Interplay of ROC and Precision-Recall AUCs: Theoretical Limits and Practical Implications in Binary Classification

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Abstract

In this paper, we present two key theorems that should have significant implications for machine learning practitioners working with binary classification models. The first theorem provides a formula to calculate the maximum and minimum Precision-Recall AUC (AUC_{PR}) for a fixed Receiver Operating Characteristic AUC (AUC_{ROC}), demonstrating the variability of AUC_{PR} even with a high AUC_{ROC}. This is particularly relevant for imbalanced datasets, where a good AUC_{ROC} does not necessarily imply a high AUC_{PR}. The second theorem inversely establishes the bounds of AUC_{ROC} given a fixed AUC_{PR}. Our findings highlight that in certain situations, especially for imbalanced datasets, it is more informative to prioritize AUC_{PR} over AUC_{ROC}. Additionally, we introduce a method to determine when a higher AUC_{ROC} in one model implies a higher AUC_{PR} in another and vice versa, streamlining the model evaluation process.

1. Introduction

Building upon existing research, this paper delves deeper into the complex relationship between Receiver Operating Characteristic (ROC) Area Under the Curve (AUC) and Precision-Recall (PR) AUC in binary classification models. Our study is different by its analytical depth, addressing specific questions directly relevant to researchers and practitioners in machine learning. This paper makes the following contributions:

1. We establish an exact analytical expression for the transformation between ROC and PR curves. This expression, that we have not found elsewhere, offers a stronger version of the theorem presented in (Davis & Goadrich, 2006) and is the basis for the two main theorems which will follow.

2. We determine, for a given AUC_{ROC}, the exact bounds for the corresponding AUC_{PR}. This finding demonstrates that a high AUC_{ROC} does not guarantee a similarly high AUC_{PR}, especially for imbalanced datasets. This challenges the conventional reliance on AUC_{ROC} as the sole metric of model performance. We mirror our analysis for AUC_{PR}, deriving the bounds for AUC_{ROC} when AUC_{PR} is fixed. This contributes a new perspective on the interplay between these two metrics.

3. Through these analytical developments, we provide a rigorous justification for preferring AUC_{PR} over AUC_{ROC} for imbalanced datasets, a debate that has been prevalent in the machine learning community.

4. We address a common comparative scenario in model evaluation: determining whether a higher AUC_{ROC} for one model implies a higher AUC_{PR} compared to another model, and vice versa. Our findings offer a more efficient approach for this comparison, potentially reducing the computational burden in model evaluation.

5. The theoretical results are complemented with graphical illustrations and empirical experiments, providing a practical and visual understanding of the implications of our findings.

Each of these contributions is aimed at enhancing the understanding and application of AUC_{ROC} and AUC_{PR} in binary classification, particularly in the context of imbalanced datasets. The analytical nature of our approach should offer a significant advancement in the field, providing clear, actionable guidance for evaluating and comparing binary classification models.

2. Related Work

In binary classification, the relationship between Receiver Operating Characteristic (ROC) Area Under the Curve

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(AUC_{ROC}) and Precision-Recall (AUC_{PR}) has been extensively studied (Fawcett, 2006). A key work by (Davis & Goadrich, 2006) established the fundamental link between these metrics, especially for imbalanced datasets. Extending this, (Boyd et al., 2012) made a significant contribution by identifying an 'unachievable region' in PR space, reshaping the understanding of AUC_{PR}. This region, determined by class skew, affects the interpretation of AUC_{PR} and the effectiveness of various evaluation methodologies. To address this, they proposed the Normalized AUC_{PR} (AUC_{NPR}), a metric that adjusts for the unachievable region and offers a more meaningful comparison across datasets. Their insights allowed a deeper understanding of AUC_{PR}, especially in contexts with imbalanced class distributions.

