Proper likelihood ratio based ROC curves for general binary classification problems

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Abstract: Everybody writes that ROC curves, a very common tool in binary classification problems, should be optimal, and in particular concave, non-decreasing and above the 45-degree line. Everybody uses ROC curves, theoretical and especially empirical, which are not so. This work is an attempt to correct this schizophrenic behavior. Optimality stems from the Neyman-Pearson lemma, which prescribes using likelihood-ratio based ROC curves. Starting from there, we give the most general definition of a likelihood-ratio based classification procedure, which encompasses finite, continuous and even more complex data types. We point out a strict relationship with a general notion of concentration of two probability measures. We give some nontrivial examples of situations with non-monotone and non-continuous likelihood ratios. Finally, we propose the ROC curve of a likelihood ratio based Gaussian kernel flexible Bayes classifier as a proper default alternative to the usual empirical ROC curve.

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1. Introduction

In a binary classification problem a new object is to be assigned to one of two possible populations or conditions, conveniently represented as probability laws $P_-$ or $P_+$. A classification rule is an algorithm which tells under what conditions the new object is assigned to population $P_+$, given data collected previously on a number of similar objects, some under $P_-$ and some under $P_+$. The data can be of any kind: one or more categorical variates, one or more ordinal variates, one or more quantitative variables, a time series, an image or some other complex data. In this paper we are then using classification as a synonym for discriminant analysis (in Statistics) and for (classification supervised learning (in Machine Learning).

Typically, a classification rule is indexed by a real-valued threshold parameter $t \in \mathcal{R}$. By varying $t$, a ROC (Receiver Operating Characteristic) curve is generated. It is defined as the parametric two-dimensional locus \{(FPR(t), TPR(t)), t \in \mathcal{R}\}, where the false positive rate FPR is the probability the classification rule

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assigns the object to population $P_+$ given the object comes from population $P_-$ and the true positive rate TPR is the probability the classification rule assigns the object to population $P_+$ given the object comes from population $P_+$. A variety of other names exist, in particular sensitivity for the TPR and specificity for 1-FPR.

ROC curves have proven to be very useful tools for binary classification problems, as witnessed by the immense literature sprung up in several different disciplines (Signal Processing, Statistics, Machine Learning, Psychometry, Educational Testing) in the last 50 years. See for example [11], [15] and [19], to mention only few relatively recent books, or consult the general treatment of the topic classification in any modern Statistics or Machine Learning textbook, such as [7].

It is widely recognized that classification rules based on the likelihood ratio (LR from now on) are in some sense optimal. For example, [15] lists a series of optimal properties and [19] further discusses optimality. The construction of an optimal ROC curve under general terms is possible as long as the data is defined as a random element and the two measures $P_-$ or $P_+$ are mutually absolutely continuous. LR can then be defined, and the optimal indexed classification rule simply assigns the object to $P_+$ if the LR is greater than $t$, with the addition of a technical randomization rule to be defined properly in the next section. The definition of the LR based classifier can be considered a back-to-basics operation: optimality of our ROC curve stems directly from the Neyman-Pearson lemma ([14]), which applies to general probability measures. The properties of ROC curves based on the LR were essentially clear in the classic statistical literature about Neyman-Pearson, for example Section 3.2 in [8], even if the expression ROC was not used (the term was invented later, in the '50s).

In practice, the LR based rule and its associated ROC curve are used much less frequently than current technology allows for. This work is partly an attempt to correct that, and partly an exploration of some properties the LR based ROC curve which have been overlooked in the references mentioned above.

Clarity of thought is improved when viewing the ROC curve as a parameter in the traditional statistical sense, i.e. as a function of the probability measures characterizing our data generating process. Keeping that in mind, we would then like to prove and give examples for the following claims.

1. The LR based classification rule produces a proper ROC curve and can been constructed or estimated under very general conditions; proper and improper ROC curves were elegantly discussed in [4], section 2.6, where the optimality of ROC curves based on LR was clearly stated for data on the real line. However, improper ROC curves (in particular, not concave), continue to be used in practice, for example in the univariate normal heteroschedastic case.

2. Particularly in the multivariate setting, LR based classification rules and ROC curves can be constructed (at least from a theoretical point of view, see Section 5) which dominate the ROC curves commonly used, such as the ones based on optimal linear combinations (e.g. in the multivariate
3. Efficient estimated ROC curves based on observed data can be constructed (up to computational problems to be discussed in Section 5) in such a way that they are proper, and in particular concave and continuous; this implies in particular that the common staircase-shaped empirical estimates of the ROC curve provided by most statistical software are not always adequate and alternatives exist.

4. The definition of the LR based classification rule for general data spaces is strictly connected to a general definition of concentration function given in [3] for two probability measures whatsoever, which generalizes the concentration definition given by Gini at the beginning of the XXth century. This clarifies that the ROC curve parameter is a theoretical quantification of the relationship between two probability measures, and not merely a descriptive tool of the performance of a classifier.

5. LR based classification rules as defined in the next section entails the use of a randomized classification rule in case the distribution of the LR contains atoms. Randomization is necessary to make the ROC curve a true continuous curve, as observed in [4]; without randomization the ROC curve would degenerate to a finite set of points. This has also the advantage of unifying the definition of the ROC curve for any pair of probability measures $P_-$ or $P_+$ whatsoever. In particular, the finite case, which is seldom given any attention in the ROC literature, is encompassed under a general definition.

Our definition of ROC curve for general data spaces is given in the next section. The connection to a general definition of concentration function is given in Section 3. The section after that contains some examples and Section 5 includes a statistical discussion of the issue of estimating ROC curves. Finally, a case study is presented.

