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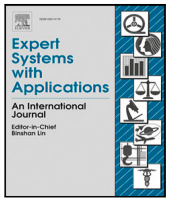

# A Rank Graduation Box for SAFE AI

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ABSTRACT

The growth of Artificial Intelligence applications requires to develop risk management models that can balance opportunities with risks.

We contribute to the development of Artificial Intelligence risk models proposing a Rank Graduation Box (RGB), a set of integrated statistical metrics that can measure the "Sustainability", "Accuracy", "Fairness" and "Explainability" of any Artificial Intelligence application.

Our metrics are consistent with each other, as they are all derived from a common underlying statistical methodology: the Lorenz curve.

The validity of the metrics is assessed by means of their practical application to both simulated and real data. The results from the comparison of alternative machine learning models to simulated data are aligned with the generating models, in general indicating linear regression models as the most accurate, regression tree models as the most fair, Random Forest models as the most robust; and leading to model explanations similar to the true ones from the generating model.

The outcomes from the application of Random Forest models to real data show that the proposed RGB metrics are more interpretable and more consistent with the expectations, with respect to standard metrics such as AUC, RMSE and Shapley values. The evidence also shows that the RGB metrics are very general and can be applied to any machine learning method, regardless of the underlying data and model.

## 1. Background and motivation

Machine Learning (ML) methods are boosting the applications of Artificial Intelligence (AI) in all human activities. Differently from ordinary computer software and applications, AI not only converts inputs into outputs, but can also change the surrounding environment, with the risk of creating harms for individuals, organisations and the environment.

This is the reason why policy makers, regulators and standard bodies around the world are issuing regulations and recommendations that AI developers, deployers and users should follow to manage the risks arising from the adoption of AI methods.

AI risk management requires to develop a consistent set of AI risk metrics that can be employed to monitor the compliance of AI applications. Such a set of metrics is not common practice, yet.

Recently, Giudici and Raffinetti (2023) have summarised the requirements in the existing regulations and recommendations into four main measurable "S.A.F.E." key principles: "S" for sustainability; "A" for accuracy; "F" for fairness; "E" for explainability.

Sustainability refers to the robustness of an AI system to extreme events, such as cyber attacks or environmental issues. The measurement of robustness is well known in the statistics and machine learning literature and it is usually conducted in terms of the difference between the accuracy of two different predictions, obtained respectively under normal and perturbed input data. Accuracy can be measured by the AUC or by the RMSE (see, e.g. Nair et al., 2022).

The measurement of Accuracy is well known in the statistics and machine learning: the Root Mean Square Error (RMSE) is routinely employed for a continuous response; the Area Under the ROC curve (AUC or AUROC) is typically employed for a binary response (see, e.g. Gneiting, 2011; Hand & Till, 2001). More recently, Raffinetti (2023) and Giudici and Raffinetti (2024) have introduced a new accuracy measure that can be applied to both types of response, generalising the AUC to the continuous case.

Fairness is one of the most important requirements for AI applications. Unfairness indicates that the output leads to an unequal treatment of different population groups, by gender, age and nationality, for example. There are several recent research papers that deal with the measurement of fairness. Most of them are based on parity measures, which calculate the difference in accuracy of the AI output obtained separately on different population groups. Accuracy can be measured employing AUC or RMSE (see, e.g. Quy et al., 2022).

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**Table 1**
Literature review on the key principles for AI risk management.

| AI principle | Main reference | Main contribution |
|---|---|---|
| *Sustainability* | Nair et al. (2022) | Change in RMSE or AUC with respect to extreme data |
| | Giudici et al. (2024) | Regularisation and model selection |
| | Giudici and Raffinetti (2023) | Concentration of Shapley–Lorenz values |
| *Accuracy* | Gneiting (2011), Hand and Till (2001) | RMSE (continuous case); AUC (binary case) |
| | Giudici and Raffinetti (2024), Raffinetti (2023) | RGA (binary and continuous case) |
| | Giudici et al. (2024) | AUC, RMSE |
| | Giudici and Raffinetti (2023) | Lorenz Zonoids |
| *Fairness* | Quy et al. (2022) | Parity measures (difference in RMSE or AUC) |
| | Giudici et al. (2024) | Variability of Shapley values |
| | Giudici and Raffinetti (2023) | Variability of Shapley–Lorenz values |
| *Explainability* | Shapley (1953) | Shapley-values in game theory |
| | Lundberg and Lee (2017) | Shapley-values in machine learning |
| | Giudici and Raffinetti (2021) | Shapley–Lorenz values: normalised Shapley values |
| | Giudici et al. (2024) | Shapley values |
| | Giudici and Raffinetti (2023) | Shapley–Lorenz values |

Explainability is a requirement that has emerged with the development of highly accurate machine learning models which have, however, so many parameters that make difficult to reconduct the output to the inputs which determine it. The measurement of explainability requires to attach to each input variable an importance weight which expresses its influence on the final output. A model is explainable if there exists at least one input variable which significantly impacts the output. In white-box models, such as regression models, such weights are functions of the estimated parameters. Instead, to explain black-box models, such as Random Forests and deep learning, further post-processing of the output is necessary. The most employed techniques are based on Shapley values and Shapley–Lorenz values (see, e.g. Giudici & Raffinetti, 2021; Lundberg & Lee, 2017; Shapley, 1953).

In a recent paper, Giudici, Centurelli, and Turchetta (2024) suggested to measure the S.A.F.E. principles using state of the art metrics, such as AUC, RMSE and Shapley values which are not, however, consistent with each other. A more consistent measurement model was put forward by Giudici and Raffinetti (2023), who replaced traditional metrics with new ones based on Lorenz Zonoids, the multivariate extension of the Gini coefficient. While mathematically sound, their approach suffers from computational complexity, especially when a large number of explanatory variables is considered.

What described so far can be summarised in a concise picture of the state of the art for AI risk measurement, which is reported in Table 1.

The aim of this paper is to propose a set of metrics for AI risk measurement which are consistent with each other, as the metrics proposed by Giudici and Raffinetti (2023), but also simple to understand and to implement, as the traditional metrics proposed in Giudici et al. (2024).

To this purpose, we extend the approach by Giudici and Raffinetti (2023) in two main ways: (a) we employ the Concordance curve and, specifically, the Rank Graduation Accuracy measure (RGA) to extend the AUC metric to the ordinal and continuous cases; (b) in analogy with the construction of the RGA, we propose a "Rank Graduation Box" (RGB), a set of consistent metrics, all based on the notion of concordance between two cumulative distributions. Doing so, we obtain a set of metrics which are: easy to interpret, similarly to the well known Area Under the ROC Curve (AUC); easy to implement and compute, using a similar logic; generalisable to other AI compliance principles, which may emerge from future recommendations, as long as they require a comparison between two cumulative distributions.

We remark that both Giudici et al. (2024) and Giudici and Raffinetti (2023) consider financial applications. Finance provides very challenging machine learning problems and is highly regulated, thus justifying the development of AI risk metrics. However, the AI risk metrics that we are going to present can be similarly applied to other important fields of application of AI, such as medicine, automotive, robotics and fault tolerance.

The rest of the paper is organised as follows: Section 2 introduces the theoretical framework of our proposal and the description of the proposed RGB metrics; Section 3 presents the application of our proposal, respectively to a simulated and a real dataset, to assess the validity of the proposal; Section 4 concludes the paper with some final remarks and comments.

## 2. Methodology

In this section, we describe our proposal. Specifically, in Section 2.1, we show the functioning of the Lorenz, dual Lorenz and Concordance curves, which represent the common mathematical background of all our proposed metrics; in Section 2.2 we define the proposed Rank Graduation Box metrics to assess "Sustainability", "Accuracy", "Fairness" and "Explainability" of AI applications. Finally, in Section 2.3, we introduce a set of statistical tests that can be employed to assess the statistical significance of the proposed metrics.

### 2.1. Theoretical background

The basic ingredients of our proposal are the Lorenz curve and the related notions of dual Lorenz curve and Concordance curve, which are statistical tools widely used to summarise the distribution of income and wealth (see, e.g. Lorenz, 1905).

Formally, let $Y^*$ and $Y^{**}$ be any two statistical distributions (continuous, ordinal or binary), each defined on a set of $n$ data points, which we are going to compare.

The $Y^*$ values can be ordered in a non-decreasing sense to build the Lorenz curve $L_{Y^*}$. For $i = 1, \dots, n$, the Lorenz curve is defined by the pairs: $(i/n, \sum_{j=1}^{i} y^*_{r^*_j}/(n\bar{y}^*))$, where $r^*_j$ indicates the non-decreasing ranks of $Y^*$ and $\bar{y}^*$ indicates the mean of $Y^*$.

The same $Y^*$ values can be ordered in a non-increasing sense to build the dual Lorenz curve, $L'_{Y^*}$. For $i = 1, \dots, n$, the dual Lorenz curve is defined by the pairs: $(i/n, \sum_{j=1}^{i} y^*_{r^*_{n+1-j}}/(n\bar{y}^*))$, where $r^*_{n+1-j}$ indicates the non-increasing ranks of $Y^*$.

The Concordance curve C can be derived ordering the $Y^*$ values with respect to the ranks of the $Y^{**}$ values. Let $r^{**}_i$, for $i = 1, \dots, n$, denote the non-decreasing ranks of $Y^{**}$. For $i = 1, \dots, n$, the Concordance curve is defined by the pairs: $(i/n, \sum_{j=1}^{i} y^*_{r^{**}_j}/(n\bar{y}^*))$.

