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A Straight Forward Approach in Understanding the Improperness of ROC Curve

R. Vishnu Vardhan[1], S. Balaswamy[2] and G. Sameera[3]
[1]*Department of Statistics, Pondicherry University, Puducherry*
[2]*Department of Statistics, Indira Gandhi National Tribal University, Madhya Pradesh*
[3]*Biostatistics and Pharmacometrics, Global Drug Development, Novartis Healthcare Private Limited, Hyderabad*

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Abstract

The present paper is based on the framework of a classification tool namely, Multivariate Receiver Operating Characteristic (MROC) curve, which is modelled to provide a better classification. In general, there are certain properties where the proposed ROC curve has to satisfy, violating any of such property leads to inappropriate conclusions about the classifier. In this paper, a straight forward approach is presented to explain the nature of 'Proper' and 'Improper' ROC curves. The methodology is supported with both simulated and real data sets.

Key words: MROC curve; AUC, Improper MROC curve; Inflection point; Crossing point.

AMS Subject Classifications: 92B15, 62P10

1. Introduction

Over the past seven to eight decades, the problem of detecting/identifying one's behavior and allocating them into one of the population gained lot of attention. Such work was majorly observed and initially related in the fields of Experimental Psychology and Signal Detection Theory (Tanner and Swets, 1954, Green and Swets, 1966). However, with the involvement of statistical essentials, this area branched to diversified fields of Science and Technology, namely Diagnostic Medicine, Banking, Finance and many more (Lusted, 1971, Krzanowski and Hand, 2009). All these come under the hub of classification tools/techniques (Statistical Decision Theory). The practice of allocation or separation is based on certain characteristics of univariate or multivariate in nature.

Initial application of this was in Medicine and used majorly to identify the individual's health status by defining an optimal threshold for a biomarker observed in the case of that particular disease. The first parametric ROC is the Binormal ROC Curve where the

Correponding Author: S. Balaswamy
Email:balaswamy.stats@gmail.com
(The third author, G. Sameera works for Novartis. Views expressed in this work are her own)

variable under study for two independent populations (healthy/diseased or signal/noise) follow Normal distributions (Green and Swets, 1966). The important properties of ROC curve are:

(i) $y = h(x)$ is the mathematical model of the ROC curve, where y denotes the true positive rate and x denotes the false positive rate. The curve is a monotonic increasing function in the positive quadrant, lying between $y = 0$ at $x = 0$ and $y = 1$ at $x = 1$.

(ii) The ROC curve is unaltered if the classification scores undergo a strictly increasing transformation.

(iii) The slope of the ROC curve (likelihood ratio of ROC curve) at threshold value 'c' is always positive and given by

$$\frac{dy}{dx} = \frac{P(U > c|1)}{P(U > c|0)}$$

When dealing with practical problems, we often come across the presence or involvement of several variables to have a classifier rule for a better classification. Su and Liu (1993), Reiser and Ferragi (1997), Schisterman *et al.* (2004), Liu *et al.* (2005), Yuan and Ghosh (2008), Chang and Park (2009) and Sameera *et al.* (2016) are a few to cite among those who proposed an extension of univariate ROC model to multivariate. However the present work is based upon the Multivariate ROC (MROC) model proposed by Sameera *et al.* (2016), as they showed that this model works better than the model proposed by Su and Liu (1993) and their model is applicable to data where the covariance structures of two populations can be proportional or non-proportional. As mentioned about the properties of the ROC curve, the most important one to verify is its concavity *i.e.*, slope of the ROC curve is always positive. Now the question that arises is, what happens if a curve is not satisfying the concavity property? If the curve violates this property, it might affect the accuracy of the test as well as the optimal cutoff point defined for that particular test. Mathematically, a meaningful decision variable should be an increasing function of the likelihood ratio (Pepe, 2003) and such MROC curve is said to be "Proper". A function whose first derivative is decreasing throughout an open interval is called concave in that interval, and a function whose first derivative is increasing throughout an open interval is called convex in that interval. Since the slope of an MROC curve for a continuous decision variable is equal to the likelihood ratio at the corresponding threshold, it follows that the slope of a MROC curve decreases as the false positive rate (FPR) increases, that is, a MROC curve will be concave everywhere ($0 \leq FPR \leq 1$). If the decision variable is not an increasing function of the likelihood function, then its model and corresponding MROC curve are said to be improper.

