Scalable Assessment and Mitigation Strategies for Fairness in Rankings

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Abstract
Motivated by industrial-scale applications, we consider two specific areas of fairness, one connected to the notion of equality of opportunity, and the other one generally tied to fair model performance. Throughout the paper, we consider only methods that can be scaled to Internet-industry size datasets. With this in mind, we propose a simple post-processing method to achieve equality of opportunity and discuss challenges and some solutions in the specific cases of recommendation systems and rankings. We then discuss a class of model performance fairness measures based on conditional ROC curves. We propose both scalable uncertainty assessment tools (that improve upon recent research) as well as scalable penalized methods to improve fairness with respect to these metrics. We provide fast algorithms with an emphasis on making few passes over the data when possible.

1 Introduction
The receiver-operating characteristic (ROC) curve plays a key role in much work on fairness. It has classically been used to characterize points where equalized odds hold [8]. Naturally and as we will explain in Section 2, aspects of the ROC curve are also connected to the problem of equality of opportunity. It is also important in its own rights in assessing the quality of a classifier [9], and is widely used and intuitively understood by practitioners. In industrial applications, it - or the derived metric of the area under this curve (AUC) - is often a metric that is tracked and optimized for. As such it is an interesting object to consider for use in fairness applications - see also [6] - especially when comparing the performance of a classifier across protected characteristics and hence when one is interested in fair model performance. Its interpretability for a wide range of machine learning practitioners gives it a substantial industrial advantage over probabilistically natural but less interpretable measures of distance, such as Wasserstein distance or various f-divergences [15, 16, 2].

The ROC curve plots power as a function of type I error/size and as such it is clear that most practitioners care particularly about the bottom left part of this curve. Indeed, few would use a test with a type I error above e.g. 20%. Hence we argue in Section 3 for the use of weights in computing the AUC. In fairness applications, it is important to assess statistical errors and therefore methods of uncertainty assessment are needed, and at a very large scale, it is intractable to use resampling methods. Therefore central limit theorems (CLTs) and fast methods for variance computation are desired. We describe solutions to this problem in Section 3.

We discuss in Section 4 various methods targeted towards large scale implementation for mitigation with the fairness metric described above in mind, through using a fairness penalty. This is a classic line of work in fairness [11, 4, 13, 21, 1], though most methods do not scale well to extremely large datasets. These penalized methods are particularly helpful when practitioners do not have access to protected characteristic information when they need to perform classification out-of-sample.

When they do, however, post-processing methods can be used. In other words, after the model is trained, one can learn a transformation of the scores to achieve various fairness objectives. This is
very appealing in industrial practice as it does not require to change the pipeline of model training. These transformations are protected-characteristic-specific and hence can only be used when the protected characteristic is available at (out-of-sample) classification time. We discuss our work on this topic in Section 2 for achieving equality of opportunity as well as some challenges and solutions in applying this technique in the context of ranked data and more generally data gathered with biased feedback.

2 Equality of opportunity in rankings through post-processing

We first recall the definition of Equality of Opportunity (EO) [8].

**Definition 1 (Equality of Opportunity (EO) in classification).** A binary predictor satisfies equal opportunity with respect to (protected) characteristic $C$ and (decision) $\hat{Y}$ if

$$P(\hat{Y} = 1 \mid C = c_1, Y = 1) = P(\hat{Y} = 1 \mid C = c_2, Y = 1), \ \forall c_1, c_2.$$  

In other words, $\hat{Y}$ is independent of $C$ given that $Y = 1$.

It is natural to extend this requirement to non-binary $\hat{Y}$, for instance if they are scores. In this case, if $X$ are features, and $s$ is a score function we would want $s(X) \mid (C = c_1, Y = 1) \overset{d}{=} s(X) \mid (C = c_2, Y = 1)$, for all $c_1, c_2$, where $\overset{d}{=}$ stands for equality in distribution. In other words, the distribution of the scores are independent of $C$ given that $Y = 1$ (see, e.g., [13], Section 2.1). For threshold classifiers (i.e. $\hat{Y}(X) = 1$ iff $s(X) > t$, for a certain threshold $t$), this would ensure EO for the associated classifiers at all thresholds. In industrial applications, this is a natural requirement as scores could be passed downstream to other machine learning systems for various tasks to yield final recommendations for instance.

2.1 A simple algorithm to achieve EO

Here is a simple post-processing algorithm that achieves EO at all thresholds.

**Lemma 1 (Algorithm for EO).** Let $F_{c,1}$ be the cumulative distribution function (CDF) of scores in group $C = c$ and $Y = 1$. Then for each $c$ we transform the scores of group $C = c$ as $s(X) \to F_{c,1}(s(X))$. These transformations guarantee EO for all thresholds $t$ in the range of $s(X)$.