To illustrate the construction of the Lorenz, dual Lorenz and Concordance curves, we now introduce a toy example. Let $Y^*$ and $Y^{**}$ be two vectors of $n = 10$ points, with $Y^* = \{12, 27, 48, 3, 34, 11, 0, 46, 75, 28\}$ and

**Table 2**
Construction of the Lorenz curve.

| ID | $y_i^*$ | $y^*_{r_i^*}$ | $\sum_{j=1}^{i} y^*_{r_j^*}$ | $y$-axis values $\left(\frac{\sum_{j=1}^{i} y^*_{r_j^*}}{n\bar{y}^*}\right)$ | $x$-axis values $\left(\frac{i}{n}\right)$ |
|---|---|---|---|---|---|
| 1 | 12 | 0 | 0 | 0 | 0.1 |
| 2 | 27 | 3 | 3 | 0.01 | 0.2 |
| 3 | 48 | 11 | 14 | 0.05 | 0.3 |
| 4 | 3 | 12 | 26 | 0.09 | 0.4 |
| 5 | 34 | 27 | 53 | 0.19 | 0.5 |
| 6 | 11 | 28 | 81 | 0.29 | 0.6 |
| 7 | 0 | 34 | 115 | 0.40 | 0.7 |
| 8 | 46 | 46 | 161 | 0.57 | 0.8 |
| 9 | 75 | 48 | 209 | 0.74 | 0.9 |
| 10 | 28 | 75 | 284 | 1 | 1 |

**Table 3**
Construction of the dual Lorenz curve.

| ID | $y_i^*$ | $y^*_{r^*_{n+1-j}}$ | $\sum_{j=1}^{i} y^*_{r^*_{n+1-j}}$ | $y$-axis values $\left(\frac{\sum_{j=1}^{i} y^*_{r^*_{n+1-j}}}{n\bar{y}^*}\right)$ | $x$-axis values $\left(\frac{i}{n}\right)$ |
|---|---|---|---|---|---|
| 1 | 12 | 75 | 75 | 0.26 | 0.1 |
| 2 | 27 | 48 | 123 | 0.43 | 0.2 |
| 3 | 48 | 46 | 169 | 0.60 | 0.3 |
| 4 | 3 | 34 | 203 | 0.71 | 0.4 |
| 5 | 34 | 28 | 231 | 0.81 | 0.5 |
| 6 | 11 | 27 | 258 | 0.91 | 0.6 |
| 7 | 0 | 12 | 270 | 0.95 | 0.7 |
| 8 | 46 | 11 | 281 | 0.99 | 0.8 |
| 9 | 75 | 3 | 284 | 1 | 0.9 |
| 10 | 28 | 0 | 284 | 1 | 1 |

**Table 4**
Construction of the Concordance curve C..

| ID | $y_i^*$ | $y^*_{r_j^{**}}$ | $\sum_{j=1}^{i} y^*_{r_j^{**}}$ | $y$-axis values $\left(\frac{\sum_{j=1}^{i} y^*_{r_j^{**}}}{n\bar{y}^*}\right)$ | $x$-axis values $\left(\frac{i}{n}\right)$ |
|---|---|---|---|---|---|
| 1 | 12 | 27 | 27 | 0.10 | 0.1 |
| 2 | 27 | 12 | 39 | 0.14 | 0.2 |
| 3 | 48 | 48 | 87 | 0.31 | 0.3 |
| 4 | 3 | 34 | 121 | 0.43 | 0.4 |
| 5 | 34 | 3 | 124 | 0.44 | 0.5 |
| 6 | 11 | 11 | 135 | 0.48 | 0.6 |
| 7 | 0 | 46 | 181 | 0.64 | 0.7 |
| 8 | 46 | 0 | 181 | 0.64 | 0.8 |
| 9 | 75 | 75 | 256 | 0.90 | 0.9 |
| 10 | 28 | 28 | 284 | 1 | 1 |

$Y^{**} = \{15, 12, 18, 24, 21, 27, 33, 30, 36, 39\}$. It follows that the mean value of $Y^*$, $\bar{y}^*$, is equal to 28.4. The $x$-axis and $y$-axis values of the Lorenz curve are reported in Table 2. The curve is then obtained joining $(n+1)$ points: the $(0, 0)$ point with all points whose coordinates are specified in Table 2.

The $x$-axis values of the dual Lorenz curve are the same as those of the Lorenz curve, whereas the $y$-axis values are obtained cumulating the $Y^*$ values in the reverse order. The resulting coordinate pairs of the dual Lorenz curve are reported in Table 3, and the dual Lorenz curve is then obtained joining the $(0, 0)$ point with all the other points in Table 3.

For the Concordance curve, the $x$-axis values are as before, whereas the $y$-axis are obtained cumulating the $Y^*$ values according to the ranks of $Y^{**}$. Both are reported in Table 4. The Concordance curve connects the $(0, 0)$ point with all the other points in Table 4.

Having clarified the calculation of the coordinates of the Lorenz, dual Lorenz and Concordance curves with a toy example, we now represent them in four distinct stylised scenarios, in Fig. 1.

Reading Fig. 1, from the top left diagram and clockwise, it follows that: [a] when $r_i^{**} = r_i^*$, for all $i = 1, \ldots, n$, the Concordance curve C coincides with the Lorenz curve (full concordance); [b] when $r_i^{**} = r^*_{n+1-i}$, for all $i = 1, \ldots, n$, the Concordance curve C coincides with the dual Lorenz curve (full discordance); [c] when $r_i^{**}$ are all equal to each other, for all $i = 1, \ldots, n$, the Concordance curve C overlaps with the 45-degree line (no association) meaning that, as all the $Y^{**}$ values are tied, the $Y^*$ values have to be replaced by their mean value $\bar{y}^*$ (see Ferrari & Raffinetti, 2015); [d] in general, the distance between the Concordance curve C and the Lorenz curve measures how the ranks of $Y^{**}$ differ from the ranks of $Y^*$, in terms of the ranked values.

Fig. 1 shows that the Concordance curve C is always between the $L_{Y^*}$ Lorenz curve and the $L'_{Y^*}$ dual Lorenz curve.

We can leverage this observation building a summary measure of the distance between the Concordance curve and the two Lorenz curves, which will be the kernel of all our Rank Graduation Box risk metrics. We can divide the area between the Concordance curve C and the dual Lorenz curve by its maximum value, corresponding to the area between the Lorenz and dual Lorenz curves. Such a normalised summary will be named "Rank Graduation" (RG·) measure. More formally, the Rank Graduation measure is defined as:

$$RG\cdot = \frac{\sum_{i=1}^{n}\left\{\frac{1}{n\bar{y}^*}\left(\sum_{j=1}^{i} y^*_{r^*_{n+1-j}} - \sum_{j=1}^{i} y^*_{r_j^{**}}\right)\right\}}{\sum_{i=1}^{n}\left\{\frac{1}{n\bar{y}^*}\left(\sum_{j=1}^{i} y^*_{r^*_{n+1-j}} - \sum_{j=1}^{i} y^*_{r_j^*}\right)\right\}} = \frac{\sum_{i=1}^{n} i y^*_{r_i^{**}} - \sum_{i=1}^{n} i y^*_{r^*_{n+1-i}}}{\sum_{i=1}^{n} i y^*_{r_i^*} - \sum_{i=1}^{n} i y^*_{r^*_{n+1-i}}}, \quad (1)$$

where, for any $i = 1, \ldots, n$: $r_i^*$ are the non-decreasing ranks of the $y_i^*$ values; $r_i^{**}$ are the non-decreasing ranks of the $y_i^{**}$ values; $r^*_{n+1-i}$ are the non-increasing ranks of the $y_i^*$ values; $\bar{y}^*$ is the mean of the $y_i^*$ values.

In summary, in this subsection we have shown how to extend the mathematical framework underlying the Lorenz curve to obtain a Rank Graduation measure, which will be the common basis of the Rank Graduation Box that is going to be described in the next subsection.

### 2.2. Rank Graduation Box metrics

In this section, we will describe how to employ the Rank Graduation measure to derive AI risk metrics for "Sustainability", "Accuracy", "Fairness" and "Explainability". We remark that the derivation is rather general, and other metrics can be developed, once specified from regulatory viewpoint, using the same logic, and put in a comprehensive "Rank Graduation Box" aimed at assessing the overall risk of AI applications.

We first consider "Accuracy". Accuracy requires that the output of an AI application is "close" to the observed (or expected) output.

Given a target variable $Y$ and a set of $K$ predictors, a machine learning model can be applied to obtain predictions, $\hat{Y}$. The RGA measure can then be derived from RG· in Eq. (1) letting $Y^* = Y$ and $Y^{**} = \hat{Y}$.

We can then interpret Fig. 1 in terms of accuracy, once $Y^*$ is replaced by $Y$ and $Y^{**}$ by $\hat{Y}$. The best scenario [a] occurs when the predicted ranks of the response variable $Y$ are equal to the observed ranks, with the Concordance curve C perfectly overlapping the Lorenz curve $L_Y$ (top left graph); the worst scenario [b] occurs when the predicted ranks of the response variable are equal to the reversed observed ranks, with the Concordance curve C perfectly overlapping the dual Lorenz curve $L'_Y$ (top right graph); the no association [c] scenario is achieved for a model that produces random predictions, leading to a Concordance curve C overlapping the 45 degree-line (bottom left graph); in the general scenario [d] (bottom right graph), the Concordance curve C lies in the area between the $Y$ response variable Lorenz curve, $L_Y$, and its dual, $L'_Y$.