2. Illustration of Improper MROC (iMROC) Curve

Consider the following example which illustrates the Indian Liver Patients (ILP) dataset for which the MROC curve has been drawn and depicted in Figure 1. The fitted MROC curve seems to be proper but when observed keenly; the improperness of the curve can be

witnessed. In such situation, the usual MROC curve methodology might not project the true accuracy of a test and will not be used for future classification. Figure 1 visualizes the two crucial points namely, Crossing Reference line ((t_0) or Crossing Point) and Inflection Reference line ((t_1) or Inflection Point). Figure 1 shows the corresponding fitted MROC curve; note that there is a visible 'dip' in the curve crossing the chance line near the upper right hand corner of the unit square plot. In Figure 1, MROC curve crosses the chance line at the point (1-Specificity, Sensitivity) = (0.96, 0.96), shown by the intersection of the "crossing" reference line with the MROC curve. Furthermore, this MROC curve is concave for $FPR < 0.76$, but is convex for $FPR > 0.76$. Therefore, the MROC curve which separates the concave and convex portions of the curve is called the "Inflection Point (t_1)". Similarly, the MROC curve which crosses the chance line at the point where FPR=TPR is called the "Chance line crossing point or Crossing Point (t_0)". From Figure 1, though the

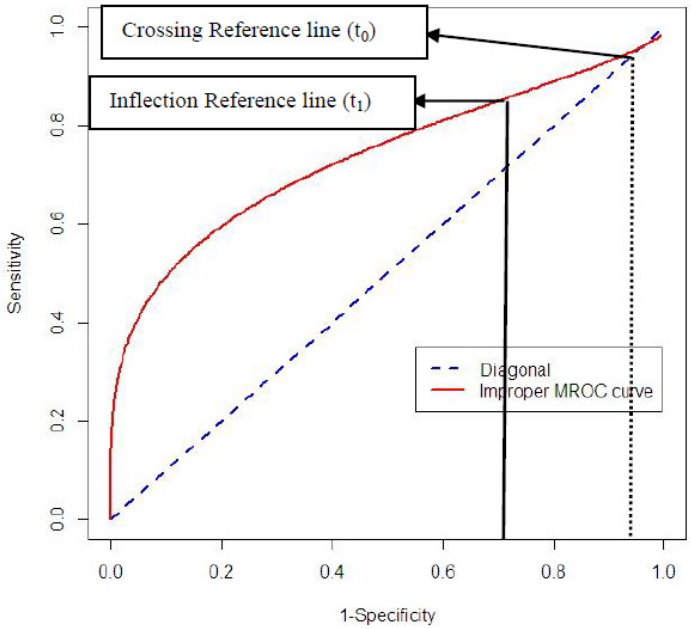

Figure 1: Improper MROC curve for ILP dataset

dip of the curve is visible *i.e.* the MROC curve is not concave everywhere, it is not possible to identify the inflection point visually. Even in the case of improper MROC curves, it is not that easy to identify the point where the curve changes from concave to convex. In order to deal with this situation, the ways to measure the improperness of an MROC curve is shown in subsequent sections with the help of real and simulated data sets.

2.1. MROC curve

Let U_0 and $U_0 \in$ U be the vectors of test scores of two independent multivariate normal populations with mean vectors μ_0, μ_1 and co-variance matrices Σ_0 and Σ_1 with m and n sample sizes respectively.

$$U_i \sim MVN(\mu_i, \Sigma_i); i = 0, 1$$

$$f(X|\mu_i, \Sigma_i) = \frac{1}{(2\Pi)^{\frac{p}{2}}|\Sigma_i|^{\frac{N}{2}}} e^{\frac{-1}{2}(X-\mu_i)'\Sigma_i^{-1}(X-\mu_i)}$$

Let $x(c)$ denote the false positive rate (FPR) and $y(c)$ denote the true positive rate (TPR) where 'c' is the threshold value. The expressions for FPR, TPR are

$$FPR = x(c) = P(U > c|0) = 1 - \Phi\left(\frac{c - b'\mu_0}{\sqrt{(b'\Sigma_0 b)}}\right) \tag{1}$$

$$TPR = y(c) = P(U > c|1) = \Phi\left(\frac{b'\mu_1 - c}{\sqrt{(b'\Sigma_1 b)}}\right) \tag{2}$$

where $b(\neq 0)$ be a $k \times 1$ vector. The threshold value thus obtained using (1) is given as

$$c = b'\mu_0 + \sqrt{(b'\Sigma_0 b)}\Phi^{-1}(1-x) \tag{3}$$

where $\Phi^{-1}(.)$ is the inverse function of $\Phi(.)$

substituting (3) in (2) implies that

$$TPR = y(c) = \Phi\left(\frac{b'(\mu_1 - \mu_0) - \sqrt{(b'\Sigma_0 b)}\Phi^{-1}(1-x)}{\sqrt{(b'\Sigma_1 b)}}\right) \tag{4}$$

which is the form of Multivariate ROC model (Sameera *et al.*, 2016)