2. Definition of the LR based ROC curve for general types of data

Assume that $P_+$ and $P_-$ are absolutely continuous with respect to one another and have densities $f_+$ and $f_-$, respectively, with respect to a common dominating measure. Then, without loss of generality, $f_-$ can be taken to be positive, so that the Likelihood Ratio

$$L = \frac{f_+}{f_-}$$

(2.1)

is a well defined nonnegative random variable. As such, $L$ then has distribution functions under $P_-$ and $P_+$, which we denote by $H_-$ and $H_+$ respectively. More precisely, for each $l \in \mathcal{R}$:

$$H_-(l) = P_-(L \leq l)$$

and

$$H_+(l) = P_+(L \leq l).$$
Next, define the quantile function associated with $H_-$ in the usual way as follows:

$$q_t = \inf\{y \in \mathbb{R} : H_-(y) \geq t\} \quad 0 < t < 1$$

and recall that, for any real number $l$,

$$q_t \leq l \quad \text{if and only if} \quad H_-(l) \geq t.$$

For any given value $t \in (0, 1)$, it may or may not happen that $t = H_-(q_t)$, depending on whether $t$ does not correspond or does correspond to a jump of $H_-$. More specifically, if $t \neq H_-(q_t)$, then $H_-(q_t^-) \leq t < H_-(q_t)$, where the notation $^-$ indicates left limits (nothing to do with $P_-$), a particularly relevant occurrence for the discussion below.

$H_-$ and $H_+$ may have jumps, even if $P_+$ and $P_-$ are, say, absolutely continuous laws on the real line. $H_-$ and $H_+$ do not have jumps for, say, two normal (or Gaussian) probability measures, but $P_+$ and $P_-$ may be absolutely continuous yet $L$ be a finite random variable which takes on a finite set of values, almost surely. This happens, for example, if $P_+$ and $P_-$ have piecewise constant densities; we will provide an example in the next section.

The following definition of LR based classification rule will be used throughout this paper.

**Definition 2.1.** Given two alternative probability laws $P_-$ or $P_+$ mutually absolutely continuous with respective densities $f_-$ and $f_+$, define the likelihood ratio $L = f_+/f_-$, its respective distribution functions $H_-$ and $H_+$ and the following classification rule. For each $0 < t < 1$:

1. if $L > q_t$, declare positive;
2. if $L < q_t$, declare negative;
3. if $L = q_t$, then perform an auxiliary independent randomization and declare positive with probability

$$r(t) = \frac{H_-(q_t) - t}{H_-(q_t) - H_-(q_t^-)}$$

and negative otherwise.

This definition parallels the definition of a randomized LR test (in [8], for example), but it is presented here in a classification context.

**Theorem 2.1.** The ROC function of the classification rule of Definition 2.1 is

$$\text{ROC}(x) = 1 - H_+(q_{1-x}) + q_{1-x}(H_-(q_{1-x}) - (1 - x)), \quad 0 < x < 1.$$  

As usual, we can complete the result by setting $\text{ROC}(0) = 0$ and $\text{ROC}(1) = 1$. 


Proof. We first compute separately the FPR and the TPR.

\[
\text{FPR} = P_-(\text{declare positive}) \\
= P_-(L > q_t) + P_-(L = q_t)r(t) \\
= 1 - H_-(q_t) + (H_-(q_t) - H_-(q_t^-))r(t) \\
= 1 - H_-(q_t) + H_-(q_t) - t \\
= 1 - t.
\]

Notice that if \( t = H_-(q_t) \) then \( H_-(q_t^-) - H_-(q_t) = 0 \); in other words the expression simplifies for points which are not \( H_- \)-atoms.

\[
\text{TPR} = P_+(\text{declare positive}) \\
= P_+(L > q_t) + P_+(L = q_t)r(t) \\
= 1 - H_+(q_t) + (H_+(q_t) - H_+(q_t^-)) \frac{H_-(q_t) - t}{H_-(q_t^-) - H_-(q_t)} \\
= 1 - H_+(q_t) + q_t(H_-(q_t) - t)
\]

since, \( P_+ \) and \( P_- \) being mutually absolutely continuous, they will both have or not have an atom in \( q_t \) and their LR in \( q_t \) will be exactly \( (H_+(q_t) - H_+(q_t^-))/(H_-(q_t^-) - H_-(q_t)) \), i.e. \( q_t \) itself. Next, set \( \text{FPR} = x \), i.e. \( t = 1 - x \), to eliminate the parameter \( t \) and obtain the explicit form of the ROC curve:

\[
\text{TPR} = 1 - H_+(q_{1-x}) + q_{1-x}(H_-(q_{1-x}) - (1 - x)).
\]

3. Relationship with a general concentration function

Expression (2.3) does not come out of nowhere. It corresponds to a definition of concentration function given in [3], and further expanded in [16], with the aim of extending the classical definition of concentration given by Gini. Such a definition is naturally based on the LR, and given the strict relationship existing between ROC curves and LRs, the connection comes easily.

We recall the definition of concentration given by [3] for the case \( P_+ \) and \( P_- \) are mutually absolutely continuous:

**Definition 3.1.** Let \( P_+ \) and \( P_- \) be mutually absolutely continuous probability measures, let \( f_+ \) and \( f_- \) be their respective derivatives with respect to a common dominating measure \( \mu \), let their LR be defined as the real-valued random variable \( L = f_+/f_- \), let \( H_- \) be its distribution function under \( P_- \) and let \( q_x \) be its quantile function. Then [3] define the concentration function of \( P_+ \) with respect to \( P_- \) as \( \varphi(0) = 0 \), \( \varphi(1) = 1 \) and

\[
\varphi(x) = P_+(L < q_x) + q_x(x - H_-(q_x^-)).
\]

The connection between this definition and the classification rule of the previous section is established in the next Theorem.
\textbf{Theorem 3.1.} Under the hypotheses described in Definition 2.1,
\[ \text{ROC}(x) = 1 - \varphi(1 - x) \quad \forall 0 \leq x \leq 1. \]
where \( \varphi(\cdot) \) is the concentration function of \( P_+ \) with respect to \( P_- \).