It can be shown that $0 \leq \text{RGA} \leq 1$, with RGA = 1 for a perfectly concordant model ($C \equiv L_Y$); RGA = 0 for a perfectly discordant model ($C \equiv L'_Y$); RGA = 0.5 for random predictions (C coincides with the 45-degree line).

We remark that the RGA metric was originally introduced by Raffinetti (2023) to measure accuracy, independently of the nature of the response variable. Indeed, when the response is binary, the RGA

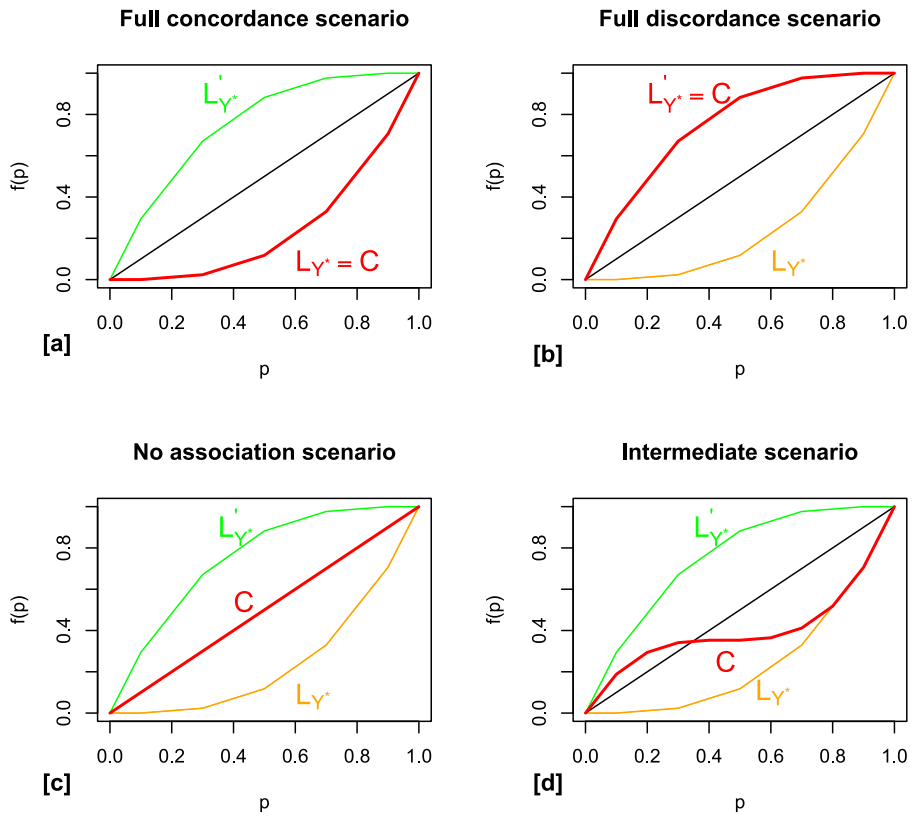


**Fig. 1.** The $L_{Y^*}$ and $L'_{Y^*}$ Lorenz curves, the Concordance curve C and the 45-degree line in the case of: [*a*] a full concordance scenario; [*b*] a full discordance scenario; [*c*] a no association scenario; [*d*] an intermediate scenario. Note that $p$ (on the $x$-axis) and $f(p)$ (on the $y$-axis) are the cumulative values of the $x$ and $y$ coordinates of the $L_{Y^*}$, $L'_{Y^*}$ and C curves.

measure coincides with the AUC (see, e.g. Giudici & Raffinetti, 2024). It can however be calculated, in the same manner, also for ordinal and continuous responses. In the remaining part of this subsection we show how the reasoning behind the RGA can be extended to other metrics, leading to a unified framework to assess the compliance and risk of AI, based on the RG· metric.

We now consider "Sustainability". Sustainability is related to the robustness of AI applications. The output of AI may be affected by extreme data, either internal or generated by cyber attacks, which can distort the inputs of an AI application and, consequently, its output.

The measurement of robustness is usually conducted in terms of an appropriate distance between the model predictions and those obtained under (intentional or non intentional) data perturbations.

The distance provided by the RG· metric can be quite useful in this context, as it is based on a distance between ranks which is, by definition, more robust to outliers and extreme data than distances based on the actual values, such as the Root Mean Square Error.

We propose to measure the robustness of AI applications by means of a "Rank Graduation Robustness" measure, denoted with RGR, which can be obtained setting in Eq. (1) $Y^* = \hat{Y}$ and $Y^{**} = \hat{Y}^p$, with $\hat{Y}$ and $\hat{Y}^p$ the predicted values obtained using the non-perturbed data and the predicted values obtained using perturbed data, respectively.

We can then interpret Fig. 1 in terms of robustness, once $Y^*$ is replaced by $Y^* = \hat{Y}$ and $Y^{**}$ by $Y^{**} = \hat{Y}^p$.

From Fig. 1, note that the case of maximum robustness [a] occurs when the ranks of the response predicted values $\hat{Y}$ correspond to the ranks of the predicted values obtained using the perturbed data, with the Concordance curve C perfectly overlapping the Lorenz curve $L_{\hat{Y}}$; the worst case [b] occurs when the ranks of the $\hat{Y}$ response predicted values are in inverse correspondence with the ranks of the predicted values obtained using the perturbed data, with the Concordance curve C perfectly overlapping the dual Lorenz curve $L'_{\hat{Y}}$; the [c] case occurs when the Concordance curve C overlaps the 45-degree implying that perturbations on the input data lead to random predictions; the general case [d] occurs when the Concordance curve C lies in the area between the $\hat{Y}$ Lorenz curve, $L_{\hat{Y}}$, and its dual, $L'_{\hat{Y}}$.

One can prove that RGR takes values in the close range $[0, 1]$. RGR = 1 for a fully robust model ($C \equiv L_{\hat{Y}}$); RGR = 0 for a fully perturbed model ($C \equiv L'_{\hat{Y}}$); RGR = 0.5 if the perturbations lead to a random model.

We now consider the measurement of "Explainability".

The standard metrics for explainability are Shapley values and their variants, such as Shapley–Lorenz values. Both are computationally intensive and their calculation, when a large amount of input variables is involved, may become infeasible.

In this paper, we propose to overcome this drawback adapting Eq. (1) to the measurement of explainability, leading to a "Rank Graduation Explainability" (RGE) metric. More precisely, we let $Y^* = \hat{Y}$ and $Y^{**} = \hat{Y}^{(-X_k)}$, where $\hat{Y}$ are the predicted values from a full model (which includes all $K$ predictors) and $\hat{Y}^{(-X_k)}$ are the predicted values from a reduced model (which excludes the $k$-th predictor under evaluation).

We remark that the stronger is the effect of a variable $X_k$ on explaining $Y$, the larger is the divergence between the ranks of the full model predicted values and those associated with the reduced model. Thus, for interpretational purpose, once let $Y^* = \hat{Y}$ and $Y^{**} = \hat{Y}^{(-X_k)}$, we will define RGE as RGE = 1− RG·.

Interpreting Fig. 1 in terms of explainability, note that the case of minimum explainability [a] occurs when the ranks of the response predicted values $\hat{Y}$ correspond to the ranks of the $\hat{Y}^{-X_k}$ predicted values (obtained by fitting the model without the $k$-th predictor), with the Concordance curve C perfectly overlapping the Lorenz curve $L_{\hat{Y}}$ (left graph); the case of maximum explainability [b] occurs when the ranks of the $\hat{Y}$ response predicted values is in inverse correspondence with

the ranks of the $\hat{Y}^{(-X_k)}$ predicted values (obtained by fitting the model on the data without the $k$-th predictor), with the Concordance curve C perfectly overlapping the dual Lorenz curve $L'_{\hat{Y}}$; the case [c] arises when the Concordance curve C is equivalent to the 45-degree line meaning that the $\hat{Y}^{-X_k}$ predicted values are random predictions; the general case [d] occurs when the Concordance curve C lies in the area between the $\hat{Y}$ Lorenz curve, $L_{\hat{Y}}$, and its dual, $L'_{\hat{Y}}$. Based on the previous considerations, it holds that $0 \leq \text{RGE} \leq 1$. Specifically: $RGE = 1$ if the $k$-th predictor provides the maximum explanation ($C \equiv L'_{\hat{Y}}$); $RGE = 0$ if the $k$-th predictor does not contribute to the explanation of the response ($C \equiv L_{\hat{Y}}$); $RGE = 0.5$ if the model without the $k$-th predictor corresponds to the random model (C coincides with the 45-degree line).

We finally consider the measurement of "Fairness".

Fairness is typically measured by parity measures, which compare the AI outputs obtained separately on different population groups. This group based comparison is unconditional on the values of the other input variables, and it is not useful to assess, besides unfairness, its reasons. Furthermore, it may lead to paradoxes: the output may be fair marginally, but not conditionally on a control variable. For example, a credit score may be fair with respect to the gender of the borrower overall, but not conditionally on the level of income of the borrower.