The discourse on the preference of AUC_{PR} over AUC_{ROC} in scenarios involving imbalanced datasets has been furthered by several studies. (Saito & Rehmsmeier, 2015) made significant contributions to this conversation, providing valuable insights for practitioners dealing with class imbalances. (Ozenne et al., 2015) focused on the advantages of PR curves in medical data analysis, especially in the context of rare diseases, arguing for the superiority of AUC_{PR} in such imbalanced situations. Similarly, (Sofaer et al., 2019) extended the application of AUC_{PR} to ecological studies, such as rare species distribution, thereby broadening the relevance of AUC_{PR} across diverse fields. (Cook & Ramadas, 2020) also underscores the importance to use AUC_{PR} for imbalanced datasets with a focus on fraud detection.

Recent discussions have also brought to light the usefulness of the Matthews correlation coefficient (MCC) as a comprehensive alternative to AUC_{ROC} in binary classification. Studies like (Chicco & Jurman, 2023) have emphasized the MCC's ability to reflect all aspects of a confusion matrix, making a strong case for its adoption in binary classification evaluation. It is interesting to mention that papers studying MCC tend not to discuss AUC_{PR}.

Collectively, these papers enhance the understanding of when and how AUC_{ROC} and AUC_{PR} should be applied, highlighting their strengths and limitations in various contexts. Our work integrates these perspectives and offers new analytical expressions and insights into the AUC relationships.

3. Results

In this section we will present and demonstrate the main results.

3.1. Notations

We denote by N the size of the dataset, N^+ the number of positive examples and N^- the number of negatives ones. N^+ and N^- are assumed to be fixed and let's denote by $a = \frac{N^-}{N^+}$ a coefficient which measures the imbalanced nature of the dataset and which we will subsequently assume is strictly positive.

We use the usual notations TP the number of true positives, FP the number of false positives, TN the number of true negatives and FN the number of False negatives.

The metrics considered below are:

$$\text{Recall} = \frac{TP}{TP + FN}$$

$$\text{Precision} = \frac{TP}{TP + FP}$$

$$\text{True Positive Rate (TPR)} = \frac{TP}{TP + FN} = \text{Recall}$$

$$\text{False Positive Rate (FPR)} = \frac{FP}{FP + TN}$$

The area under the ROC curve will be denoted AUC_{ROC} and the area under the precision recall curve will be denoted AUC_{PR}.

3.2. Transformation between ROC and Precision Recall (PR) space

Theorem 3.1. *The transformation between a point (x, y) on the ROC curve and a point on the PR curve is given by the following expression:*

$$(x, y) \to (y, \frac{y}{y + ax}) \tag{1}$$

The transformation between a point (x, y) in the PR curve and a point in the ROC curve has the simple form:

$$(x, y) \to (\frac{1}{a}\frac{x(1 - y)}{y}, x) \tag{2}$$

Demonstration 3.2. *Let (x, y) be a point on the ROC curve then x is the TPR and y is the FPR. By definition we have: $x = \frac{FP}{N^-}$ and $y = \frac{TP}{N^+}$ and then $Precision = \frac{TP}{TP+FP} = \frac{N^+y}{N^+y+N^-x} = \frac{y}{y+ax}$. As $recall = y$ the corresponding point in PR space will be $(y, \frac{y}{y+ax})$*

By reversing this relation we find the expression of the transformation between a point on the PR curve and a point on the ROC curve

Remark 3.1. *Let's denote by $\widehat{ROC}$ the space (TPR, FPR) which is just a symmetry by the first* *bisector of the ROC space. The calculation will be easier in this space. In fact, the transformation between $\widehat{ROC}$ and PR space is:*

$$(x, y) \to (y, x) \to (x, \frac{x}{x + ay}) \tag{3}$$

using equation 1

Corollary 3.3. *We say that one curve dominates another curve if it is always above (for all abscissa). The theorem 3.2 in (Davis & Goadrich, 2006) which stipulates that: one curve dominates a second curve in ROC space if and only if the first dominates the second in Precision-Recall space can then be proven faster than in their article.*

Demonstration 3.4. *One curve dominates a second in the ROC space if and only if the first curve is below the second one in the $\widehat{ROC}$ space.*

At fixed $x \in (0, 1)$, if we denote by $y_1(x)$ the value of the first curve in the $\widehat{ROC}$ space at abscissa x and $y_2(x)$ the value of the second curve, we have the following equivalences:

$$\begin{aligned} y_1(x) \leq y_2(x) &\Leftrightarrow x + ay_1(x) \leq x + ay_2(x) \\ &\Leftrightarrow \frac{x}{x + ay_1(x)} \geq \frac{x}{x + ay_2(x)} \end{aligned} \tag{4}$$

which means than in the PR space, the first curve is above the second one with equation 3.