\textit{Proof.} The equivalent relationship
\[ 1 - \text{ROC}(1 - x) = \varphi(x) \quad \forall 0 \leq x \leq 1. \]
can be verified directly for \( x = 0, 1 \) and as follows for \( 0 < x < 1 \):
\[
1 - \text{ROC}(1 - x) = H_+(q_x) - q_x(H_-(q_x) - x)
= H_+(q_x) + q_x(H_-(q_x) - x)
= H_+(q_x) + q_x(x - H_-(q_x)) + H_-(q_x) - H_-(q_x)
= H_+(q_x) + q_x(x - H_-(q_x)) + H_-(q_x) - H_-(q_x)
= P_+(L < q_x) + q_x(x - H_-(q_x))
= \varphi(x).
\]
\( \square \)

\textbf{Corollary 3.1.} Under the hypotheses described in Definition 2.1, \( \text{ROC}(\cdot) \) is a nondecreasing, continuous and concave function on \([0, 1]\). In particular, \( \text{ROC}(\cdot) \) is proper.

\textit{Proof.} This is a consequence of Theorem 2.3 in [3]. In particular, \( \varphi(x) \) is always convex over its domain, i.e. \( \forall x_1, x_2 \) and \( \nu \in [0, 1], \varphi(\nu x_1 + (1 - \nu)x_2) \leq \nu \varphi(x_1) + (1 - \nu)\varphi(x_2). \) By Theorem 3.1:
\[
1 - \text{ROC}(1 - (\nu x_1 + (1 - \nu)x_2)) \leq \nu(1 - \text{ROC}(1 - x_1)) + (1 - \nu)(1 - \text{ROC}(1 - x_2)).
\]
The left hand side of the previous equality becomes:
\[
1 - \text{ROC}(1 - (\nu x_1 + (1 - \nu)x_2)) = 1 - \text{ROC}(\nu + (1 - \nu) - \nu x_1 - (1 - \nu)x_2)
= 1 - \text{ROC}(\nu(1 - x_1) + (1 - \nu)(1 - x_2)),
\]
while the right hand side can be rewritten as:
\[
\nu(1 - \text{ROC}(1 - x_1)) + (1 - \nu)(1 - \text{ROC}(1 - x_2)) =
\nu - \nu \text{ROC}(1 - x_1) + 1 - \nu - (1 - \nu)\text{ROC}(1 - x_2) =
1 - \nu \text{ROC}(1 - x_1) - (1 - \nu)\text{ROC}(1 - x_2).
\]
Therefore:
\[
\text{ROC}(\nu t_1 + (1 - \nu)t_2) \geq \nu \text{ROC}(t_1) + (1 - \nu)\text{ROC}(t_2), \quad \forall t_1, t_2, \nu \in [0, 1]
\]
where \( t_1 = 1 - x_1, t_2 = 1 - x_2. \)
\( \square \)
As mentioned in the Introduction, we would like to stress that a proper ROC curve is possible under the very general assumption that a LR is meaningful. Instead, in the applied literature, the existence of a proper ROC curve is often believed to be limited to models with a monotone likelihood ratio on a certain score.

Finally, we conclude by stating a precise relationship between ROC curves and the Lorenz-Gini curve. Such a relationship belongs to the folklore on ROC curves, since their affinity is apparent, but it has been seldom clearly stated due to the persistence of improper ROC curves in current applications. Now that we have shown that a proper curve can be constructed, we are able to make a clear statement, building again on results in [3].

**Corollary 3.2.** If \( P_- \) is a probability measure on the positive real line with distribution function \( F_- \) and finite mean \( m = \int tP_-(dt) \) and if \( P_+ \) has distribution function

\[
F_+(y) = \frac{\int_{[0,y]} tP_-(dt)}{m}, \quad y \geq 0,
\]

then

\[
1 - \text{ROC}(1 - x) = \lambda(x) \quad \forall 0 \leq x \leq 1.
\]

where \( \lambda(\cdot) \) is the Lorenz-Gini curve.

This is a consequence of Theorem 2.4 in [3], where further details on the Lorenz-Gini curve can be found. In particular, in the economic applications where the Lorenz-Gini scheme is usually employed, \( F_+(y) \) is the fraction of total income owned by the poorest fraction \( F_-(y) \) of the population. Finally notice that, in other contexts, under the assumptions of the Corollary 3.2 \( P_+ \) is also called a length-biased version of \( P_- \).

4. Examples

4.1. **Two absolutely continuous measures with discrete LR**

Let \( P_- \) be an absolutely continuous probability measure on the real line with density \( f_- \) uniform between 0 and 3 and let \( P_+ \) have a piecewise constant density \( f_+ \) defined as follows:

\[
f_+(s) = \frac{1}{18} (0 < s \leq 1) + \frac{10}{18} (1 < s \leq 2) + \frac{7}{18} (2 < s \leq 3) = \begin{cases} 
\frac{1}{18} & \text{if } 0 < s \leq 1 \\
\frac{10}{18} & \text{if } 1 < s \leq 2 \\
\frac{7}{18} & \text{if } 2 < s \leq 3 \\
0 & \text{otherwise}
\end{cases}
\]

where we write \( (A) \) as an indicator function for the event \( A \), i.e. the function which equals 1 if \( A \) is true and 0 otherwise. Suppose \( S \) is a real random variable
Fig 1. Proper ROC curve based on the LR of $S$ (solid line); improper ROC curve based on $S$ (dashed line).

with density $f_-$ under $P_-$ and $f_+$ under $P_+$. It is easy to see that the LR $L = f_+/f_-$ is piecewise constant and not monotone in $S$, being:

$$L = \begin{cases} 
\frac{1}{6} & \text{if } 0 < s \leq 1 \\
\frac{10}{7} & \text{if } 1 < s \leq 2 \\
\frac{7}{6} & \text{if } 2 < s \leq 3.
\end{cases}$$

