners are always advised to have a basic level of mathematical rigor and understanding of these foundations, even if they do not produce research or contribute to theoretical discoveries in the field.

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