Remark 3.2. *Moreover, the expression found in equation (3) gives a more precise information than the theorem 3.2 in (Davis & Goadrich, 2006) because it shows that if, at a given abscissa, a curve is below another one in the $\widehat{ROC}$ space then, in the PR space, the first one will be above the second.*

3.3. Main theorem: Minimum and Maximum of AUC_{PR} at fixed AUC_{ROC}

We will denote by $AUC'_{ROC} = 1 - AUC_{ROC}$ the area under the curve in the $\widehat{ROC}$ space. We will see that the results will be expressed more easily as a function of AUC'_{ROC}.

Theorem 3.5. *At $AUC'_{ROC} = 1 - AUC_{ROC} = c$ fixed, the maximum of the AUC_{PR} is equal to:*

$$AUC_{PR}^{max} = 1 - a \ln(\frac{1 + a}{1 - c + a}). \tag{5}$$

and the minimum of the AUC_{PR} is equal to:

$$AUC_{PR}^{min} = 1 - ac \ln(\frac{1 + ac}{ac}). \tag{6}$$

Remark 3.3. *Here we find relatively simple analytical expressions.*

Demonstration 3.6. *For this demonstration we will place ourselves in $\widehat{ROC}$ space.*

First, let's remark that the ROC curve is always increasing, not necessarily continuously. As a result, in the $\widehat{ROC}$ space, the curve will also be increasing. Here we fix $c \in (0, 1)$ and we want to answer the question: at fixed $AUC' = c$ what is the maximum of the AUC_{PR}?

Mathematically, with equation (3) the problem takes the form:

$$\begin{cases} \sup\limits_{\text{increasing function } f} \int_0^1 \frac{x}{x + af(x)}\, dx \\ \qquad \textit{subject to} \\ f(0) = 0,\ f(1) = 1 \textit{ and } \int_0^1 f(x)\, dx = c \end{cases} \tag{7}$$

Before proceeding to the proof of the theorem 3.5, we will demonstrate a lemma that will allow us to restrict ourselves to step functions.

Lemma 3.7. *Let's denote by $T(f) = \int_0^1 \frac{x}{x+af(x)} dx$. Then for f and g two positive and increasing functions we have:*

$$|T(f) - T(g)| \leq 2\sqrt{2a}\sqrt{||f - g||_\infty} \tag{8}$$

where $||.||_\infty$ is the infinity norm

This lemma allows us to see that if two functions f and g are close for the infinity norm, then T(f) and T(g) are also close.

Proof of the Lemma: First, we remind that as f is increasing on $[0, 1]$ then f is Lebesgue integrable (it is even Riemann integrable) and as $0 \leq \frac{x}{x+af(x)} \leq 1, \forall x \in [0, 1]$, the integral $\int_0^1 \frac{x}{x+af(x)} dx$ is well defined.

Then

$$|T(f) - T(g)| = \left| \int_0^1 \left(\frac{x}{x + af(x)} - \frac{x}{x + ag(x)} \right) dx \right| \tag{9}$$

Let's denote by α a given real number in $(0, 1)$, we have by triangular inequality:

$$\begin{aligned} |T(f) - T(g)| \leq &\left| \int_0^\alpha \left(\frac{x}{x + af(x)} - \frac{x}{x + ag(x)} \right) dx \right| \\ &+ a \left| \int_\alpha^1 \frac{x}{(x + af(x))(x + ag(x))} (g(x) - f(x)) dx \right| \end{aligned} \tag{10}$$

And then, by applying the triangular inequality and observing that for all $x \in [0,1]$ we have:

$$0 \leq \frac{x}{(x+af(x))} \leq 1, \tag{11}$$

and

$$0 \leq \frac{x}{(x+ag(x))} \leq 1, \tag{12}$$

and for $x \in [\alpha, 1]$ we have:

$$\frac{x}{(x+af(x))(x+ag(x))} \leq \frac{1}{x} \leq \frac{1}{\alpha}, \tag{13}$$

we thus have for every $\alpha \in (0,1)$:

$$|T(f) - T(g)| \leq 2\alpha + \frac{a}{\alpha}||f-g||_\infty) \tag{14}$$

By studying the variations of the function

$$h : \alpha \longmapsto 2\alpha + \frac{1}{\alpha}||f-g||_\infty$$

and by taking it's minimum, we then find (8) which completes the proof of the lemma.