A classification rule based only on $S$ gives rise to a ROC curve

$$\text{ROC}_S(x) = \begin{cases} 
\frac{21}{18}x & \text{if } 0 \leq x < 1/3 \\
\frac{4}{18} + \frac{30}{18}x & \text{if } 1/3 \leq x < 2/3 \\
\frac{15}{18} + \frac{3}{18}x & \text{if } 2/3 \leq x < 1
\end{cases}$$

which is not concave, shown as dashed line in Figure 1. Using instead the LR based classification rule, the ROC curve is:

$$\text{ROC}_L(x) = \begin{cases} 
\frac{30}{18}x & \text{if } 0 \leq x < 1/3 \\
\frac{3}{18} + \frac{21}{18}x & \text{if } 1/3 \leq x < 2/3 \\
\frac{15}{18} + \frac{3}{18}x & \text{if } 2/3 \leq x < 1
\end{cases}$$

which is concave and dominates the previous one as shown in Figure 1. This example deals with absolutely continuous densities which, nonetheless, have a
finite discrete likelihood ratio. As mentioned in the Introduction, this case is particularly difficult for the usual approaches to ROC curves, which emphasize a continuous score is necessary.

4.2. Two finite measures

The following example is taken from [1]. Suppose 109 patients have been classified as diseased (D+) or not diseased (D-), based on a gold standard such as biopsy or autopsy. On the basis of radiological exams, they have also been classified over five ordinal levels

\[ - = \text{very mild} \]
\[ - = \text{mild} \]
\[ ++ = \text{neutral} \]
\[ = \text{serious} \]
\[ ++ = \text{very serious} \]

Here are the results:

|       | – | – | + | + | ++ | total |
|-------|---|---|---|---|----|-------|
| D-    | 33 | 6 | 6 | 11| 2  | 58    |
| D+    | 3  | 2 | 2 | 11| 33 | 51    |

Define as \( P_+ \) and \( P_- \) the two empirical measures, relative to the diseased and not diseased population respectively, derived from data. There are four possible values for the LR:

\[
L = \begin{cases}
\frac{58}{561} & \text{if } -- \\
\frac{58}{153} & \text{if } - - \text{ or } +- \\
\frac{58}{51} & \text{if } + \\
\frac{58}{17} & \text{if } ++ 
\end{cases}
\]

which give rise to four empirical ROC points \{ (25/58, 48/51); (19/58, 46/51); (13/58, 44/51); (2/58, 33/51)\}, shown in Figure 2. Now we can see that, thanks to the randomization device, we can... connect the dots! This is so since the distribution functions of \( L \) under \( P_- \) and \( P_+ \) are

\[
H_-(l) = \begin{cases}
0 & \text{if } 0 \leq l < \frac{58}{561} \\
33 & \text{if } \frac{58}{561} \leq l < \frac{58}{153} \\
45 & \text{if } \frac{58}{153} \leq l < \frac{58}{51} \\
56 & \text{if } \frac{58}{51} \leq l < \frac{58}{17} \\
58 & \text{if } \frac{58}{17} \leq l < \frac{19}{17} \\
1 & \text{if } \frac{19}{17} \leq l 
\end{cases}
\]
Fig 2. The proper ROC curve based on the LR interpolates the empirical ROC points.

and

\[ H_+(l) = \begin{cases} 
0 & \text{if } 0 \leq l < \frac{58}{561} \\
\frac{3}{51} & \text{if } \frac{58}{561} \leq l < \frac{58}{153} \\
\frac{5}{7} & \text{if } \frac{58}{153} \leq l < \frac{58}{51} \\
\frac{18}{51} & \text{if } \frac{58}{51} \leq l < \frac{319}{77} \\
1 & \text{if } \frac{319}{77} \leq l.
\end{cases} \]

Therefore, the ROC curve can be calculated using Equation (2.3):

\[ \text{ROC}(x) = \begin{cases} 
\frac{319}{77} x & \text{if } 0 \leq x < \frac{2}{58} \\
\frac{31}{51} + \frac{58}{51} x & \text{if } \frac{2}{58} \leq x < \frac{13}{58} \\
\frac{2}{9} + \frac{58}{153} x & \text{if } \frac{13}{58} \leq x < \frac{25}{58} \\
\frac{503}{561} + \frac{58}{561} x & \text{if } \frac{25}{58} \leq x < 1
\end{cases} \]

The continuous ROC curve interpolates the empirical ROC points, as shown in Figure 2.

The example illustrates the crucial role played by randomization in order to obtain a proper ROC curve in the finite case. Even more so, if we consider that hardly any attention is ever given to the finite case in the ROC literature.
4.3. Two multivariate normal measures: Fisher’s LDA and QDA

Assume \( P_- \) is multivariate normal with mean \( \mu_- \) and variance \( \Sigma_- \) and \( P_+ \) is multivariate normal with mean \( \mu_+ \) and variance \( \Sigma_+ \) and both densities exist. By taking the logarithmic transformation of the LR, it can easily be seen that for the normal case the LR based classification rule in Definition (2.1) declares positive if the quadratic score

\[
(X - \mu_-)'\Sigma_-^{-1}(X - \mu_-) - (X - \mu_+)'\Sigma_+^{-1}(X - \mu_+) \tag{4.1}
\]

is large. This is the well known Fisher’s Quadratic Discriminant Analysis (QDA) rule ([5], which reduces to linear – hence the corresponding Linear Discriminant Analysis (LDA) – in the case \( \Sigma_- = \Sigma_+ \) (homoschedasticity). The original work by Fisher did not actually focus on the normality assumption, but QDA and LDA are well established terminology in the literature. Being based on the LR, QDA has a proper ROC curve and it is optimal under the stated assumptions; the score in Equation (4.1) is a continuous random variable and no randomization device is needed.