We propose to overcome the difficulties of parity measures adapting formula (1) to the fairness context, leading to the "Rank Graduation Fairness" (RGF) metric.

More precisely, given a set $G$ of group variables, converted into $G$ binary variables, to calculate RGF we let $Y^* = \hat{Y}$ and $Y^{**} = \hat{Y}^{(-X_g)}$, where $\hat{Y}$ are the predicted values obtained with a full model (including all the $G$ group variables as predictors); and $\hat{Y}^{(-X_g)}$ are the predicted values obtained with a reduced model (that excludes the $g$-th group binary variable under evaluation).

We can now interpret Fig. 1 in terms of the RGF measure. The maximum fairness scenario [a] arises when the ranks of the response predicted values $\hat{Y}$ correspond to the ranks of the $\hat{Y}^{(-X_g)}$ predicted values (obtained by fitting the model without the $g$-th group variable), with the Concordance curve C perfectly overlapping the Lorenz curve $L_{\hat{Y}}$ (left graph); the maximum unfairness condition [b] arises when the ranks of the $\hat{Y}$ response predicted values are in inverse correspondence with the ranks of the $\hat{Y}^{(-X_g)}$ predicted values (obtained by fitting the model on data without the $g$-th group variable), with the Concordance curve C perfectly overlapping the dual Lorenz curve $L'_{\hat{Y}}$; in the case [c], the Concordance curve C coincides with the 45-degree line, indicating that the $\hat{Y}^{(-X_g)}$ predicted values without the $g$-th group variable correspond to a random model; in the intermediate scenario [d], the Concordance curve C lies in the area between the $\hat{Y}$ Lorenz curve, $L_{\hat{Y}}$ and its dual, $L'_{\hat{Y}}$. It can be shown that $0 \leq \text{RGF} \leq 1$. More precisely: $RGF = 1$ ($C \equiv L_{\hat{Y}}$) in the case of maximum fairness; $RGF = 0$ ($C \equiv L'_{\hat{Y}}$) in the case of maximum unfairness. $RGF = 0.5$ if the model without the $g$-th group variable corresponds to the random model.

For the sake of clarity, the toy example introduced in Section 2.1 is further exploited in the Appendix section to show how the RGA, RGR, RGE and RGF can be practically computed.

In summary, in this subsection we have shown how to adapt the Rank Graduation measure, illustrated in the previous subsection, to measure different compliance aspects of AI: Accuracy, by means of RGA; Sustainability, by means of RGR; Explainability, by means of RGE; and fairness, by means of RGF. The application of the metrics to an AI application can assess its compliance and risks.

### 2.3. Statistical tests

The introduced $RG\cdot$ metric can be complemented with statistical tests that can indicate whether the found degree of sustainability, accuracy, fairness or explainability is significantly high or not, taking into account the sampling variability.

To this aim, we now derive two statistical tests based on the RG· metric. The first test can be applied to RGA and RGR. For both cases, RG· can be expressed in terms of the covariance operator as follows:

$$RG\cdot = \frac{1}{2}\frac{cov(Y^*_{r(Y^{**})}, F(Y^*))}{cov(Y^*, F(Y^*))} + \frac{1}{2}, \tag{2}$$

where $Y^*_{r(Y^{**})}$ represents the $Y^*$ variable re-ordered according to the ranks of $Y^{**}$ and $F$ is the cumulative continuous distribution function of $Y^*$.

It follows that the RG· is a linear function of the ratio:

$$\psi(Y^*, Y^{**}) = cov(Y^*_{r(Y^{**})}, F(Y^*))/cov(Y^*, F(Y^*)). \tag{3}$$

We recall that $Y^*$ and $Y^{**}$ have two different roles: for RGA, they represent the target variable $Y$ to be predicted (i.e., $Y^* = Y$) and the predicted values $\hat{Y}$ (i.e., $\hat{Y} = Y^{**}$); for RGR, they represent the predicted values $\hat{Y}$, provided by the model fitted on non-perturbed data (i.e., $Y^* = \hat{Y}$), and the predicted values $\hat{Y}^p$, derived from the same model fitted on perturbed data (i.e., $Y^{**} = \hat{Y}^p$).

Given two alternative models ($Mod_1$ and $Mod_2$), the statistics in (3) can be used to test the following hypotheses:

$$\begin{aligned} &H_0 : \psi(Y^*_{Mod_1}, Y^{**}_{Mod_1}) = \psi(Y^*_{Mod_2}, Y^{**}_{Mod_2}) \quad \text{vs} \\ &H_1 : \psi(Y^*_{Mod_1}, Y^{**}_{Mod_1}) \neq \psi(Y^*_{Mod_2}, Y^{**}_{Mod_2}), \end{aligned} \tag{4}$$

where

$$\psi(Y^*_{Mod_1}, Y^{**}_{Mod_1}) = cov(Y^*_{r(Y^{**}_{Mod_1})}, F(Y^*_{Mod_1}))/cov(Y^*_{Mod_1}, F(Y^*_{Mod_1}))$$

and

$$\psi(Y^*_{Mod_2}, Y^{**}_{Mod_2}) = cov(Y^*_{r(Y^{**}_{Mod_2})}, F(Y^*_{Mod_2}))/cov(Y^*_{Mod_2}, F(Y^*_{Mod_2}))$$

are functions that derive from the application of (3), respectively to $RG\cdot_{Mod_1}$ and $RG\cdot_{Mod_2}$.

Note that the estimator of $\psi(Y^*_{Mod_1}, Y^{**}_{Mod_1})$ can be expressed as a function of two dependent U-statistics, denoted with $U_1$ and $U_2$:

$$\hat{\psi}(Y^*_{Mod_1}, Y^{**}_{Mod_1}) = \frac{U_1}{U_2} = \frac{\frac{1}{4\binom{n}{2}}\sum_{i=1}^{n}(2i-1-n)Y^*_{r(Y^{**}_{i_{Mod_1}})}}{\frac{1}{4\binom{n}{2}}\sum_{i=1}^{n}(2i-1-n)Y^*_{r(Y^{*}_{i_{Mod_1}})}}. \tag{5}$$

Similarly, the estimator of $\psi(Y^*_{Mod_2}, Y^{**}_{Mod_2})$ can be defined as a function of two dependent U-statistics, $U_3$ and $U_4$:

$$\hat{\psi}(Y^*_{Mod_2}, Y^{**}_{Mod_2}) = \frac{U_3}{U_4} = \frac{\frac{1}{4\binom{n}{2}}\sum_{i=1}^{n}(2i-1-n)Y^*_{r(Y^{**}_{i_{Mod_2}})}}{\frac{1}{4\binom{n}{2}}\sum_{i=1}^{n}(2i-1-n)Y^*_{r(Y^{*}_{i_{Mod_2}})}}. \tag{6}$$

It follows that $\delta = \psi(Y^*_{Mod_1}, Y^{**}_{Mod_1}) - \psi(Y^*_{Mod_2}, Y^{**}_{Mod_2})$ can be estimated by $\hat{\delta}$, a function of four dependent U-statistics:

$$\hat{\delta} = \hat{\psi}(Y^*_{Mod_1}, Y^{**}_{Mod_1}) - \hat{\psi}(Y^*_{Mod_2}, Y^{**}_{Mod_2}) = \frac{U_1}{U_2} - \frac{U_3}{U_4}. \tag{7}$$

According to Hoeffding (1948), a function of several dependent U-statistics has a normal distribution, provided that the sample size is large enough. Thus, the estimator in Eq. (7) has a limiting normal distribution, whose variance $\widehat{Var(\hat{\delta})}$ can be estimated by means of the Jackknife method (see, e.g. Efron & Stein, 1981) each time omitting the pairs $(Y^*_{Mod_1}, Y^{**}_{Mod_1})$ and $(Y^*_{Mod_2}, Y^{**}_{Mod_2})$.

Therefore, a test statistic for testing the null hypothesis $H_0 : \psi(Y^*_{Mod_1}, Y^{**}_{Mod_1}) = \psi(Y^*_{Mod_2}, Y^{**}_{Mod_2})$ is:

$$Z = \frac{\hat{\delta}}{\sqrt{\widehat{Var(\hat{\delta})}}} \rightarrow N(0,1), \tag{8}$$

where, for $i = 1, \ldots, n$: $\widehat{Var(\hat{\delta})} = \frac{n-1}{n}\sum_{i=1}^{n}(\hat{\delta}_{(-i)} - \bar{\delta})^2$; $\hat{\delta}_{(-i)}$ are the values of $\hat{\delta}$ by omitting the pairs $(Y^*_{Mod_1}, Y^{**}_{Mod_1})$ and $(Y^*_{Mod_2}, Y^{**}_{Mod_2})$ at a time; $\bar{\delta}$ is the average of the values $\hat{\delta}_{(-i)}$.

For a fixed significance level $\alpha$, a rejection region for the test corresponds to the region $|Z| \geq z_{\alpha/2}$. If the test statistic falls in this region, $Mod_1$ and $Mod_2$ are significantly different from each other.