With Lemma 3.7, as the step functions are dense in the increasing space function for the infinity norm ($||.||_\infty$), we can restrict ourselves to step functions.

We will then prove that the step function which maximizes the system 7 is the following step function (see figure 1):

$$f : \begin{cases} [0,1] \longrightarrow [0,1] \\ x \longmapsto \begin{cases} 0 & \text{if } x \in [0, 1-c) \\ 1 & \text{if } x \in [1-c, 1] \end{cases} \end{cases} \tag{15}$$

Demonstration 3.8. *In order to prove that the step function which maximizes (7) is the function describe above (15) we will prove that if we have an increasing step function denoted f_0 with $f_0(0) = 0$ and $f_0(1) = 1$ and with $\int_0^1 f_0 = c$ which is not equal to 0 before $1-c$, then we can construct an other increasing step function denoted f_1 with $f_1(0) = 0$ and $f_1(1) = 1$ and $\int_0^1 f_1 = c$ and $T(f_1) > T(f_0)$. The result will follow.*

As the value of the integral does not depend on the values of the function at a few points, we will assume, without loss of generality, that the step functions are right continuous.

Let's denote by $x_0 \in [0, 1-c)$ the point such that f_0 is equal to 0 on $[0, x_0)$ and $f_0(x_0) = y_0 > 0$. Let's denote by $x_1 \in (x_0, 1)$ such that $\forall x \in [x_0, x_1)\,, f_0(x) = f_0(x_0) = y_0$

Then, let's take ϵ small enough and define the following f_1 function (see Figure 1):

$$f_1 : \begin{cases} [0,1] \longrightarrow [0,1] \\ x \longmapsto \begin{cases} 0 & \text{if } x \in [0, x_0+\epsilon) \\ y_1 = y_0 \frac{x_1 - x_0}{x_1 - x_0 - \epsilon} & \text{if } x \in [x_0+\epsilon, x_1) \\ f_0(x) & \text{otherwise} \end{cases} \end{cases}$$

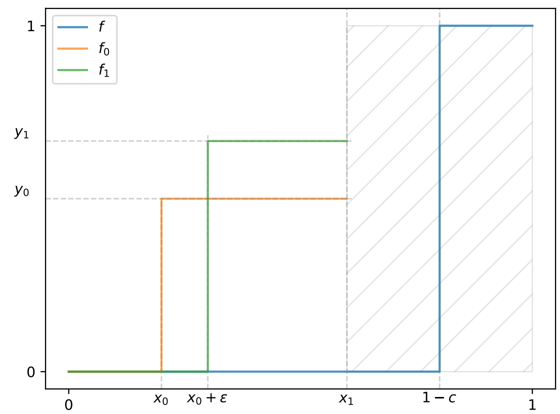

Figure 1. Step Functions. f is the step function that maximizes equation (7)

We can take ϵ small enough such that f_1 is well defined and increasing. Moreover, the condition on y_1 implies that $\int_0^1 f_1 = \int_0^1 f_0$

As f_1 and f_0 are equal outside $[x_0, x_1]$ we have:

$$\begin{aligned} T(f_1) - T(f_0) &= \int_{x_0}^{x_1} \left(\frac{x}{x+af_1(x)} - \frac{x}{x+af_0(x)}\right)dx \\ &= \int_{x_0}^{x_0+\epsilon} 1\,dx + \int_{x_0+\epsilon}^{x_1} \frac{x}{x+ay_1}dx - \int_{x_0}^{x_1} \frac{x}{x+ay_0}dx \end{aligned} \tag{16}$$