Insisting on a linear classifier leads to suboptimal procedures in the case of heteroscedasticity. The classifier which is optimal within the class of linear classifiers is considered in [18] and it declares positive if

\[
(\mu_+ - \mu_-)'(\Sigma_- + \Sigma_+)^{-1}X \tag{4.2}
\]

is large. It gives an improper ROC curve, which always has a “hook” and which is dominated by the ROC curve of the corresponding quadratic score in Expression (4.1). It may be worth providing an example, since the optimality of the quadratic score in the normal case is being continuously rediscovered, see for example [12] and [10], but it actually boils down to [5].

Consider a bivariate normal vector \((X, Y)\) which in population \( P_- \) has a bivariate standard normal distribution, whereas in population \( P_+ \) has independent components \( X \) distributed normally with mean \( \mu_x > 0 \) and variance \( \sigma^2_x \) and \( Y \) distributed normally with mean \( \mu_y > 0 \) and variance \( \sigma^2_y \neq \sigma^2_x \). According to Equation (4.1), the QDA classifier declares positive if

\[
\left(\frac{X - \mu_x}{\sigma_x}\right)^2 + \left(\frac{Y - \mu_y}{\sigma_y}\right)^2 - X^2 - Y^2 < c
\]

where \( c \) is an arbitrary threshold. By varying \( c \) and calculating the appropriate probabilities under \( P_- \) and \( P_+ \), we can obtain the ROC curve, by simulation or, if greater precision is needed, by using non-central chi-square distributions. The ROC curve for the case \( \mu_x = 1, \mu_y = 2, \sigma_x = 2, \sigma_y = 4 \) is plotted as a solid line in Figure 3.

The best linear classifier according to Expression (4.2) is instead

\[
S = \frac{\mu_x}{1 + \sigma^2_x}X + \frac{\mu_y}{1 + \sigma^2_y}Y.
\]
Fig 3. QD (solid) and best linear ROC (dashed) curves for the bi-bivariate normal case, assuming $\mu_x = 1$, $\mu_y = 2$, $\sigma_x = 2$, $\sigma_y = 4$.

$S$ has normal distributions under $P_-$ and $P_+$ and by a well-known result its ROC is

$$\text{ROC}(t) = \phi(A + \phi^{-1}(t)B)$$

(4.3)

where $\phi(\cdot)$ is the standard normal distribution function,

$$A = \frac{\mu_x^2(1 + \sigma_y^2) + \mu_y^2(1 + \sigma_x^2)}{\sqrt{\mu_x^2\sigma_y^2(1 + \sigma_y^2)^2 + \mu_y^2\sigma_x^2(1 + \sigma_x^2)^2}}$$

and

$$B = \frac{\sqrt{\mu_x^2(1 + \sigma_y^2)^2 + \mu_y^2(1 + \sigma_x^2)^2}}{\sqrt{\mu_x^2\sigma_y^2(1 + \sigma_y^2)^2 + \mu_y^2\sigma_x^2(1 + \sigma_x^2)^2}}$$

This ROC curve for the case $\mu_x = 1$, $\mu_y = 2$, $\sigma_x = 2$, $\sigma_y = 4$ is plotted as a dashed line in Figure 3. We can easily see that the QDA ROC curve is concave and dominates the best linear ROC curve.

4.4. Two point process measures: Polya versus Poisson

Suppose we can observe the times $T_1, \ldots, T_n$ of the first consecutive $n$ failures of a repairable engine under the assumption of instant repair. Under the further assumption of perfect repair, after each failure the engine is restored to the
original state of perfect reliability and the failure counting process \( \{N_-(t), t > 0\} \) is then a homogeneous Poisson process with parameter, say, \( \lambda > 0 \); the times \( T_1, \ldots, T_n \) are partial sums of independent and identically distributed negative exponential times. Take then as \( P_- \) their probability law. Now recall that 

\[
E(N_-(t)) = \lambda t
\]

and the intensity function of the process \( \{N_-(t), t > 0\} \) is constant

\[
\lambda_-(t) = \lim_{\Delta t \to 0} \frac{P(N(t + \Delta t) - N(t) = 1|F_t^-)}{\Delta t} = \lambda,
\]

where \( F_t^- \) is the internal filtration of the process in \([0, t)\). The observable data \( T_1, \ldots, T_n \) have density

\[
f_-(t_1, \ldots, t_n) = \lambda^n e^{-\lambda t_n} (4.4)
\]

for \( 0 < t_1 < t_2 < \ldots < t_n \). The data \( T_1, \ldots, T_n \) provide a non-trivial multivariate example based on which we can classify the object (the repairable engine) as having perfect repair or not. Consider as alternative law \( P_+ \) the distribution of \( T_1, \ldots, T_n \) under the simplest self-exciting point processes, the Polya process, discussed for example in [2], having intensity function

\[
\lambda_+(t) = \frac{1 + N_+(t^-)}{1 + \lambda t} \lambda,
\]

where \( N_+(t^-) \) is the number of failures observed in \([0, t)\). The intensity function is scaled in such a way that \( N_+(t) \) has the same expectation function as \( N_-(t) \):

\[
E(N_+(t)) = \lambda t.
\]

For such process the density of \( T_1, \ldots, T_n \) is

\[
f_+(t_1, \ldots, t_n) = \frac{n! \lambda^n}{(1 + \lambda T_n)^{n+1}}. (4.5)
\]

The likelihood ratio is then

\[
L = \frac{e^{\lambda T_n}}{(1 + \lambda T_n)^{n+1}}
\]

and our LR based classification rule declares positive (i.e., not perfect repair) if \( L \) is large. The classification rule is simple since it is a function of \( T_n \) only, due to the fact that, in both expressions (4.4) and (4.5), \( T_n \) is a sufficient statistic. It would not be difficult to construct a more complicated example using self-exciting processes where that is not the case.
5. Estimated ROC curves

The examples chosen in the previous section are intentionally simple but of growing complexity, since they are meant to illustrate some theoretical points about ROC curves. In particular, in all examples, \( P_- \) and \( P_+ \) were assumed to be known measures. As already mentioned, the ROC curve has been treated in this context as a parameter, a function of the underlying measures, and the examples were meant to study how this special parameter function looks like. If \( P_- \) and \( P_+ \) are not known, the problem arises to estimate them and any parameter which is a function of them based on data, via statistics which are functions of the data.