Note that: in the case of RGA, $Y^*_{Mod_1} = Y^*_{Mod_2}$, being $Y^* = Y$, i.e. the observed target variable to be predicted based on two alternative models $Mod_1$ and $Mod_2$; in the case of RGR, $Y^*_{Mod_1} \neq Y^*_{Mod_2}$, being $Y^*_{Mod_1} = \hat{Y}_{Mod_1}$ and $Y^*_{Mod_2} = \hat{Y}_{Mod_2}$, i.e. the predicted values computed on non-perturbed data and provided by $Mod_1$ and $Mod_2$, respectively.

We now derive a second test, aimed to assess the significance of RGE and RGF. In this case $Y^*$ corresponds to the predicted values obtained with a full model while $Y^{**}$ corresponds to the predicted values generated by the reduced model, that is the model without the $k$-th variable, for RGE; and without the $g$-th group variable for RGF. It follows that a suitable test statistic can be defined as the difference between the denominator and the numerator of (3):

$$\gamma(Y^*, Y^{**}) = cov(Y^*, F(Y^*)) - cov(Y^*_{r(Y^{**})}, F(Y^*)). \tag{9}$$

By resorting to $\gamma(Y^*, Y^{**})$, the hypotheses

$$H_0 : \gamma(Y^*, Y^{**}) = 0 \quad \text{vs} \quad H_1 : \gamma(Y^*, Y^{**}) \neq 0, \tag{10}$$

can be tested.

Note that the estimator of $\gamma(Y^*, Y^{**})$ can be expressed as a function of two dependent U-statistics, denoted with $\tilde{U}_1$ and $\tilde{U}_2$:

$$\hat{\gamma}(Y^*, Y^{**}) = \tilde{U}_1 - \tilde{U}_2 = \frac{1}{4\binom{n}{2}} \sum_{i=1}^{n} (2i-1-n) Y^*_{r(Y^*_i)} - \frac{1}{4\binom{n}{2}} \sum_{i=1}^{n} (2i-1-n) Y^*_{r(Y^{**}_i)}. \tag{11}$$

By exploiting Hoeffding's Theorem (see, e.g. Hoeffding, 1948), (11) has a limiting normal distribution whose variance $Var(\hat{\gamma})$ can be estimated through the Jackknife method giving rise to the test statistic:

$$Z = \frac{\hat{\gamma}}{\sqrt{\widehat{Var(\hat{\gamma})}}} \to N(0,1), \tag{12}$$

where, for $i = 1, \ldots, n$: $\widehat{Var(\hat{\gamma})} = \frac{n-1}{n} \sum_{i=1}^{n} (\hat{\gamma}_{(-i)} - \bar{\gamma})^2$; $\hat{\gamma}_{(-i)}$ are the values of $\hat{\gamma}$ by omitting one pair $(Y^*, Y^{**})$ at a time; $\bar{\gamma}$ is the average of the values $\hat{\gamma}_{(-i)}$.

For a fixed significance level $\alpha$, a rejection region for the test corresponds to the region $|Z| \geq z_{\alpha/2}$.

In summary, in this subsection we have shown how to improve the robustness of the results from the application of the proposed RGB metrics. Essentially, by means of statistical tests that can verify whether the obtained assessments for Sustainability, Accuracy, Fairness and Explainability are statistically significant.

## 3. Empirical analysis

In this section we apply the described Rank Graduation Box metrics. We consider both a simulated and a real data set.

Specifically, the simulation settings and the related results are presented and discussed in Section 3.1, whereas the application of our proposal to real surveys is described in Section 3.2.

### 3.1. Simulated data

For simulated data, we illustrate the experimental designs in Section 3.1.1 and the obtained empirical findings in Section 3.1.2.

**Table 5**
Correlation matrix $S_1$.

| | $Y$ | $X_1$ | $X_2$ | $X_3$ | $X_4$ |
|---|---|---|---|---|---|
| $Y$ | 1 | 0.6 | 0.4 | 0.3 | 0.1 |
| $X_1$ | | 1 | 0.2 | 0.7 | 0.3 |
| $X_2$ | | | 1 | 0.05 | 0.1 |
| $X_3$ | | | | 1 | 0.5 |
| $X_4$ | | | | | 1 |

**Table 6**
Correlation matrix $S_2$.

| | $Y$ | $X_1$ | $X_2$ | $X_3$ | $X_4$ |
|---|---|---|---|---|---|
| $Y$ | 1 | 0.1 | 0.5 | 0.2 | 0.8 |
| $X_1$ | | 1 | 0.3 | 0.6 | 0.3 |
| $X_2$ | | | 1 | 0.05 | 0.1 |
| $X_3$ | | | | 1 | 0.5 |
| $X_4$ | | | | | 1 |

#### 3.1.1. Experimental designs

We simulate 1000 times 100 five-dimensional samples $(Y, X_1, X_2, X_3, X_4)$, from a five-dimensional Normal distribution, with mean $\boldsymbol{\mu}$ and correlation matrix $\boldsymbol{\Sigma}$. We assume, without loss of generality, that $\boldsymbol{\mu} = \{150, 20, 72, 5, 200\}$. For the correlation matrix, we consider two alternative specifications: $\Sigma = S_1$, as in Table 5; and $\Sigma = S_2$, as in Table 6, with different correlations between the target variable and the predictors. We also simulate the 1000 samples from a non-Normal distribution, with mean and correlation matrices as before, plus a skewness parameter at $\nu = 3$ and a kurtosis parameter at $\kappa = 61$.

We thus obtain four experimental settings: (A) 1000 samples of size 100 from a Normal distribution with correlation matrix $S_1$; (B) 1000 samples of size 100 from a Normal distribution with correlation matrix $S_2$; (C) 1000 samples of size 100 from a non-Normal distribution with correlation matrix $S_1$; (D) 1000 samples of size 100 from a non-Normal distribution with correlation matrix $S_2$.

To measure robustness, in all four scenarios the predictors are then perturbed in the train set by replacing the left and right tails of the related distributions with outliers. Specifically, the values lower than the 15% percentile are replaced by observations sampled from a $U(-6, -4)$ distribution, whereas the values greater than the 85% percentile are replaced by observations sampled from a $U(15, 22)$ distribution.

To measure fairness, in all four scenarios the predictor $X_1$ is binarised assigning a level of 1 to the values greater than the corresponding mean and a level of 0 otherwise.

We have then run three alternative machine learning models on the simulated data: a linear regression model, a regression tree model and a Random Forest model. While the linear regression model is explainable by design and the regression tree can be explained by visualising its tree, the Random Forest is a full black-box model.

The proposed metrics (RGA, RGR, RGE and RGF) have then been applied to compare the three machine learning models in terms of accuracy, robustness, explainability and fairness. All models have been fit on the same training set (80% of the observations) and evaluated on the same test set (20% of the observations).

#### 3.1.2. Experimental results

The results of the RGA, RGR, RGF and RGE metrics can be summarised by their mean and standard deviations along the 1000 considered samples.

Tables 7 and 8 show the results for experiment (A).

From Table 7, note that the linear regression model is the most accurate model, followed by the Random Forest and by the regression tree model. This is not surprising, as the generating model is a multivariate Gaussian distribution. On the contrary, the linear regression model appears as the least robust and fair. Whereas the Random Forest and regression tree models appear as the most robust and fair, respectively.

**Table 7**
Summary statistics for RGA, RGR and RGF metrics in experiment (A).

| RGA | Mean | Standard deviation ($sd$) |
|---|---|---|
| Linear regression | 0.8297 | 0.0722 |
| Regression tree | 0.7569 | 0.0882 |
| Random Forest | 0.7911 | 0.0835 |
| RGR | Mean | Standard deviation ($sd$) |
| Linear regression | 0.6543 | 0.1943 |
| Regression tree | 0.8222 | 0.1111 |
| Random Forest | 0.9445 | 0.0465 |
| RGF | Mean | Standard deviation ($sd$) |
| Linear regression | 0.7252 | 0.2465 |
| Regression tree | 0.9668 | 0.0946 |
| Random Forest | 0.9142 | 0.0729 |

**Table 8**
Summary statistics for the RGE metric in experiment (A).

| $RGE_{X_1}$ | Mean | Standard deviation ($sd$) |
|---|---|---|
| Linear regression | 0.0307 | 0.0733 |
| Regression tree | 0.2379 | 0.1623 |
| Random Forest | 0.1116 | 0.0709 |
| $RGE_{X_2}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.0242 | 0.0483 |
| Regression tree | 0.1388 | 0.1491 |
| Random Forest | 0.0703 | 0.0545 |
| $RGE_{X_3}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.2594 | 0.2253 |
| Regression tree | 0.1371 | 0.1340 |
| Random Forest | 0.0354 | 0.0290 |
| $RGE_{X_4}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.0031 | 0.0130 |
| Regression tree | 0.0466 | 0.0885 |
| Random Forest | 0.0436 | 0.0387 |

**Table 9**
Summary statistics for the RGA, RGR and RGF metrics in experiment (B).

| RGA | Mean | Standard deviation ($sd$) |
|---|---|---|
| Linear regression | 0.9736 | 0.0149 |
| Regression tree | 0.8828 | 0.0483 |
| Random Forest | 0.9323 | 0.0353 |
| RGR | Mean | Standard deviation ($sd$) |
| Linear regression | 0.2335 | 0.1431 |
| Regression tree | 0.9010 | 0.0700 |
| Random Forest | 0.9591 | 0.0312 |
| RGF | Mean | Standard deviation ($sd$) |
| Linear regression | 0.6355 | 0.2295 |
| Regression tree | 0.9999 | 0.0032 |
| Random Forest | 0.9616 | 0.0352 |

Moving to explainability, Table 8 shows that, in general, the most explainable predictor is $X_1$, which is indeed the variable with the highest correlation with $Y$. Removing variable $X_1$ from any of the three models leads to a change in the ranked values of about 3%–24%. The importance ranking of the predictors is almost the same for the tree models: $X_1$ is followed by $X_2$ and, then, by $X_3$ and $X_4$. This is as expected, being the true correlations with $Y$ equal to 0.4, 0.3 and 0.1, respectively. A notable exception is the explanation for $X_3$ with the linear regression model, which has a very high mean, but also a very high standard deviation. Taking into account all four metrics, we can conclude that the Random Forest model is the best model, as the high performance of the linear regression on RGA may be due to its low robustness.