The CDF transformations in Lemma 1 would map the scores into $[0, 1]$. We can apply an additional transformation $F^{-1}(s)$ to bring the scores back to the original scale, where $F$ is the CDF of the original scores before applying any transformation and irrespective of group membership and value of $Y$. Note that this step will not affect the EO problem - or the ROC curve, since the latter is invariant under increasing transformations - but this step might be useful in industrial settings where scores are used in more than one machine learning systems. This line of idea is related to quantile normalization in (bio)statistics [3, 5]. We further discuss interesting variants in the Appendix, Subsection A.1.

2.2 Learning the CDF from clicks and ranked data

Consider a recommendation system where for each query $q$ a candidate set of $K$ documents $\{d_1^{(q)}, \ldots, d_K^{(q)}\}$ are ranked according to a scoring function $s(X)$ defined on a set of features $X$. The viewer’s response to $d_i^{(q)}$ in the recommended list not only depends on the quality of $d_i^{(q)}$ (relative to the viewer) but also depends on the position of $d_i^{(q)}$ in the list. The position bias refers to the fact that the chance of observing a positive response (e.g., click) on a document appearing at a higher position (where the highest position is Position 1) is higher than the chance of observing the same in a lower position. To achieve EO for recommendation systems, we need to adjust for the effect of the position bias in learning the CDFs.

**Definition 2.** A scoring function $s(X)$ of a recommendation system satisfies EO with respect to a characteristic $C$ if $s(X) \mid (C = c_1, Y(\gamma) = 1) \overset{d}{=} s(X) \mid (C = c_2, Y(\gamma) = 1)$, for all $c_1, c_2$, where $\overset{d}{=}$ denote equality in distribution over all queries and candidate documents, $Y(j)$ denotes the counterfactual response when an item appears at position $j$ and $\gamma$ denotes the position of an item in the ranking generated by $s(X)$.
Note that if \( Y(j) \) does not depend on \( j \), then Definition 2 coincides with Definition 1, the classification case. Suppose we learn the conditional CDF transformations described in Section 2.1 from the observational distribution \((s(X), C, Y(\gamma))\) to have the scoring function \( \tilde{s}(X) := \sum_{C} F_{c,1}(s(X))1_{\{C=c_{1}\}} \) that satisfy

\[
\tilde{s}(X) \mid (C = c_{1}, Y(\gamma) = 1) \overset{d}{=} \tilde{s}(X) \mid (C = c_{2}, Y(\gamma) = 1), \text{ for all } c_{1}, c_{2}. \tag{1}
\]

Then the scoring function \( \tilde{s}(X) \) is not guaranteed to satisfy EO (Definition 2) due to the presence of the position bias. To understand this, let \( \tilde{\gamma} \) denote the position of an item based on \( \tilde{s}(X) \). Since \( \tilde{\gamma} \neq \gamma \) could imply \( Y(\tilde{\gamma}) \neq Y(\gamma) \), (1) cannot guarantee

\[
\tilde{s}(X) \mid (C = c_{1}, Y(\tilde{\gamma}) = 1) \overset{d}{=} \tilde{s}(X) \mid (C = c_{2}, Y(\tilde{\gamma}) = 1), \text{ for all } c_{1}, c_{2}. \tag{2}
\]

Under the following assumption, we achieve (2) by learning the conditional CDFs of weighted scores where the weights are given by the inverse of the position bias \( w_{\gamma} = \mathbb{P}(Y(\gamma) = 1 \mid Y(1) = 1) \).

**Assumption 1.** Let \( s(X), Y(j) \) and \( C \) be as in Definition 2. For all query \( q \) and all candidate document \( d^{(q)}_{i} \) and all \( j > 1 \), we assume that

1. (Homogeneity) \( \mathbb{P}(Y(j) = 1 \mid Y(1) = 1) = d^{(q)}_{i} = \mathbb{P}(Y(j) = 1 \mid Y(1) = 1) \), and
2. (Preservation of Hierarchy) \( \mathbb{P}(Y(j) = 1 \mid Y(1) = 0, d^{(q)}_{i}) = 0 \).

The first assumption states that the position bias is homogeneous over all queries and candidate documents. This is common assumption in the literature (see, for example, [17, 20, 18]). The second assumption states that if a candidate document does not get a positive response, then it cannot get a positive response in a lower position.