Example 4.2 blurred the difference between theoretical and empirical measures, since \( P_- \) and \( P_+ \) were derived from the data. But, except for this detail, the theoretical framework was the same as the other examples. Finite measures are a particularly simple case, since the empirical frequencies are often a good estimate of the theoretical point masses at each atom and can leisurely be substituted for them.

In practice, many of the interesting applications arise when \( P_- \) and \( P_+ \) are unknown multivariate probability measures of a set of \( p \) continuous real covariates, or features. \( P_- \) and \( P_+ \) must then be estimated, or learned, from data, which are realizations of such covariates. The words feature and learning belong to the Machine Learning dictionary. As a matter of fact, binary classification problems of this sort constitute a great portion of the contemporary literature at the intersection of Statistics and Machine Learning, which nowadays is the theoretical foundation of Data Science. An example is the very popular textbook [7], where several chapters are devoted to finding efficient estimates of \( P_- \) and \( P_+ \) and of their densities.

The usual assumption within a statistical approach is that the data from \( P_- \) and \( P_+ \) are two random samples from the respective populations. By far the most popular estimate of the ROC parameter is the empirical ROC curve, a plot of the empirical true positive versus false positive sample frequencies for varying threshold \( t \). Often, the ROC curve is actually defined as the empirical ROC curve, to avoid reference to any underlying model (by the same ideology, TPR is often defined as the empirical TPR, hiding the fact that the empirical TPR changes from sample to sample). The empirical ROC curve is also often used not as an estimate of an underlying parameter, but as a simple descriptive tool of the performance of a classifier. The frequencies are calculated from the set of predictions, i.e. a score for each of the statistical units, obtained from the classifier. Empirical ROC curves are pro-bono estimates on the grounds of the law of large numbers, which ensures that for every fixed threshold the empirical TPR converges to TPR and the empirical FPR converges to FPR. However, empirical ROC curves are generally improper: they easily switch from roughly concave to roughly convex and vice versa. Actually, to speak of convexity or concavity it is not even applicable, since they are staircase-shaped functions, which are therefore neither convex nor concave.

It is of interest to propose a LR based proper estimated ROC curve, not
staircase-shaped. Such a nonparametric but still model-based proposal was made in the univariate continuous case by [20]. In the multivariate continuous case, the problem is that there is no universally accepted optimal estimate of the density, in the way sample frequencies are optimal in the discrete case. In addition to that, the computational problems for large $p$ are conspicuous. This has led some of the same authors to express skepticism, see for example Section 4.2.1 of [19]. But, if LR based ROC curves are optimal and interesting parameters, then we should not be discouraged by difficulties in estimating them. The weaponry to do so has been overweamly enriched in the last few decades with contributions coming from both Statistics and Machine Learning, as hinted above. A minimal proposal is an estimated ROC curve associated to a nonparametric extension of naive Bayes estimation, a method which has proved its validity in a great deal of applied work (see for example Section 6.6.3 of [7]). Such a nonparametric extension has been know in the Machine Learning literature at least since [6], where it is called Flexible Bayes, and we now discuss a proper estimated ROC curve for it.

Assume two multivariate random samples $\{x_{ik}^i; i = 1, \ldots, n_-, k = 1, \ldots, p\}$ and $\{x_{ik}^i; i = 1, \ldots, n_+, k = 1, \ldots, p\}$ have been observed, where $x_{ik}^i$ (resp. $x_{ik}^+$) is the value of the $k$-th feature previously recorded on the $i$-th object under condition $P_-$ (resp. $P_+$). A kernel estimate of the $k$-th marginal density $f_{ik}^s, k = 1, \ldots, p, s \in \{-, +\}$ has the well-known form

$$\hat{f}_k^s(x) = \frac{1}{n_s \lambda_k^s} \sum_{i=1}^{n_s} K_\lambda(x, x_{ik}^s) \quad -\infty < x < +\infty \quad (5.1)$$

which, in the Gaussian case (other options exist), has

$$K_\lambda(x, x_{ik}^s) = \phi(\frac{x - x_{ik}^s}{\lambda_k^s}) = \frac{1}{\sqrt{2\pi}} \exp\{\frac{1}{2} (\frac{x - x_{ik}^s}{\lambda_k^s})^2 \}.$$

$\lambda_k^s$ is generally called the bandwidth, and it equals the standard deviation in the Gaussian kernel case. Gaussian kernels are widely used in density estimation and dedicated software exists; we will use some default proposals for bandwidth selection.

A LR based Gaussian kernel flexible Bayes classifier is a nonparametric classification rule which assigns a new object $X = (X_1, \ldots, X_p)$ to $P_+$, given a fixed threshold $t$, if

$$\hat{L} = \prod_{k=1}^{p} \frac{\hat{f}_k^+}{\hat{f}_k^-} (X_k) > t. \quad (5.2)$$

Notice that this is a LR based classification rule, which assumes as $P_-$ (resp. $P_+$) the product measure with density $\prod_{k=1}^{p} \hat{f}_k^-$ (resp. $\prod_{k=1}^{p} \hat{f}_k^+$). The implied independence of the features is an often unrealistic but parsimonious assumption.