Then by integrating the previous relation we find that:

$$\begin{aligned} T(f_1) - T(f_0) = \epsilon + [x - ay_1 \ln(x+ay_1)]_{x_0+\epsilon}^{x_1} - \\ [x - ay_0 \ln(x+ay_0)]_{x_0}^{x_1} \end{aligned} \tag{17}$$

And thus:

$$\begin{aligned} T(f_1) - T(f_0) = &- ay_1 \ln(x_1 + ay_1) \\ &+ ay_1 \ln(x_0 + \epsilon \\ &\quad + ay_1) \\ &+ ay_0 \ln(x_1 + ay_0) \\ &- ay_0 \ln(x_0 + ay_0) \end{aligned} \tag{18}$$

By doing a first-order Taylor expansion in ϵ, after a few calculations, we find that:

$$ay_1 \ln(x_1 + ay_1) = ay_0 \ln(x_1 + ay_0)+ \epsilon(\frac{ay_0}{x_1 - x_0} \ln(x_1 + ay_0) + \frac{a^2 y_0^2}{(x_1 - x_0)(x_1 + ay_0)}) + o(\epsilon) \tag{19}$$

and

$$ay_1 \ln(x_0 + \epsilon + ay_1) = ay_0 \ln(x_0 + ay_0)+ \epsilon\left(\frac{ay_0}{x_1 - x_0} \ln(x_0 + ay_0) + \frac{ay_0}{x_0 + ay_0}\right)+ \frac{\epsilon a^2 y_0^2}{(x_1 - x_0)(x_0 + ay_0)} + o(\epsilon) \tag{20}$$

By replacing the expressions of (19) and (20) in (18) we find that:

$$T(f_1) - T(f_0) = \epsilon(-\frac{ay_0}{x_1 - x_0} \ln(x_1 + ay_0)+ \frac{ay_0}{x_1 - x_0} \ln(x_0 + ay_0) + \frac{ay_0}{x_0 + ay_0}- \frac{a^2 y_0^2}{(x_1 - x_0(x_1 + ay_0)} + \frac{a^2 y_0^2}{(x_1 - x_0)(x_0 + ay_0)}) + o(\epsilon) \tag{21}$$

Thus

$$T(f_1) - T(f_0) = \epsilon(-\frac{ay_0}{x_1 - x_0} \ln(\frac{x_1 + ay_0}{x_0 + ay_0})+ \frac{ay_0}{x_0 + ay_0} + \frac{ay_0}{(x_0 + ay_0)} \frac{ay_0}{(x_1 + ay_0)}) + o(\epsilon) \tag{22}$$

By writing

$$\ln(\frac{x_1 + ay_0}{x_0 + ay_0}) = \ln(1 + \frac{x_1 - x_0}{x_0 + ay_0}) \tag{23}$$

and using the concavity inequality for the logarithm:

$$\ln(1 + \frac{x_1 - x_0}{x_0 + ay_0}) < \frac{x_1 - x_0}{x_0 + ay_0} \tag{24}$$

we find that the first term in ϵ in $T(f_1) - T(f_0)$ is greater than:

$$\frac{ay_0}{(x_0 + ay_0)} \frac{ay_0}{(x_1 + ay_0)} \tag{25}$$

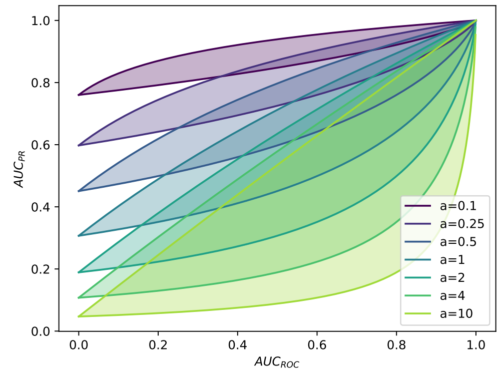

Figure 2. Maximum and Minimum of the AUC_{PR} as a function of the AUC_{ROC}

which is strictly positive.

Thus, for ϵ small enough, $T(f_1) - T(f_0) > 0$ which completes the demonstration.