The results for experiment (B) are displayed in Table 9 and in Table 10.

**Table 10**
Summary statistics for the RGE metric in experiment (B).

| $RGE_{X_1}$ | Mean | Standard deviation ($sd$) |
|---|---|---|
| Linear regression | 0.0634 | 0.0951 |
| Regression tree | 0.0077 | 0.0247 |
| Random Forest | 0.0285 | 0.0243 |
| $RGE_{X_2}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.1312 | 0.1270 |
| Regression tree | 0.0461 | 0.0742 |
| Random Forest | 0.0770 | 0.0487 |
| $RGE_{X_3}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.1176 | 0.1370 |
| Regression tree | 0.0254 | 0.0489 |
| Random Forest | 0.0183 | 0.0147 |
| $RGE_{X_4}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.2579 | 0.2264 |
| Regression tree | 0.3926 | 0.1365 |
| Random Forest | 0.1750 | 0.0883 |

**Table 11**
Summary statistics for the RGA, RGR and RGF metrics in experiment (C).

| RGA | Mean | Standard deviation ($sd$) |
|---|---|---|
| Linear regression | 0.8263 | 0.0819 |
| Regression tree | 0.7707 | 0.0914 |
| Random Forest | 0.7994 | 0.0876 |
| RGR | Mean | Standard deviation ($sd$) |
| Linear regression | 0.9743 | 0.0268 |
| Regression tree | 0.9378 | 0.0859 |
| Random Forest | 0.9613 | 0.0364 |
| RGF | Mean | Standard deviation ($sd$) |
| Linear regression | 0.7757 | 0.1185 |
| Regression tree | 0.8794 | 0.1436 |
| Random Forest | 0.8837 | 0.0749 |

Table 9 highlights that the linear regression model is again the most accurate model, followed by the Random Forest and the regression tree models.

As in Scenario (A), the linear regression has a worse performance in robustness and fairness. The Random Forest and the regression tree perform better.

In terms of explainability, Table 10 shows that, for all three models, the predictor $X_4$ contributes the most to the explanation of the target variable $Y$. Removing $X_4$ from any of the three models leads to a change in the ranked values of about 17.5%–39%. On the other hand, $X_1$ in general provides the smallest contribution in explaining the target variable $Y$. These findings are coherent with our expectations as $X_1$ and $X_4$ have, respectively, a low and a strong correlation with $Y$ in experiment (B). Overall, we can conclude that, for this experiment, both linear regression and Random Forest are good models, the choice depends on which metric is retained more important.

Consider now experiment (C), whose results are displayed in Tables 11 and in Table 12.

From Table 11, it turns out that the linear regression model has again the highest accuracy. The regression model has also a good performance in robustness, but it is low performing in fairness with respect to Random Forest.

Table 12 shows that, also in case of non-normally distributed data, the most important predictor is $X_1$, followed by $X_2$, $X_4$ and $X_3$. The highest explanation for $X_1$ is reached with the regression tree, which, however, is also the model where the RGE metric achieves the largest variability. In this scenario, removing predictor $X_1$ from any of the three models leads to a change in the ranked values of about 9.5%–25%. Overall, no one of the three models dominate the others in terms of all metrics. The choice therefore depends on which metric is considered most important.

**Table 12**
Summary statistics for the RGE metric in experiment (C).

| $RGE_{X_1}$ | Mean | Standard deviation ($sd$) |
|---|---|---|
| Linear regression | 0.0955 | 0.0698 |
| Regression tree | 0.2502 | 0.1234 |
| Random Forest | 0.1069 | 0.0657 |
| $RGE_{X_2}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.0641 | 0.0578 |
| Regression tree | 0.1212 | 0.1101 |
| Random Forest | 0.0752 | 0.0543 |
| $RGE_{X_3}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.0068 | 0.0133 |
| Regression tree | 0.0204 | 0.0458 |
| Random Forest | 0.0217 | 0.0185 |
| $RGE_{X_4}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.0086 | 0.0155 |
| Regression tree | 0.0250 | 0.0542 |
| Random Forest | 0.0231 | 0.0233 |

**Table 13**
Summary statistics for the RGA, RGR and RGF metrics in experiment (D).

| RGA | Mean | Standard deviation ($sd$) |
|---|---|---|
| Linear regression | 0.9666 | 0.0239 |
| Regression tree | 0.8666 | 0.0598 |
| Random Forest | 0.9134 | 0.0523 |
| RGR | Mean | Standard deviation ($sd$) |
| Linear regression | 0.9820 | 0.0200 |
| Regression tree | 0.9398 | 0.0742 |
| Random Forest | 0.9673 | 0.0295 |
| RGF | Mean | Standard deviation ($sd$) |
| Linear regression | 0.7282 | 0.1819 |
| Regression tree | 0.9994 | 0.0063 |
| Random Forest | 0.9774 | 0.0236 |

**Table 14**
Summary statistics for the RGE metric in experiment (D).

| $RGE_{X_1}$ | Mean | Standard deviation ($sd$) |
|---|---|---|
| Linear regression | 0.0073 | 0.0112 |
| Regression tree | 0.0070 | 0.0212 |
| Random Forest | 0.0126 | 0.0105 |
| $RGE_{X_2}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.0697 | 0.0541 |
| Regression tree | 0.1016 | 0.0815 |
| Random Forest | 0.0828 | 0.0498 |
| $RGE_{X_3}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.0036 | 0.0076 |
| Regression tree | 0.0082 | 0.0238 |
| Random Forest | 0.0110 | 0.0091 |
| $RGE_{X_4}$ | Mean | Standard deviation ($sd$) |
| Linear regression | 0.1823 | 0.0938 |
| Regression tree | 0.3163 | 0.1349 |
| Random Forest | 0.1750 | 0.0862 |

We finally consider experiment (D), whose results are displayed in Table 13 and in Table 14.

Table 13 shows that the linear regression is more accurate than the Random Forest and regression tree. And it also appears as the most robust model in presence of extreme observations, followed by Random Forest and regression tree. Differently, in terms of fairness, the linear regression model has the worst performance.

In terms of explainability, from Table 14 it arises that the predictor which mostly affect the target variable $Y$ is $X_4$, followed by predictor $X_2$. Removing predictor $X_4$ from any of the three models would imply a change in the ranked values of about 17.5%–32%.

To robustify the presented results, helping the final choice between the three models, we now carry out statistical tests to check whether the difference in the values of the metrics among the three models is statistically significant. To this aim, we apply the tests presented in Section 2.3 to compare $s = 3$ metrics. Under the null hypotheses, there is no difference among the expected value of the $s$ metrics. Whereas, under the alternative hypotheses the expected values differ.

The results of the test, in terms of $p$-values, are reported in Table 15, for the RGA, RGR and RGF metrics, and in Table 16 for RGE.

The results of the statistical tests, reported in Tables 15 and 16, highlight that the metrics computed on the different models are all significantly different ($p$-value $< 0.01$) in all the considered experiments.

We can therefore conclude that the values of the metrics, previously discussed, are all statistically significant.

### 3.2. Real data

In this section, we show how the proposed metrics can be actually employed to check the compliance of AI applications on real data.

We consider the publicly available "employee" dataset, which can be directly uploaded from the **stima** package in **R**. The data derive from a study carried out on the 473 employees of a bank, and include information on their gender, age, educational degree (in terms of years of education), employment category (custodial, clerical, or manager), job time in months since hire, previous experience (job time in months from previous experiences), minority classification (that is, whether of an ethnic minority), starting salary (in dollars), and current salary (in dollars). For a better description see e.g. Ferrari and Raffinetti (2015).

We consider both classification and prediction machine learning problems for the employee data. In the classification problem, the response variable is binary. It is defined as a "doubling salary", obtained assigning a level of 1 to the employees who achieve a salary growth rate (ratio of the current salary to the starting salary) greater or equal to two, and a level of 0 otherwise. In the prediction problem, the response variable is directly the "salary growth", defined as the difference between two variables, the current salary and the starting salary.

We consider, for both the prediction and the classification problems, a Random Forest model. More specifically, the predicted values for the response variable are estimated for the test data (corresponding to the 30% of the whole dataset), employing the model fitted on the train dataset, using all explanatory variables, and including the 70% of the observations. We remark that the choice of a Random Forest model is taken without loss of generality, as it can ease the interpretation of the results, as we use the same type of models for both classification and prediction.

We apply the proposed RGA, RGR, RGE and RGF metrics to the predictions from the Random Forest model. In the case of RGR we consider perturbing all input variables, with a perturbation scheme different from what seen for the simulated data: we replace the values smaller than the 5% percentile with the values greater than the 95% percentile.