Let $\hat{H}_-$ and $\hat{H}_+$ be the distributions of $\hat{L}$ induced by $\prod_{k=1}^{p} \hat{f}_k^-$ and $\prod_{k=1}^{p} \hat{f}_k^+$ respectively and let $\hat{q}$ be the quantile function of $\hat{H}_-$. The ROC curve associated
with rule (5.2) is
\[
\widehat{\text{ROC}}(x) = 1 - \hat{H}_+(\hat{q}_1-x) + \hat{q}_1-x(\hat{H}_-(\hat{q}_1-x) - (1-x)), \quad 0 < x < 1
\]
which, for Gaussian kernels, reduces to
\[
\widehat{\text{ROC}}(x) = 1 - \hat{H}_+(\hat{q}_1-x) \quad 0 < x < 1, \quad (5.3)
\]
since the LR does not have atoms, almost surely. Notice ROC curve (5.3) is proper by Corollary 3.1. In addition, the particular shape of the kernel estimate (5.1) lends itself to a simple simulation procedure which allows for reliable Monte Carlo calculation of formula (5.3).

The key of the simulation algorithm is that equation (5.1) is formally the density of a mixture of kernel distributions and it is therefore easy to simulate from it by choosing at random (i.e. with equal probabilities) one among the \(n_s\) random variables with densities centered at the observations \(x^k_i, i = 1, \ldots, n_s, s \in \{-, +\}\). We have therefore the following algorithm, which is stated for the Gaussian kernel Flexible Bayes case, but generalizes easily to other options.

**Algorithm 5.1.** To draw the graph of curve (5.3), proceed parameterically in \(t\) as follows:
- for \(t\) taking values on a finite positive grid
  - for \(k = 1, \ldots, p\)
    - for \(b = 1 \ldots B, \text{ with large } B\)
      - draw \(x_{-b}^*\) uniformly from one of the \(n_-\) Gaussian variables with mean \(x^k_i, i = 1, \ldots, n_-\) and standard deviation \(\lambda_-^k\)
      - compute \(\hat{f}^k_-(x_{-b}^*)\) and \(\hat{f}^k_+(x_{-b}^*)\)
      - draw \(x_{+b}^*\) uniformly from one of the \(n_+\) Gaussian variables with mean \(x^k_i, i = 1, \ldots, n_+\) and standard deviation \(\lambda_+^k\)
      - compute \(\hat{f}^k_-(x_{+b}^*)\) and \(\hat{f}^k_+(x_{+b}^*)\)
    - compute \(\hat{\text{FPR}}(t) = \frac{1}{B} \sum_{b=1}^B \left( \prod_{k=1}^p \frac{\hat{f}^k_-(x_{+b}^*)}{\hat{f}^k_+(x_{-b}^*)} > t \right)\)
    - compute \(\hat{\text{TPR}}(t) = \frac{1}{B} \sum_{b=1}^B \left( \prod_{k=1}^p \frac{\hat{f}^k_+(x_{+b}^*)}{\hat{f}^k_-(x_{-b}^*)} > t \right)\)
  - plot \((\hat{\text{FPR}}(t), \hat{\text{TPR}}(t))\)

where \((A)\) is the indicator function of event \(A\), which equals 1 if \(A\) is true and 0 otherwise.

[6] contains a discussion of the consistency of the Flexible Bayes estimate which could be extended to consistency of the estimated ROC function of Equation (5.3) via a continuous mapping argument.
6. Case study: diagnosis of prostate cancer using biomarkers

Prostate cancer (PCa) is the most frequent neoplasia diagnosis in men in Europe and one of the most common causes of cancer related death. Nowadays its correct diagnosis requires invasive tests (such as biopsy and digital rectal examination), because the standard and still widely used prostate specific antigen measurement (PSA, a non-invasive tool) leads to high percentages of false positives and false negatives and it is no longer recommended for screening purposes. A lot of efforts are currently devoted worldwide to finding non-invasive and easy-to-detect biomarkers to improve the diagnostic route for prostate cancer. The biomarkers are meant to be used in combination, possibly with PSA itself.

This diagnosis can be considered a classification problem, and a binary one if it is simplified to PCa versus non-PCa. ROC curves are used to evaluate the performance of the classifiers.

A dataset was provided by Fondazione Edo e Elvo Tempia (Biella, Italy) and described in the article by [13], in which microRNAs and other clinical variables for prostate cancer detection were investigated. MicroRNAs, small non coding RNA molecules which can be release in body fluids (blood, urine, saliva) and are highly stable, can control major cell pathways and can act as tumour suppressor or oncogene. They were analysed by real-time quantitative polymerase chain reaction, a biological technique which produces a continuous measurement of each microRNAs (namely the $C_t$ level, i.e. the point in time when DNA amplification is first detected).

The dataset consists of 58 PCa (the $P_+$ sample) and 170 non-PCa patients (the $P_-$ sample), including 89 benign hyperplasias, 8 precancerous lesions and 73 healthy controls – but this finer subdivision is not used here. For each patient, two microRNAs and (log-transformed) PSA were combined to build the classifier. The two microRNAs were selected after a cumbersome feature selection procedure which combined statistical and practical aspects and it is ignored here for the sake of simplicity. Let $X = (X_1, X_2, X_3)$ be the observation vector (microRNA1, microRNA2, log(PSA)).