It follows directly that the maximum of the AUC_{PR} is equal to:

$$\int_0^{1-c} 1 + \int_{1-c}^1 \frac{x}{x+a} dx = 1 - c + \int_{1-c}^1 1 - \frac{a}{x+a} dx \tag{26}$$

And therefore, by integrating in the previous equation (26), the maximum value is equal to:

$$AUC_{PR}^{max} = 1 - a \log(\frac{1+a}{1-c+a}) \tag{27}$$

With the same arguments, we demonstrate that the minimum is reached for the function constant equal to c. And therefore, the minimum of the AUC_{PR} is equal to:

$$AUC_{PR}^{min} = \int_0^1 \frac{x}{x+ac} dx = 1 - ac \ln(\frac{1+ac}{ac}) \tag{28}$$

3.4. Minimum and Maximum of AUC_{ROC} at fixed AUC_{PR}

We can reverse the formulas of theorem 3.5 to find the minimum and the maximum of AUC_{ROC} at fixed AUC_{PR}. More precisely we have the following theorem:

Theorem 3.9. *At $AUC_{PR} = k$ fixed, if we denote by F the function:* $\begin{array}{rccc} F & : & (0, +\infty) & \to & \mathbb{R} \\ & & x & \mapsto & x \ln(\frac{1+x}{x}) \end{array}$, *the maximum of the AUC_{ROC} is equal to:*

$$AUC_{ROC}^{max} = 1 - \frac{F^{-1}(1-k)}{a} \tag{29}$$

and the minimum of the AUC_{ROC} is equal to:

$$AUC_{ROC}^{min} = 1 - \frac{(e^{\frac{1-k}{a}} - 1)}{e^{\frac{1-k}{a}}}(1+a) \tag{30}$$

Demonstration 3.10. *Let's denote as previously, $AUC'_{ROC} = 1 - AUC_{ROC}$. We suppose that $k \in [1 - a\ln(\frac{1+a}{a}), 1]$ is the AUC_{PR} and is fixed.*

With theorem 3.5, and as illustrated by the Figure 2 we have that $c = AUC_{ROC}^{min'}$ satisfies

$$1 - ac\ln(\frac{1+ac}{ac}) = k \tag{31}$$

and thus, by setting $x = ac$, we have $F(x) = 1 - k$ then $x = F^{-1}(1-k)$ and then $c = \frac{F^{-1}(1-k)}{a}$.

Finally:

$$AUC_{ROC}^{max} = 1 - AUC_{ROC}^{min'} = 1 - \frac{F^{-1}(1-k)}{a} \tag{32}$$

Regarding the minimum we use the same method, $AUC_{ROC}^{max'} = c$ satisfies with theorem 3.5 the relationship:

$$1 - a\ln(\frac{1+a}{1-c+a}) = k \tag{33}$$

and then:

$$\ln(\frac{1+a}{1-c+a}) = \frac{1-k}{a}, \tag{34}$$

then:

$$(1+a) = e^{\frac{1-k}{a}}(1-c+a), \tag{35}$$

then:

$$c = \frac{(e^{\frac{1-k}{a}} - 1)}{e^{\frac{1-k}{a}}}(1+a). \tag{36}$$

As $AUC_{ROC}^{max'} = 1 - AUC_{ROC}^{min}$, we find the expression of AUC_{ROC}^{min}.

3.5. Short demonstration of the global minimum of AUC_{PR}

In their article (Boyd et al., 2012), the authors find in their Theorem 2 an expression of the global minimum of the AUC_{PR}, that is to say the minimum over all the possible AUC_{ROC} which is naturally achieved for an $AUC_{ROC} = 0$. They use this minimum value to define a normalized AUC_{PR} which, like the AUC_{ROC}, can take all values between 0 and 1.