The AUC of MROC curve is

$$AUC = \Phi\left\{\frac{b'(\mu_1 - \mu_0)}{\sqrt{(b'(\Sigma_0 + \Sigma_1)^{-1}b}}\right\} \tag{5}$$

2.2. Crossing point

In order to verify whether the generated ROC curve is 'proper' or 'improper', Balaswamy *et al.* (2020) came out with two measures namely crossing point and inflection point. The mathematical framework of these measures are adopted here to maintain the continuity of explanation about proper vs improper ROC curves. Let 'c' denote threshold to a chance line crossing FPR, then

$$P(U > c|0) = P(U > c|1)$$

$$\Rightarrow \Phi\left(\frac{c - b'\mu_0}{\sqrt{(b'\Sigma_0 b)}}\right) = \Phi\left(\frac{c - b'\mu_1}{\sqrt{(b'\Sigma_1 b)}}\right)$$

on further simplification, the expression for c_0 crossing threshold is

$$c_0 = \frac{(b'\mu_0)\sqrt{(b'\Sigma_1 b)} - (b'\mu_1)\sqrt{(b'\Sigma_0 b)}}{\sqrt{(b'\Sigma_1 b)} - \sqrt{(b'\Sigma_0 b)}} \tag{6}$$

Let t_0 denote the chance line crossing FPR corresponding to c_0. Then

$$t_0 = P(U > c_0|0) = 1 - \Phi\left(\frac{c_0 - b'\mu_0}{\sqrt{(b'\Sigma_0 b)}}\right)$$

on substituting (6) in the above expression, we obtain the expression for crossing point as,

$$t_0 = \Phi\left(\frac{b'\mu_1 - b'\mu_0}{\sqrt{(b'\Sigma_1 b)} - \sqrt{(b'\Sigma_0 b)}}\right) \tag{7}$$

Uniqueness of t_0 follows from the uniqueness of c_0.

2.3. Inflection point

The slope of ROC curve is twice differentiable. From basic calculus results concerning concave functions it follows that the MROC curve is concave (convex) over an open interval if its second derivative is negative (positive) throughout the interval (0, 1). The approach is to show that the second derivative of the MROC curve is negative throughout $(0, t_1)$ and positive throughout $(t_1, 1)$ if $v < 1$, and positive throughout $(0, t_1)$ and negative throughout $(t_1, 1)$ if $v > 1$.

Let t denote an FPR with corresponding threshold c. The derivative of the MROC curve evaluated at t is equal to the likelihood ratio evaluated at c, *i.e.*,

$$\frac{\partial ROC(t)}{\partial t} = LR(c)$$

i.e., at $t = t_0$

$$\frac{\partial ROC(t)}{\partial t}/t = t_0 = LR(c_0)$$

it follows, using the chain rule, that

$$\frac{\partial^2 ROC(t)}{\partial^2 t} = \frac{\partial LR(c)}{\partial c}\frac{\partial c}{\partial t} \tag{8}$$

since,

$$t = P(U > c|0) = 1 - P(U < c|0) = 1 - \Phi\left(\frac{c_0 - b'\mu_0}{\sqrt{(b'\Sigma_0 b)}}\right)$$

then t is a strictly decreasing function of c and

$$\frac{\partial c}{\partial t} = -\frac{1}{\sqrt{(b'\Sigma_0 b)}}\varphi\left(\frac{c_0 - b'\mu_0}{\sqrt{(b'\Sigma_0 b)}}\right)$$

therefore, the equation (8) can be rewritten as,

$$\frac{\partial^2 ROC(t)}{\partial^2 t} = \frac{\partial LR(c)}{\partial c}\left[-\frac{1}{\sqrt{(b'\Sigma_0 b)}}\varphi\left(\frac{c_0 - b'\mu_0}{\sqrt{(b'\Sigma_0 b)}}\right)\right]^{-1} \tag{9}$$

Since $\varphi\left(\frac{c_0-b'\mu_0}{\sqrt{(b'\Sigma_0 b)}}\right) > 0$, it follows from Equation (9) that the second derivative of the MROC curve and the derivative of the likelihood ratio have opposites signs when evaluated at t and c, respectively (Balaswamy *et al.*, 2020).