The maximum likelihood estimates of means and variance covariance matrices under $P_-$ and $P_+$ are:

$$\hat{\mu}_- = \begin{pmatrix} 4.952 \\ 5.463 \\ 1.403 \end{pmatrix}, \quad \hat{\Sigma}_- = \begin{pmatrix} 7.233 & 5.260 & 1.639 \\ 5.259 & 4.927 & 1.165 \\ 1.638 & 1.165 & 2.490 \end{pmatrix},$$

$$\hat{\mu}_+ = \begin{pmatrix} 6.833 \\ 6.939 \\ 2.518 \end{pmatrix}, \quad \hat{\Sigma}_+ = \begin{pmatrix} 3.570 & 3.167 & -0.098 \\ 3.167 & 3.086 & -0.150 \\ -0.098 & -0.149 & 0.656 \end{pmatrix}.$$  

If we assume $X$ is multivariate normal, then we estimate $X \sim \text{MVN}(\hat{\mu}_-, \hat{\Sigma}_-)$ under $P_-$ and $X \sim \text{MVN}(\hat{\mu}_+, \hat{\Sigma}_+)$ under $P_+$. The best parametric classifier is Fisher QDA in Equation (4.1), since the covariance matrices differ. The associated ROC curve is displayed in Figure 4, left panel, dashed line. If we insist on
linear transformations of $X$, then the best one by [18], given in Equation 4.2, is
\[
0.09872 \times X_1 + 0.04335 \times X_2 + 0.29222 \times X_3
\]
with Gaussian univariate distributions $\mathcal{N}(1.13560, 0.46137)$ under $P_-$ and $\mathcal{N}(1.71123, 0.11426)$ under $P_+$. The associated ROC curve is displayed in Figure 4, left panel, solid line.

On the other hand, adopting a less restrictive nonparametric point of view, we could apply Algorithm 5.1 to get a good approximation of a nonparametric LR based estimated ROC curve for the Flexible Bayes classifier, displayed in Figure 4, right panel, dashed line. The solid line on the right panel is instead the usual staircase-shaped empirical ROC curve obtained by pairing the empirical frequencies of the predictions for various thresholds (obtained in this case with the R library described by [17]). The ROC of the Flexible Bayes classifier is different from and on average lower than the QDA ROC, since there is a price to pay for the greater generality of the nonparametric approach, but it exhibits a definite advantage over the empirical ROC, which appears to be a less efficient estimate of the underlying true ROC.

7. Conclusion

This work focuses on ROC curves associated with LR based binary classification methods. Nowadays, many new classification methods not based on the
likelihood are being proposed, especially in the Machine Learning literature. The properties of these new classification methods will have to be studied with mathematical methods. From a statistical point of view, LR methods remain a fundamental reference which provide principled and mathematically sound methods. “There is nothing more useful than a good theory”, said once Kurt Lewin.

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References

[1] Armitage, P. and Colton, T. (2005). *Encyclopedia of biostatistics*. Wiley.
[2] Bailey N. (1964). *The elements of stochastic processes with applications to natural sciences*. Wiley.
[3] Cifarelli D.M. and Regazzini E. (1987). On a general definition of concentration function. *Sankhya B*, vol. 49; p. 307-319.
[4] Egan J.P. (1975). *Signal detection theory and ROC analysis*. Academic Press.
[5] Fisher R. A. (1936). The Use of Multiple Measurements in Taxonomic Problems. *Annals of Eugenics*, 7 (2): 179-188. doi:10.1111/j.1469-1809.1936.tb02137.x
[6] John G.H. and Langley P. (1995). Estimating continuous distributions in Bayesian classifiers. In *Proceedings of the 11th Conference on Uncertainty in Artificial Intelligence*. Morgan Kaufmann Publishers, San Mateo.
[7] Hastie T., Tibshirani R. and Friedman J. (2008). *The Elements of Statistical Learning*. Springer.
[8] Lehmann E.L. (1986). *Testing Statistical Hypotheses*. Wiley. Second Edition.
[9] Green D.M. and Swets J.A. (1966). *Signal detection theory and Psychophysics*. Wiley.
[10] Hillis S.L. (2016). Equivalence of binormal likelihood-ratio and bi-chi-squared ROC curve models. *Statistics in Medicine*, 35(12): 2031-2057. doi:10.1002/sim.6816.
[11] Krzanowski W.J. and Hand D.J. (2009). *ROC Curves for Continuous Data*. Chapman & Hall.
[12] Metz C.E. and Pan X.C. (1999). Proper binormal ROC curves: theory and maximum-likelihood estimation. *Journal of Mathematical Psychology*, 43:133.
[13] Mello-Grand M., Gregnanin I., Sacchetto L., Ostano P., Zitella A., Bottone G., Oderda M., Marra G., Munegato S., Par- dini B., Naccarati A. Gasparini M., Gonteno P. and Chiorino G. (2018). Circulating microRNAs combined with PSA for accurate and non- invasive prostate cancer detection. Submitted Manuscript.

[14] Neyman, J. and Pearson, E.S. (1933). On the problem of the most effi- cient tests of statistical hypothesis. Philosophical Transactions of the Royal Society of London, Series A 231: 289337.

[15] Pepe M.S. (2003). The statistical evaluation of medical tests for classification and prediction. Oxford University Press.

[16] Regazzini E. (1992). Concentration comparisons between probability measures. SANKHYA B, vol. 54: 129-149.

[17] Sing T., Sander O., Beerenwinkel N., Lengauer T. (2005). ROCR: visualizing classifier performance in R. Bioinformatics, 21(20):3940-3941.

[18] Su J.Q. and Liu J.S. (1993). Linear combinations of multiple diagnos- tic markers. Journal of the American Statistical Association, 88(424):1350 - 1355.

[19] Zou K.H., Liu A., Bandos A.I., Ohno-Machado L. and Rockette H.E. (2012). Statistical Evaluation of Diagnostic Performance Topics in ROC Analysis. Chapman & Hall.

[20] Zou K.H., Hall W.J. and Shapiro D.E. (1997). Smooth non- parametric receiver operating characteristic (ROC) curves for continuous di- agnostic tests. Statistics in Medicine, 16: 21432156. doi:10.1002/sim.6816.