**Theorem 1.** Under Assumption 1, let \( w_{j} := \mathbb{P}(Y(j) = 1 \mid Y(1) = 1) \) and let \( F^{*}_{c,1} \) denote the CDF of the conditional scores \( s(X) \) given \( Y(\gamma) = 1 \) and \( C = c \) with weights \( 1/w_{\gamma} \) (see Equation (5)). Then the transformed scores \( \tilde{s}(X) := \sum_{C} F^{*}_{c,1}(s(X))1_{\{C=c_{1}\}} \) satisfy

1. \( \tilde{\gamma} \mid (C = c_{1}, Y(1) = 1) \overset{d}{=} \tilde{\gamma} \mid (C = c_{2}, Y(1) = 1) \), and
2. \( \tilde{s}(X) \mid (C = c_{1}, Y(\tilde{\gamma}) = 1) \overset{d}{=} \tilde{s}(X) \mid (C = c_{2}, Y(\tilde{\gamma}) = 1) \),

for all \( c_{1}, c_{2} \), where \( \tilde{\gamma} \) denote the position of an item based on \( \tilde{s}(X) \).

The first part Theorem 1 shows the weighted CDF transformations guarantees the “fairness of exposure” with respect to the documents with a (counterfactual) positive response at position 1. This is also related to the notion of group fairness parity defined in Section 2.2 of [18].

**Corollary 1.** For a group \( C = c \), let \( M_{c} := \mathbb{P}(Y(1) = 1 \mid C = c) \) and \( v_{obs}(c) := \mathbb{P}(Y(\gamma) = 1 \mid C = c) \) be the average merit and the observed exposure (with respect to the scoring function \( \tilde{s}(X) \) defined in Theorem 1) respectively. Then under Assumption 1, \( \tilde{s}(X) \) achieves the group fairness parity, given by the following constraint: \( v_{obs}(c_{1})/M_{c_{1}} = v_{obs}(c_{2})/M_{c_{2}} \), for all \( c_{1}, c_{2} \).

**Weight estimation:** The weighted CDF transformations defined in Theorem 1 requires the weights to be known. To estimate the position bias \( w_{j} \), we may collect data by randomizing slots and estimate the ratio of click-through-rates (CTRs) at position \( j \) and position 1, i.e.

\[
\hat{w}_{j} = \left[ \frac{\sum_{i} 1_{\{Y(\gamma)=1, \gamma=j\}}}{\sum_{i} 1_{\{\gamma=j\}}} \right] / \left[ \frac{\sum_{i} 1_{\{Y(\gamma)=1, \gamma=1\}}}{\sum_{i} 1_{\{\gamma=1\}}} \right]. \tag{3}
\]

Without the randomization, we will end up underestimating the CTR ratio by using (3) as the items served at position \( j \) is expected to have a lower quality than the items served at position 1. More precisely, in the observational data where the items are ranked according to \( s(X) \), the conditional distribution of \( s(X) \) given \( \gamma = 1 \) is expected to be stochastically larger than the conditional distribution of \( s(X) \) given \( \gamma = j \).

However, randomly shuffling all documents can undesirably harm the user experience. A less harmful alternative is to shuffle pairs of documents randomly [10, 20]. To estimate the weights from observational data [20] applied the EM algorithm with a parametric click model. Below, we propose a non-parametric approach based on importance sampling. To this end, we first estimate the response bias at position \( j \) relative to position \( j-1 \) by correcting for the discrepancy in the distribution of scores in those positions with importance weighting as follows.
Let $f_j(\cdot)$ denote the conditional density of the observed score at position $j$. For $j \geq 2$, define

$$
\eta_j = E \left[ \frac{Y(\gamma) f_{j-1}(s(X))}{f_j(s(X))} \mid \gamma = j \right] / E[Y(\gamma) \mid \gamma = j - 1].
$$

It is straightforward to estimate $\eta_j$ by replacing the conditional density with its estimate and the conditional expectations with the corresponding empirical averages. We denote this estimator by $\hat{\eta}_j$.

Finally, we estimate $w_j$ by $\hat{w}_j = \prod_{r=2}^j \hat{\eta}_r$. The reason for not estimating the $w_j$ directly by using the importance weights $f_j(s(X))/f_j(s(X))$ is that the distribution of scores at position 1 might be much different from its counterpart at position $j$, even for not-so-large large $j$. Our adjacent-pairwise importance sampling approach tends to have a lower variance than the direct importance sampling approach. However, for practical purposes we recommend to use a truncated version $\hat{w}_j = \prod_{r=2}^{\min(j,T)} \hat{\eta}_r$, for some threshold $T$. Note that this is equivalent to assuming $\eta_j = 1$ for all $j > T$, which is a reasonable practical assumption for most recommendation systems.