The threshold value at the inflection point is given by

$$c_1 = \frac{(b'\Sigma_1 b)(b'\mu_0) - (b'\Sigma_0 b)(b'\mu_1)}{(b'\Sigma_1 b) - (b'\Sigma_0 b)} \tag{10}$$

then the corresponding FPR is

$$t_1 = 1 - \Phi\left(\frac{c_1 - b'\mu_0}{\sqrt{(b'\Sigma_0 b)}}\right)$$

on substituting c_1 in the above equation, the FPR at the corresponding c_1 is given by

$$t_1 = 1 - \Phi\left(\frac{\left\{\frac{(b'\Sigma_1 b)(b'\mu_0)-(b'\Sigma_0 b)(b'\mu_1)}{(b'\Sigma_1 b)-(b'\Sigma_0 b)}\right\} - b'\mu_0}{\sqrt{(b'\Sigma_0 b)}}\right) \tag{11}$$

on further simplification, the FPR value at the inflection point is as follows

$$t_1 = \Phi\left(\frac{(b'\mu_1 - b'\mu_0)\sqrt{(b'\Sigma_0 b)}}{(b'\Sigma_1 b) - (b'\Sigma_0 b)}\right) \tag{12}$$

Since the derivative of the log likelihood ratio will have opposite sign of the second derivative of the MROC curve evaluated at the corresponding FPR and thresholds less than c_1 correspond to FPRs greater than t_1 and vice versa, the FPR value

$$t_1 = \Phi\left(\frac{(b'\mu_1 - b'\mu_0)\sqrt{(b'\Sigma_0 b)}}{(b'\Sigma_1 b) - (b'\Sigma_0 b)}\right)$$

is the unique inflection point FPR and

$$c_1 = \frac{(b'\Sigma_1 b)(b'\mu_0) - (b'\Sigma_0 b)(b'\mu_1)}{(b'\Sigma_1 b) - (b'\Sigma_0 b)}$$

is its corresponding inflection point threshold.

3. Results and Discussion

3.1. Proper MROC curve

In order to explain the concept of Proper MROC curve, the Statlog (heart) data taken from UCI repository is used. The heart dataset consists of 270 samples of which 120 (44.4%) are diagnosed with presence of heart disease and 150 (55.6%) with absence of heart disease. The parameters age, sex (Male: 183, 67.78% & Female: 87, 32.22%), chest pain type

(4 nominal values), resting blood pressure, serum cholesterol, fasting blood sugar, resting electrocardiographic (ECG) results (0, 1&2), maximum heart rate achieved, exercise induced angina, oldpeak, the slope of the peak exercise ST segment, number of major vessels (0-3) colored by fluoroscopy and thal (normal, fixed defect & reversible defect) are considered for diagnosis. MROC curve is fitted and it corresponding linear combination is

$$\begin{aligned} U = &-0.022 * Age + 1.323 * Sex + 0.829 * Chestpaintype + 0.019 * Restingbloodpressure \\ &+ 0.005 * SerumCholesterol - 0.724 * Fastingbloodsugar \\ &+ 0.358 * RestingECGresults - 0.025 * Maximumheartrate \\ &+ 1.091 * Exerciseinducedangina + 0.424 * Oldpeak + 0.534 * thal \\ &+ 0.398 * SlopeofthepeakexerciseSTsegment + 1.269 * Numberofmajorvessels \end{aligned}$$

This linear combination helps us to know the status of a new individual basing on the U value. From the results, the curve is found to be proper by satisfying the property of monotonic likelihood ratio of MROC curve, hence it is a Proper MROC curve and the figure is depicted in Figure 2.

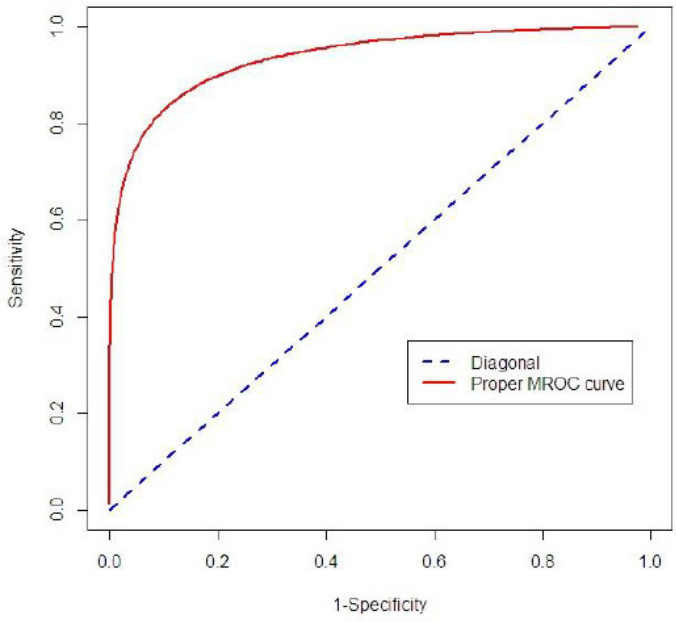

Figure 2: Proper MROC curve for Heart dataset

The optimal threshold value for identifying heart disease in an individual when the above mentioned characteristics studied is 7.27 with accuracy (AUC) of 93.7%. If score obtained for a new patient U is greater than 7.27, the individual will be allocated to heart disease group. The obtained threshold is observed to have 86.2% of sensitivity and 13.8% of 1-specificity (false positive rate). This means that the threshold is able to identify the true status of individual in a sensible manner with 86.2% by allowing 13.8% of false positive cases. This features out that the performance of the threshold has to be improved in such a way that the percentage of false positive rate can be minimized.