To improve the robustness of our results, we compare the proposed metrics with existing standard methods. This will provide a benchmark and a clearer picture of the advantages and limitations of the proposed metrics. Specifically, the RGA will be compared with the Root Mean Squared Error (RMSE) in the continuous case and to the AUC in the binary case; the RGR will be compared with the loss in accuracy when all input data are perturbed; the RGF will be compared with the difference in accuracy between the model applied separately on the different population groups; the explanations from RGE will be compared with those obtained applying Shapley values.

Table 17 displays the results from the application of RGA, RGR and RGF, along with the benchmark metrics, in the continuous case.

From Table 17, it results that the RGA is equal to about 91%. We recall that the higher the RGA value, the better the concordance between the trained model and the actual values. Here, the RGA value is close to one, meaning that the predictive accuracy of the model

**Table 15**
*p*-values for RGA, RGR, RGF.

| Experiment (A) | Alternative hypothesis | *p*-values |
|---|---|---|
| RGA | $H_1 : RGA_{\text{lin reg}} > RGA_{\text{Rand For}} > RGA_{\text{reg tree}}$ | 0.001 |
| RGR | $H_1 : RGR_{\text{Rand For}} > RGR_{\text{reg tree}} > RGR_{\text{lin reg}}$ | 0.001 |
| RGF | $H_1 : RGF_{\text{reg tree}} > RGF_{\text{Rand For}} > RGF_{\text{lin reg}}$ | 0.001 |
| Experiment (B) | Alternative hypothesis | *p*-values |
| RGA | $H_1 : RGA_{\text{lin reg}} > RGA_{\text{Rand For}} > RGA_{\text{reg tree}}$ | 0.001 |
| RGR | $H_1 : RGR_{\text{Rand For}} > RGR_{\text{reg tree}} > RGR_{\text{lin reg}}$ | 0.001 |
| RGF | $H_1 : RGF_{\text{reg tree}} > RGF_{\text{Rand For}} > RGF_{\text{lin reg}}$ | 0.001 |
| Experiment (C) | Alternative hypothesis | *p*-values |
| RGA | $H_1 : RGA_{\text{lin reg}} > RGA_{\text{Rand For}} > RGA_{\text{reg tree}}$ | 0.001 |
| RGR | $H_1 : RGR_{\text{lin reg}} > RGR_{\text{Rand For}} > RGR_{\text{reg tree}}$ | 0.001 |
| RGF | $RGF_{\text{Rand For}} > H_1 : RGF_{\text{reg tree}} > RGF_{\text{lin reg}}$ | 0.001 |
| Experiment (D) | Alternative hypothesis | *p*-values |
| RGA | $H_1 : RGA_{\text{lin reg}} > RGA_{\text{Rand For}} > RGA_{\text{reg tree}}$ | 0.001 |
| RGR | $H_1 : RGR_{\text{lin reg}} > RGR_{\text{Rand For}} > RGR_{\text{reg tree}}$ | 0.001 |
| RGF | $H_1 : RGF_{\text{reg tree}} > RGF_{\text{Rand For}} > RGF_{\text{lin reg}}$ | 0.001 |

**Table 16**
*p*-values for RGE.

| Experiment (A) | Alternative hypothesis | *p*-values |
|---|---|---|
| $\text{RGE}_{X_1}$ | $H_1 : RGE_{X_1\text{reg tree}} > RGE_{X_1\text{Rand For}} > RGE_{X_1\text{lin reg}}$ | 0.001 |
| $\text{RGE}_{X_2}$ | $H_1 : RGE_{X_2\text{reg tree}} > RGE_{X_2\text{Rand For}} > RGE_{X_2\text{lin reg}}$ | 0.001 |
| $\text{RGE}_{X_3}$ | $H_1 : RGE_{X_3\text{lin reg}} > RGE_{X_3\text{reg tree}} > RGE_{X_3\text{Rand For}}$ | 0.001 |
| $\text{RGE}_{X_4}$ | $H_1 : RGE_{X_4\text{reg tree}} > RGE_{X_4\text{Rand For}} > RGE_{X_4\text{lin reg}}$ | 0.001 |
| Experiment (B) | Alternative hypothesis | *p*-values |
| $\text{RGE}_{X_1}$ | $H_1 : RGE_{X_1\text{lin reg}} > RGE_{X_1\text{Rand For}} > RGE_{X_1\text{reg tree}}$ | 0.001 |
| $\text{RGE}_{X_2}$ | $H_1 : RGE_{X_2\text{lin reg}} > RGE_{X_2\text{Rand For}} > RGE_{X_2\text{reg tree}}$ | 0.001 |
| $\text{RGE}_{X_3}$ | $H_1 : RGE_{X_3\text{lin reg}} > RGE_{X_3\text{reg tree}} > RGE_{X_3\text{Rand For}}$ | 0.001 |
| $\text{RGE}_{X_4}$ | $H_1 : RGE_{X_4\text{reg tree}} > RGE_{X_4\text{lin reg}} > RGE_{X_4\text{Rand For}}$ | 0.001 |
| Experiment (C) | Alternative hypothesis | *p*-values |
| $\text{RGE}_{X_1}$ | $H_1 : RGE_{X_1\text{reg tree}} > RGE_{X_1\text{Rand For}} > RGE_{X_1\text{lin reg}}$ | 0.001 |
| $\text{RGE}_{X_2}$ | $H_1 : RGE_{X_2\text{reg tree}} > RGE_{X_2\text{Rand For}} > RGE_{X_2\text{lin reg}}$ | 0.001 |
| $\text{RGE}_{X_3}$ | $H_1 : RGE_{X_3\text{Rand For}} > RGE_{X_3\text{reg tree}} > RGE_{X_3\text{lin reg}}$ | 0.001 |
| $\text{RGE}_{X_4}$ | $RGE_{X_4\text{reg tree}} > H_1 : RGE_{X_4\text{Rand For}} > RGE_{X_4\text{lin reg}}$ | 0.005 |
| Experiment (D) | Alternative hypothesis | *p*-values |
| $\text{RGE}_{X_1}$ | $H_1 : RGE_{X_1\text{Rand For}} > RGE_{X_1\text{lin reg}} > RGE_{X_1\text{reg tree}}$ | 0.001 |
| $\text{RGE}_{X_2}$ | $H_1 : RGE_{X_2\text{reg tree}} > RGE_{X_2\text{Rand For}} > RGE_{X_2\text{lin reg}}$ | 0.001 |
| $\text{RGE}_{X_3}$ | $H_1 : RGE_{X_3\text{Rand For}} > RGE_{X_3\text{reg tree}} > RGE_{X_3\text{lin reg}}$ | 0.001 |
| $\text{RGE}_{X_4}$ | $H_1 : RGE_{X_4\text{reg tree}} > RGE_{X_4\text{lin reg}} > RGE_{X_4\text{Rand For}}$ | 0.001 |

**Table 17**
RGA, RGR, RGF and benchmark measures, continuous response.

| Accuracy | RGA | RMSE |
|---|---|---|
| | 0.9149 | 8107.1686 |
| Robustness | RGR | Accuracy Loss |
| | 0.4697 | 399.6947 |
| Fairness | RGF | Accuracy Difference |
| | 0.9984 | 5244.0689 |

is high. The result is statistically significant, as it turns out that, if we test the model against a random model, the *p*-value is very small, approximately equal to $10^{-253}$, thus rejecting the null hypotheses of equality.

The benchmark measure for RGA is the RMSE which, in this case, is equal to about 8107. We cannot easily interpret this value, in absolute terms; we need to make relative comparisons. For example, as the mean salary growth is about 17409$, we can conclude that the RMSE is about half of the mean. The RGA, instead, is normalised and can be interpreted in both absolute and relative terms. A possible disadvantage of RGA is that, with respect to RMSE, it requires a further computational step of ordering the response values with respect to the ranks of the predictions. This, however, allows to compare models for a continuous response with models with a binary response.

The result of the application of RGR leads to a value of about 47%, which indicates that the Random Forest model is not so robust in terms of the considered perturbation of all input variables. However, the model is significantly more robust then a random model, as the *p*-value of the RGR test is approximately equal to $10^{-27}$. The RGR can be compared with the loss in accuracy (in RMSE) obtained moving

**Table 18**
RGA, RGR, RGF and benchmark measures, binary response.

| Accuracy | RGA | AUC |
|---|---|---|
| | 0.6848 | 0.6848 |
| Robustness | RGR | Accuracy Loss |
| | 0.8591 | 0.0333 |
| Fairness | RGF | Accuracy Difference |
| | 0.9366 | 0.1116 |

from the model with non-perturbed data to a model with perturbed data. Such difference is equal to 399, about 5% of the original RMSE, indicating high robustness. This result seems, however, not very reliable, considering that all input variables have been perturbed. The RGR appears more suited to capture lack of robustness. A further advantage of RGR, with respect to the difference in accuracy, is that it is normalised. This allows an easier interpretation with respect to the accuracy loss, albeit at the cost of an extra computational cost.