We can notice that this result is weaker than ours because it determines the global minimum of the AUC_{PR} and not the minimum of the AUC_{PR} at fixed AUC_{ROC}. Moreover, this result is a simple corollary of our theorem 3.5:

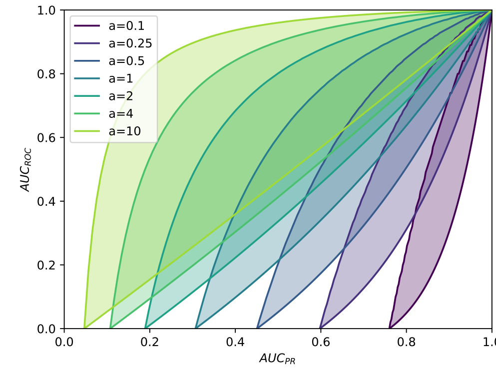

Figure 3. Maximum and Minimum of the AUC_{ROC} as a function of the AUC_{PR}

Corollary 3.11. *In their article, (Boyd et al., 2012) find that the global minimum of the AUC_{PR} is equal to:*

$$AUC_{PR}^{global\,min} = 1 + \frac{(1-\pi)\ln(1-\pi)}{\pi} \tag{37}$$

where $\pi = \frac{N^+}{N}$

Using our theorem 3.5, we can find that the global minimum of AUC_{PR} is equal to $AUC_{PR}^{global\,min} = AUC_{PR}^{max}(c := 1) = AUC_{PR}^{min}(c := 1) = 1 - a\ln(\frac{1+a}{a})$

Finally, as $1 - \pi = \frac{N^-}{N^+}$ and $1 + a = \frac{N}{N^+}$, we get $\frac{a}{1+a} = \frac{N^-}{N} = 1 - \pi$ and then we have:

$$1+\frac{(1-\pi)\ln(1-\pi)}{\pi} = 1+a\ln(\frac{a}{a+1}) = 1-a\ln(\frac{a+1}{a}) \tag{38}$$

which shows that the two results are identical.

4. Consequences of the Previous Theorems

4.1. Good AUC_{ROC} does not mean good model

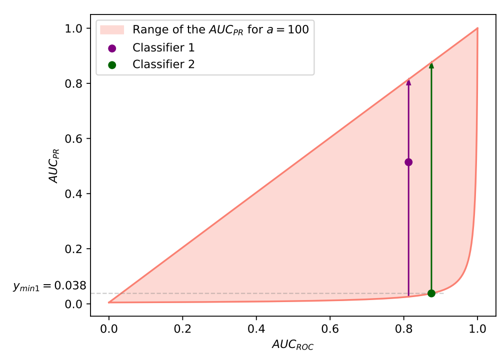

Figure 4. How the example classifiers presented by (Davis & Goadrich, 2006) compare to the range limits we found for the AUC_{PR}

In their article, (Davis & Goadrich, 2006) prove that algorithms that optimize the AUC_{ROC} do not necessarily optimize the AUC_{PR} by giving the example of 2 classifiers for a dataset with $a = 100$: $Classifier1$ and $Classifier2$. AUC_{ROC} of $Classifier2$ is greater than the $Classifier1$'s one (0.875 versus 0.813); however, the AUC_{PR} of the $Classifier1$ is way greater than the $Classifier2$'s one (0.514 versus 0.038).

Interestingly, as depicted by Figure 4, when choosing a classifier that performed really bad on the AUC_{PR} score, they found a classifier that reached the minimum given by our theorem 3.5 of the AUC_{PR} for $a = 100$ and $AUC_{ROC} = 0.875$. With our theorem, we are not only able to find examples such as the ones presented by (Davis & Goadrich, 2006) but we are now able to quantify precisely how much the AUC_{PR} can vary at fixed a and AUC_{ROC} values. For example, for $a = 100$, a classifier with a good $AUC_{ROC} = 0.875$ can have a AUC_{PR} that ranges from 0.038 to 0.876. On the other hand, if $a = 1$ the AUC_{PR} ranges from 0.725 to 0.935 (as depicted by Figure 2).

We can thus conclude that the ROC curve is not always suitable to measure the performance of a model, especially when the dataset is highly imbalanced. Nevertheless, our theorem 3.5 ensures that for a balanced dataset, a classifier with a good AUC_{ROC} is bound to have a good AUC_{PR}.