3.2. Improper MROC (iMROC) curve

The concept of iMROC curve is supported with the help of simulation studies as well as real datasets. The degree of improperness is also measured with the help of crossing point and inflection point and the results are reported along with the figures.

3.2.1. Simulation study

Two sets of multivariate normal random numbers are generated with mean vectors and covariance matrices (Table 1) for various samples sizes 25, 50, 100 and 300 respectively.

Table 1: Mean Vectors and Covariance Matrices of Simulation Studies

	μ_D	μ_H	Σ_D	Σ_H
1	$\begin{pmatrix}0.8606\\1.68\\5.1302\end{pmatrix}$	$\begin{pmatrix}0.8059\\1.5812\\4.7992\end{pmatrix}$	$\begin{pmatrix}0.0084 & 0.0057 & 0.1221\\0.0057 & 0.1183 & 0.0601\\0.1221 & 0.0601 & 2.3087\end{pmatrix}$	$\begin{pmatrix}0.0046 & 0.0001 & 0.0561\\0.0001 & 0.1274 & 0.0037\\0.0561 & 0.0037 & 0.7628\end{pmatrix}$
2	$\begin{pmatrix}0.7305\\1.39\\3.6302\end{pmatrix}$	$\begin{pmatrix}0.7057\\1.2811\\3.5992\end{pmatrix}$	$\begin{pmatrix}0.0084 & 0.0057 & 0.1221\\0.0057 & 0.1183 & 0.0601\\0.1221 & 0.0601 & 2.3087\end{pmatrix}$	$\begin{pmatrix}0.0046 & 0.0001 & 0.0561\\0.0001 & 0.1274 & 0.0037\\0.0561 & 0.0037 & 0.7628\end{pmatrix}$

The accuracy and intrinsic measures along with the linear combinations obtained for the simulated data sets are reported in Table 2.

Table 2: Measures of MROC curve for two sets of simulations at four different sample sizes

Simulation	Samples	c	AUC	TPR	FPR	Linear combination
I	25	2.1928	0.5817	0.5591	0.4408	$2.95 * X_1 + 0.50 * X_2$ - $0.12 * X_3$
	50	4.4107	0.6323	0.5979	0.4020	$6.01 * X_1$ - $0.10 * X_2$ - $0.07 * X_3$
	100	9.8698	0.6754	0.6444	0.3555	$1627 * X_1 + 0.62 * X_2$ - $0.90 * X_3$
	300	18.5639	0.7003	0.6640	0.3359	$29.69 * X_1 + 0.99 * X_2$ - $1.53 * X_3$
II	25	-1.6330	0.5713	0.5543	0.4456	$-2.93 * X_1 + 0.51 * X_2$ - $0.07 * X_3$
	50	2.0133	0.6109	0.5811	0.4188	$3.62 * X_1 + 1.05 * X_2$ - $0.53 * X_3$
	100	4.3673	0.6493	0.6111	0.3888	$5.37 * X_1 + 0.84 * X_2$ - $0.16 * X_3$
	300	2.5782	0.6519	0.5943	0.4056	$3.35 * X_1 + 1.16 * X_2$ - $0.23 * X_3$

Here, an observation made is that as the sample size increases the accuracy (AUC) is also slightly improving even though the expressions for the intrinsic measures FPR, TPR and the accuracy measure AUC are free from the sample size. This means that, there is slight deviation in the accuracy as the curve deviates from cancavity to convexity (Figure 3 and 4). Therefore, iMROC curve is not able to provide the maximum extent of correct classification with less misclassification rate due to the shift in the magnitude of the curve.

3.2.2. Real datasets

In order to demonstrate the iMROC curve, MCA and ILP datasets are used. Further, ILP dataset has been split according to gender of the patients. Of which, ILP male dataset