We now discuss the obtained value for the RGF metric, taking gender as the selected protected variable. The result is an RGF close to one, which seems to indicate that "gender" does not affect the ranks of the target variable "salary growth". The result is, however, not statistically significant, as the $p$-value for the statistical test on RGA is equal to 0.003: we reject the assumption of fairness. On the other hand, the standard "parity" measure which compares the RMSE of the model in the female and male group is equal to 5244: about 64% of the value of the overall RMSE, indicating a similar behaviour of the model in the two groups. The result is consistent with RGF, the difference is that RGF, although more expensive computationally, is normalised and, thus, easier to interpret.

We now consider the case of a binary response. Table 18 reports the results from the application of RGA, RGR and RGF, along with the benchmark metrics, in the binary case, respectively.

Table 18 highlights the clear advantage of our proposed metrics: we can compare the performance of the Random Forest model under two different configurations of the response. While it is not possible to directly compare RMSE with AUC, or accuracy loss/difference expressed as difference of RMSE rather than difference in AUC, the RGB metrics are the same for the binary and the continuous cases. Specifically, the comparison indicates that a continuous response is better predicted than a binary response (RGA = 91% vs 68%); that the model for the continuous response is less robust than the model for the binary response (47% vs 85%); that the model which predicts salary growth (continuous) is more fair than the model which predicts salary doubling (binary) (99% vs 93%). The application of the statistical tests show that the model is significantly more accurate and robust than a random model; and that, similarly to what occurs for a continuous response, the model is not significantly fair, being the $p$-value equal to 0.001.

The results for standard metrics are consistent with those from our metrics; however, the latter have the advantage of a better interpretability and of a wider comparability, against the disadvantage of an increased computational cost.

We now compare the application of RGE with the standard explainability metrics: Shapley values. Table 19 includes the results from the application of RGE, along with Shapley values, in both the continuous and binary cases.

Table 19 shows that the explanations for the binary response are higher than those for the continuous response. This highlights that, in the continuous case, there is a high interaction between the variables, and it is difficult for a single feature to have a high explainability. Overall, based on RGE, the most important explanations are jobtime, age, previous experience and also education. The standard Shapley values do not allow an easy comparison between the values of the two problems, binary and continuous. However, in both cases, the contribution of the predictors to explainability is consistent with those of the RGE. Once more, the comparison shows that our proposed metric is easier to interpret than the benchmark. From a computational complexity viewpoint, Shapley values are computationally expensive, more than the RGE, as they require calculating the difference in predictions for all possible models' combinations.

A further comparison between our proposed RGB metrics and standard ones can be conducted by means of resampling. For example, if we focus on our core metrics, without loss of generality, and for the sake of space, we can calculate the value of RGA and of RMSE, for a continuous response, in 100 different train/sample tests. We can then compute the mean and standard deviation of the values which are provided in Table 20.

From Table 20, note that the RGA has a low standard deviation, about 50 times smaller than the mean. An approximate 99.7% empirical confidence interval ranges from 0.84 to 0.94, indicating a high value of accuracy. On the other hand, the RMSE has a higher standard deviation, about 10 times smaller than the mean. An approximate 99.7% empirical confidence interval ranges from 5069 to 9226, indicating a variable degree of accuracy.

## 4. Concluding remarks

The paper has presented a set of consistent statistical metrics, all rooted in the framework of the rank graduation approach introduced by Lorenz (1905).

The implementation instructions of the proposed metrics, along with their corresponding Python code and all data analysed in the paper are available at: https://github.com/GolnooshBabaei/safeaipackage. The results of the paper are therefore fully transparent and reproducible.

In this contribution we illustrated how these metrics can practically assess the compliance of any AI application to regulatory requirements such as Sustainability (Robustness), Accuracy, Fairness and Explainability.

Our experimental results show that the proposed metrics work quite effectively and can thus be a useful tool for the different stakeholders involved in the assessment of compliance of AI applications and their risks: developers, deployers, consumers, regulators.

Further research is needed, from a methodological viewpoint, to enhance the robustness of the proposed methodology by comparing it with alternative modelisations. Additional research is also needed, from an applied viewpoint, to test the functioning of the methodology on different field domains and applications, such as insurance, health and robotics, to name a few.

We would like to mention that what presented can be enriched by new developments, without altering the reference framework. For example, different types of adversarial attacks can be considered, as different types of perturbations; explainability of group of variables could be considered; other ethical requirements can be included, such as human oversight and environmental sustainability.

Overall, our proposed approach to assess the compliance of AI applications is scientifically sound and relatively simple to implement and interpret. It has two possible limitations, which may be overcome in future research work. First, it assumes that the response variable to be predicted is unidimensional. A multidimensional response would require a multidimensional generalisation of the Lorenz curves. Second, it has been applied to numerical data but it can be extended to deal with non-numerical data, such as text and images.

We finally remark that our devised approach is based only on the comparison of the outputs of machine learning models. It is therefore rather secure, as it does not involve neither new data inputs nor new model elaborations.

**Table 19**
RGE and Shapley values for a Random Forest model to predict a continuous response (left) and a binary response (right).

| Variable | RGE | Shapley values |
|---|---|---|
| Jobtime | 0.0355 | 0.0830 |
| Age | 0.0151 | 0.1018 |
| Previous experience | 0.0130 | 0.0888 |
| Education | 0.0180 | 0.0193 |
| Manager | 0.0129 | 0.0221 |
| Clerical | 0.0004 | 0.0263 |
| Minority | 0.0016 | 0.0180 |
| Gender | 0.0015 | 0.0120 |
| Custodial | 0.0004 | 0.0085 |

| Variable | RGE | Shapley values |
|---|---|---|
| Jobtime | 0.2112 | 1939.8556 |
| Age | 0.1901 | 2050.5184 |
| Previous experience | 0.1197 | 557.7384 |
| Education | 0.1056 | 1143.2048 |
| Manager | 0.0986 | 526.5470 |
| Clerical | 0.0985 | 221.5846 |
| Minority | 0.0915 | 284.7139 |
| Gender | 0.0633 | 208.1586 |
| Custodial | 0.0563 | 208.2397 |

**Table 20**
Robustness comparison between RGA and RMSE.

| RGA | Mean | Standard deviation ($sd$) |
|---|---|---|
| | 0.8962 | 0.0167 |
| RMSE | Mean | Standard deviation ($sd$) |
| | 7,148.0864 | 693.8385 |

**Table 21**
The terms of the RG· formula.

| ID | $y^*_{r^*_i}$ | $iy^*_{r^*_i}$ | $y^*_{r^*_{n+1-i}}$ | $iy^*_{r^*_{n+1-i}}$ | $y^*_{r^{**}_i}$ | $iy^*_{r^{**}_i}$ |
|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 75 | 75 | 27 | 27 |
| 2 | 3 | 6 | 48 | 96 | 12 | 24 |
| 3 | 11 | 33 | 46 | 138 | 48 | 144 |
| 4 | 12 | 48 | 34 | 136 | 34 | 136 |
| 5 | 27 | 135 | 28 | 140 | 3 | 15 |
| 6 | 28 | 168 | 27 | 162 | 11 | 66 |
| 7 | 34 | 238 | 12 | 84 | 46 | 322 |
| 8 | 46 | 368 | 11 | 88 | 0 | 0 |
| 9 | 48 | 432 | 3 | 27 | 75 | 675 |
| 10 | 75 | 750 | 0 | 0 | 28 | 280 |

## CRediT authorship contribution statement

**Golnoosh Babaei:** Coding, Investigation. **Paolo Giudici:** Methodology, Supervision, Revision of the paper. **Emanuela Raffinetti:** Methodology, Investigation, Coding, Revision of the final version to be submitted.

## Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Paolo Giudici reports financial support was provided by The European Union - NextGenerationEU in the framework of the GRINS- Growing Resilient, INclusive and Sustainable (GRINS PE00000018). If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Data availability

https://github.com/GolnooshBabaei/safeaipackage.

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## Appendix

With this Appendix we aim at showing how the RG· metric is calculated, based on data reported in Tables 2–4.

The single terms involved in formula (1) are displayed in Table 21.

By summing all the terms appearing in the third, fifth and seventh column of Table 21 across the 10 observations, from formula (1) it results that RG· = 0.6031.

The proposed metrics can be computed based on the previous example by replacing the terms (i) $y^*_{r^*_i}$, (ii) $y^*_{r^*_{n+1-i}}$ and (iii) $y^*_{r^{**}_i}$ with:

- (i) the response variable values ordered in a non-decreasing sense; (ii) the response variable values ordered in a non-increasing sense; (iii) the response variable values ordered according to the non-decreasing ranks of the predicted values (in the case of RGA);
- the predicted values, computed on non-perturbed data, ordered in a non-decreasing sense; (ii) the predicted values, computed on non-perturbed data, ordered in a non-increasing sense; (iii) the predicted values, computed on non-perturbed data, ordered according to the non-decreasing ranks of the predicted values computed on perturbed data (in the case of RGR);
- the predicted values, provided by the full model, ordered in a non-decreasing sense; (ii) the predicted values, provided by the full model, ordered in a non-increasing sense; (iii) the predicted values, provided by the full model, ordered according to the non-decreasing ranks of the predicted values provided by the reduced model, i.e. without the predictor under evaluation (in the case of RGE);
- the predicted values, provided by the full model, ordered in a non-decreasing sense; (ii) the predicted values, provided by the full model, ordered in a non-increasing sense; (iii) the predicted values, provided by the full model, ordered according to the non-decreasing ranks of the predicted values provided by the reduced model, i.e. without the group variable under evaluation (in the case of RGF).

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