4.2. AUC_{PR} vs AUC_{ROC} for imbalanced dataset

It is unclear whether we should always prioritize AUC_{ROC} or AUC_{PR}. However, there is a general trend suggesting that in the case of imbalanced datasets, AUC_{PR} should be prioritized. This is notably described in the following articles (Saito & Rehmsmeier, 2015; Sofaer et al., 2019; Cook & Ramadas, 2020). The AUC_{PR} is more informative for imbalanced datasets due to the fact that a good AUC_{ROC} does not necessarily mean a good model when dealing with imbalanced data. Our results further illustrate this point, especially for highly imbalanced datasets with many more negative examples than positive (i.e. $a \gg 1$), which is the case for many real-world binary classification problems such as Fraud Detection, Disease Diagnosis or Spam Email Detection. In such situations, machine learning practitioners should use AUC_{PR} instead of AUC_{ROC}. Indeed, a good AUC_{PR} (above 0.7) will necessarily result in a good AUC_{ROC} but the opposite is not true as discussed in the previous section : for $a = 100$ and $AUC_{PR} = 0.7$ the AUC_{ROC} ranges from 0.697 to 0.999 while for a $AUC_{ROC} = 0.7$ the AUC_{PR} ranges from 0.016 to 0.703.

4.3. When $AUC_{ROC1} \geq AUC_{ROC2}$ implies $AUC_{PR1} \geq AUC_{PR2}$ and vice versa

It is natural to say that a model 1 is better than a model 2 when $AUC_{ROC_1} \geq AUC_{ROC_2}$ and $AUC_{PR_1} \geq AUC_{PR_2}$. However, thanks to the theorem 3.5, to check these two conditions it is sometimes unnecessary to calculate the two AUCs, which can be sometimes really time consuming. Indeed traditional AUC computation is non-differentiable and has a time complexity of $O(n^2)$. RankOpt (Herschtal & Raskutti, 2004) which reduces the time complexity to $O(n)$ and more generally the AUC maximization field, recently surveyed by (Yang & Ying, 2022), shows that optimizing the AUC computation is of interest. We show below that computing AUC_{ROC} is not always necessary anymore if AUC_{PR} is already computed and vice versa. We have the following corollary:

Corollary 4.1. *With the expressions of theorem 3.5 and 3.9, by considering the functions* $c \mapsto AUC_{PR}^{min}(c)$, $c \mapsto AUC_{PR}^{max}(c)$, $k \mapsto AUC_{ROC}^{min}(k)$, $k \mapsto AUC_{ROC}^{max}(k)$ *we have:*

If $AUC_{PR}^{min}(1 - AUC_{ROC_1}) \geq AUC_{PR}^{max}(1 - AUC_{ROC_2})$ *then* $AUC_{PR_1} \geq AUC_{PR_2}$

and

If $AUC_{ROC}^{min}(AUC_{PR_1}) \geq AUC_{ROC}^{max}(AUC_{ROC_1})$ *then* $AUC_{ROC_1} \geq AUC_{ROC_2}$

Demonstration 4.2. *By the definition of the minimum we have:* $AUC_{PR_1} \geq AUC_{PR}^{min}(1 - AUC_{ROC_1})$ *and by the definition of the maximum we have* $AUC_{PR}^{max}(1 - AUC_{ROC_2}) \geq AUC_{PR_2}$ *and thus if* $AUC_{PR}^{min}(1 - AUC_{ROC_1}) \geq AUC_{PR}^{max}(1 - AUC_{ROC_2})$ *we get* $AUC_{PR_1} \geq AUC_{PR_2}$.

Idem for the other inequality.

5. Conclusion

In this paper, we study the relationship between AUC_{ROC} and AUC_{PR} in binary classification models. We established an exact analytical expression for the transformation between ROC and PR curves. More precisely given an AUC_{ROC} we determine exact bounds for the corresponding AUC_{PR} and vice versa. Our results confirms that in certain situations, especially for imbalanced datasets, it is more informative to prioritize AUC_{PR} over AUC_{ROC}. The conventional reliance on AUC_{ROC} as the sole metric of model performance might as a result not be optimal in this situation. These findings provide clear, actionable guidance for evaluating and comparing binary classification models. We believe that these results will enhance the understanding and application of AUC_{ROC} and AUC_{PR} in binary classification, particularly in the context of imbalanced datasets.

Impact Statement

This paper presents work whose goal is to advance the field of Machine Learning. There are many potential societal consequences of our work, none which we feel must be specifically highlighted here.

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