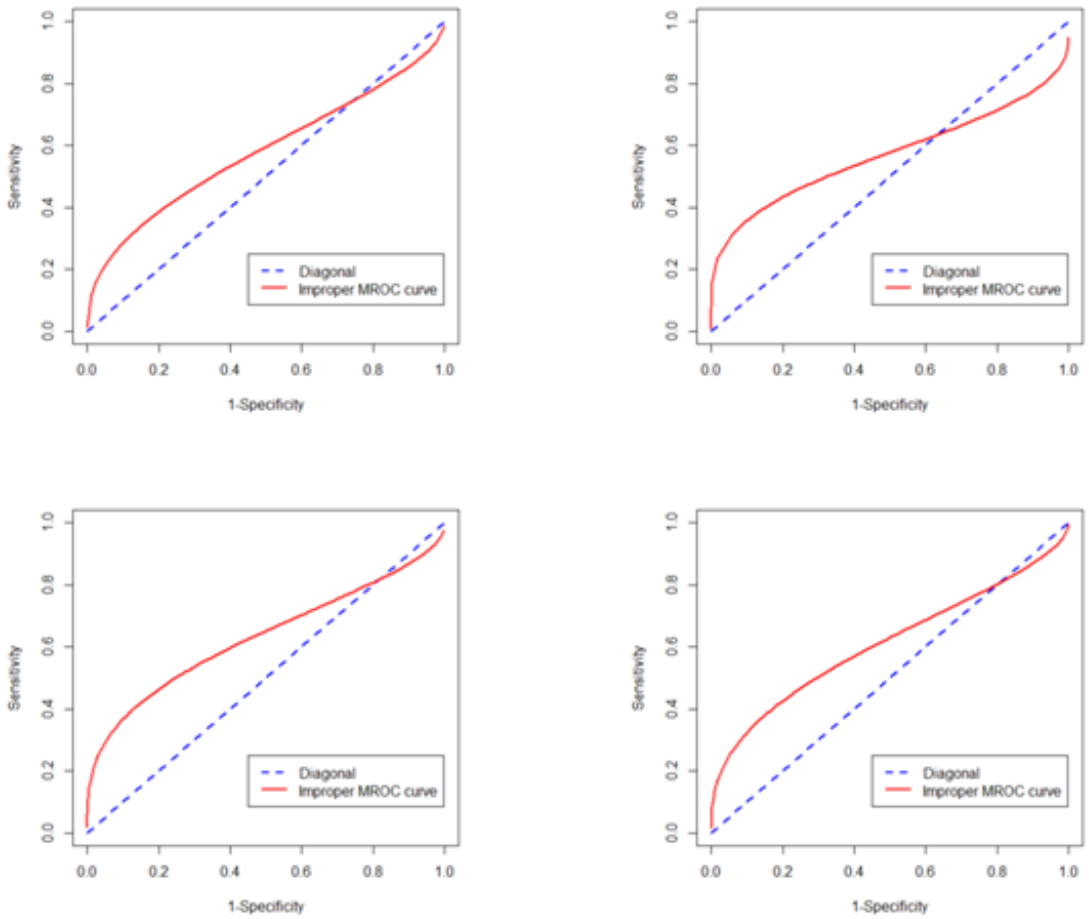

Figure 3: iMROC curves for Simulation datasets at different sample sizes with 25 and 50

has a form of Improper ROC curve and the same dataset has been chosen for demonstration purpose.

ILP Male dataset (Ramana *et al.*, 2012)

The intrinsic measures TPR and FPR, summary measure AUC and optimal cut point are computed using equations (1) to (5). The AUC observed is 0.7495 which provides moderate classification, TPR and FPR are 0.6992 and 0.3008 respectively at the optimal cutpoint c = 1.5372. The best linear combination is given by

$$U_{ILP} = 0.0172 * Age\text{–}0.0556 * TB + 0.3133 * DB + 0.0005 * Alkphos\text{–}0.0104 * sgpt + 0.0074 * sgot - 0.4164 * TP + 0.6726 * ALB\text{–}1.1341 * A.G$$

If the test score is greater than optimal cutoff *i.e.*, 1.5372 the individual is classified as diseased, otherwise healthy. The iMROC curve is drawn and depicted in the Figure (5). From Figure (5), it is clear that the fitted MROC curve crosses the chance line and is

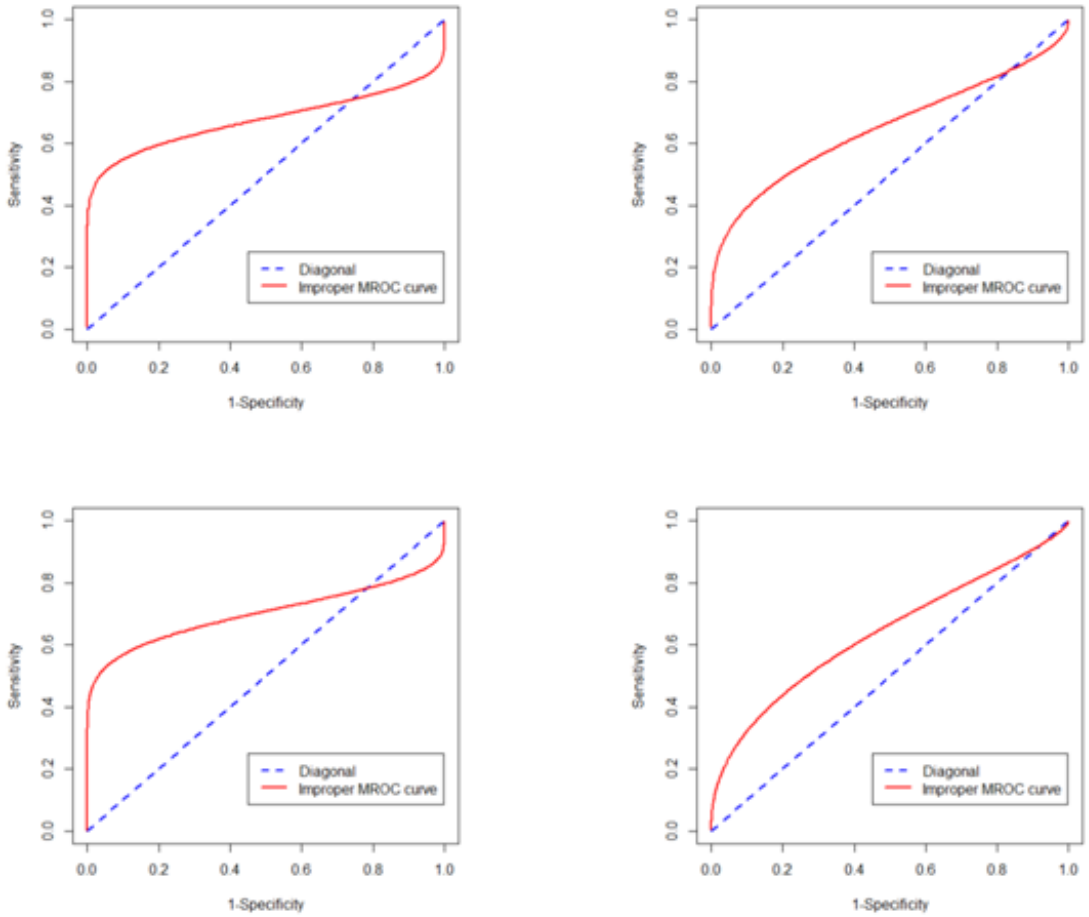

Figure 4: iMROC curves for Simulation datasets at different sample sizes with 100 and 300

moving towards the top right corner of the unit square plot, which generates an improper MROC curve. Using the proposed methodology, the inflection point (t_1) and chance line cross reference points (t_0) are obtained and are highlighted in the Figure (5). MROC curve is concave for $FPR < 0.5221$, but is convex for $FPR > 0.5221$. Due to this improperness, the true accuracy of the classifier cannot be obtained. Further, such contaminated AUC will mislead the interpretation and decision making too.

MCA dataset (Vishnu Vardhan *et al.*. 2015)

The neonatal dataset consists of two procedures: MCA and CPR used to check the blood flow from the womb of the mother to the baby for identifying the growth of the baby. Three indices were measured namely pulsatility index (PI), resistivity index (RI) and Systolic/Diastolic (S/D) ratio in all the procedures. The intrinsic measures TPR and FPR, summary measure AUC and optimal cut point are computed using equation (1) to (5). The AUC observed is 0.6253, which provides moderate classification, TPR and FPR are 0.5968

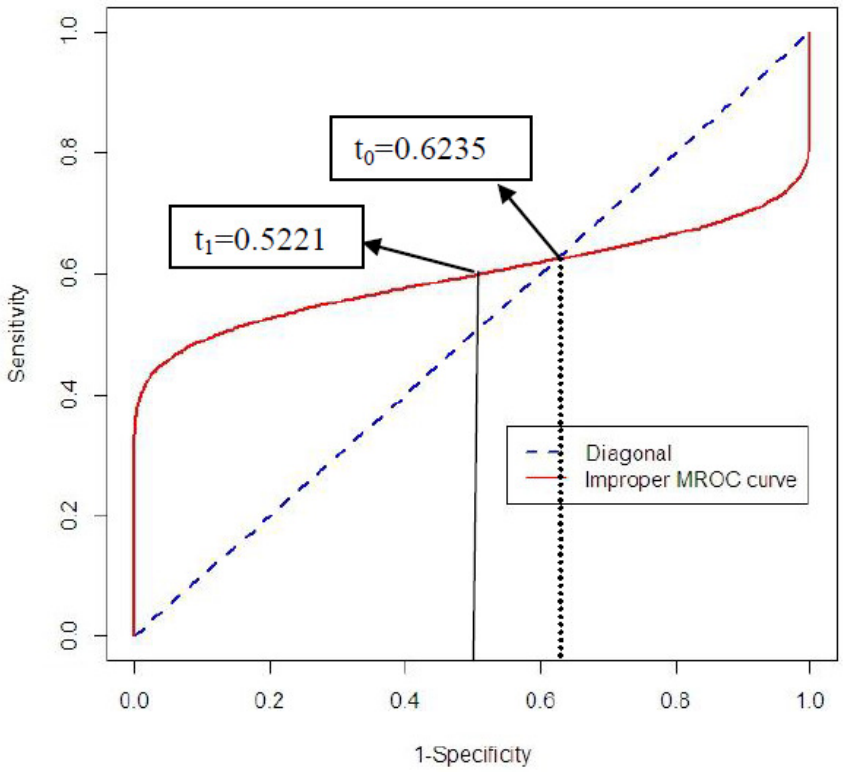

Figure 5: iMROC curve for ILP Male dataset

and 0.4032 at the optimal cutpoint $c = -3.1749$. The best linear combination is given by

$$U_{MCA} = -10.6711 * MCA.RI + 0.0226 * MCA.PI + 1.1733 * MCA.SD$$

The above linear combination can be used for identifying the status of new individual. If the test score is greater than optimal cutoff *i.e.*, -3.1749 the individual is classified as diseased, otherwise healthy.

Further, the MROC curve is drawn and depicted in Figure (6). From Figure (6), it is clear that the fitted MROC curve crosses the chance line and moves towards the top right corner of the unit square plot, which leads to an improper MROC curve. In this illustration also, it is shown that not all ROC curves that gets generated for the classification data is a "Proper" one and before fitting and computing the measures of ROC curve, one has to verify whether the data is satisfying the three properties or not. Doing so, we can overcome the misuse of the technique and misleading conclusions out of it.

4. Conclusion

In this paper, main focus was on establishing the fact that not all ROC curves that are generated through data will be "Proper", *i.e.* that they possesses the monotonic property. So, there is a need to have some mechanism to verify whether an ROC curve so obtained is proper or improper. To address this, crossing point and inflection point are defined, which work on concavity and convexity nature of the ROC curve. To have a better understanding

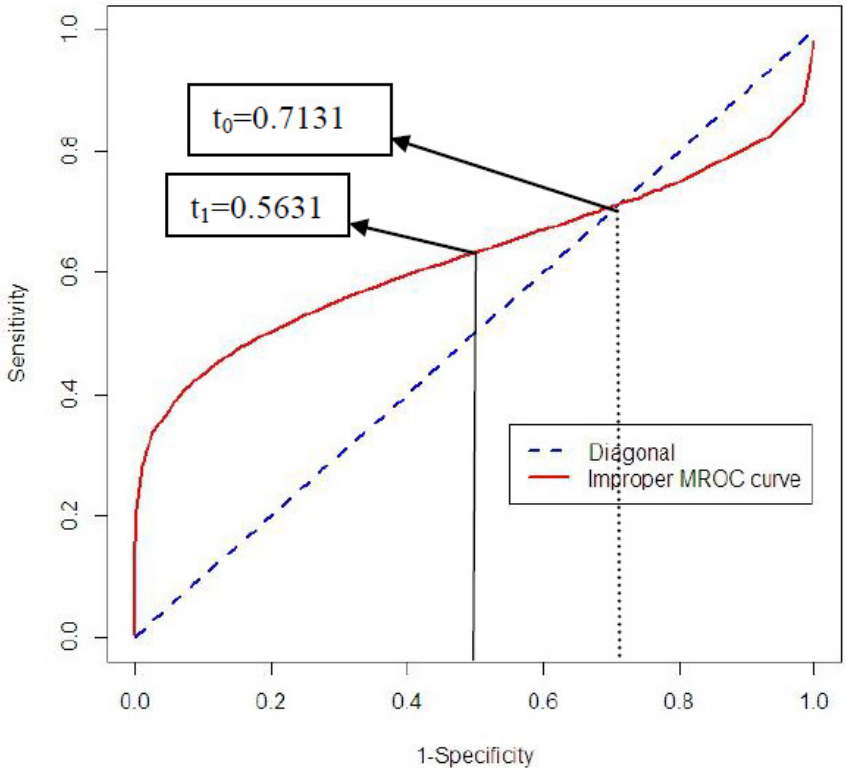

Figure 6: iMROC curve for MCA dataset

of these crossing and inflection points, simulations were carried out for different sample sizes and parameter combinations. Also support of real data sets is also taken. On the whole, the message emerging from this study is that before interpreting the outcomes of ROC curves, it is essential to check whether the curve is proper or improper. If the curve is satisfying the desirable properties then one can proceed for using the classifier for future classification, and if the curve is improper then it is not a better way to use the classifier anymore. So, here it is quite essential to work on a procedure that helps in correcting the ROC curve and making it to have the monotonicity.

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