**Simulations:** We generate a population of $p = 50000$ items, where each item consists of document id $i$, characteristic $C_i \sim \{0, 1\}$, $Y_i(1) \in \{0, 1\}$ and relevance $R_i$. We independently generate $C_i$'s from a Bernoulli(0.7) distribution. The conditional distribution $Y_i(1) \mid C_i = 0$ is Bernoulli(0.35), and the conditional distribution $Y_i(1) \mid C_i = 1$ is Bernoulli(0.45). Finally, $R_i$ is generated from

$$
R_i \mid (C_i, Y_i(1)) \sim \mathcal{N}(0.6Y_i(1) + 2C_i, 0.5) + \text{Uniform}[0, (1 - C_i) \ast (1 + Y_i(1))].
$$

We consider a recommendation system with $K = 50$ slots. For each query, we randomly select 50 documents from the population and assign a score $s_i = R_i + \mathcal{N}(0, 0.2)$ to each selected document $i \in \{1, \ldots, 50,000\}$. The selected documents are then ranked according to $s_i$ (in a descending order) and assigned position according to rank($i$). Finally, the document at position $j$ gets observed response $Y(j) = Y(1) \times \text{Bernoulli}(w_j)$ with position bias $w_j = 1/\log_2(1 + j)$. We generate a training data based on $n = 25000$ queries.

![Figure 1: Score and position distributions corresponding to online positive responses](image)

We estimate the conditional CDFs without weights and with estimated weights from the training data, where we estimate the weights using the adjacent-pairwise importance sampling approach with the threshold $T = 30$ (a plot is provided in Appendix A.3). We generate validation datasets (i) without score transformation, (ii) with CDF transformations, and (iii) with weighted CDF transformations. Figure 1 shows demonstrate that without considering position bias, we may end up over-exposing the previously under-exposed group, while the weighted CDF approach can correctly address the equality of opportunity in rankings.

### 3 A practical fairness metric: weighted AUC

A standard way to assess the quality of a classifier is to consider the Receiver-Operating characteristic (ROC) curve. The area under the curve (AUROC/AUC) is often used to assess the quality of a classifier: the higher the AUROC/AUC, the better. In the fairness context, this gives rise to the following idea (see also [6] and less directly [8]): one can compare the AUROC for a classifier measured for data taking two values of a protected characteristic. One might want the classifier to be equally good for the two values of the protected characteristic, i.e., equality of AUROC. When this is restricted to the classifier setup and hence a single point on ROC curves, this is the requirement
of Equalized Odds [8]. This is also a relaxed version of the requirement that score distributions be independent of the protected characteristic. With real data, the question then arises of assessing whether two AUROC’s are statistically significantly different. Previous work [6] addressed that problem by using a permutation test. This is very interesting but suffers from two potential pitfalls: computational expense and lack of information about effect size. We develop here an alternative approach, based on asymptotic analysis: it allows us to derive confidence intervals for the (weighted) AUROC and hence immediately for the difference of two independent (weighted) AUROCs. Weighted AUROC is more interesting from a practical standpoint as a classifier with a high false-positive rate would not be used in practice. This derivation leads to a fast algorithm which can be implemented in e.g. scala and described in Subsection 3.2. In Appendix B.2 we briefly describe how to extend the results to Precision-Recall curves, to deal with class imbalance. Throughout this section, we consider the setup where a classifier is trained on training data and then we have independent observations in a validation set with labels. This is where we measure AUROC.

Notations and reminders We call \( \{ Y_j \}_{j=1}^m \) the \((m)\) observations with true label 1 (i.e. the positives) and \( \{ X_i \}_{i=1}^n \) the \((n)\) observations with label 0. The classifier gives score \( s \) to observations; when \( s \) is large we classify to group 1. We define the notation \( \overset{d}{\sim} \) in Appendix A.4, a proxy for weak convergence.

ROC curves plot True positive rates vs False positive rates, i.e. fraction of \( Y_j \)'s correctly classified (TP/(TP+FN)) vs fraction of \( X_i \)'s incorrectly classified (FP/(FP+TN)). Suppose cutoff is at \( T \), classify to group 1 if \( s(\cdot) > T \); then \( TP_R(T) = 1 - \hat{G}_m(T) \) and \( FP_R(T) = 1 - \hat{F}_n(T) \) where \( \hat{G}_m \) is empirical cdf of \( s(Y_j) \), \( \hat{F}_n \) empirical cdf of \( s(X_i) \). Calling \( t = 1 - \hat{F}_n(T) \), the empirical ROC curve, \( \hat{ROC}_{m,n}(t) \) is just a plot of

\[
(t, 1 - \hat{G}_m(\hat{F}_n^{-1}(1-t))) , \ 0 \leq t \leq 1.
\]

This is well known ([9]) but will be central to our analysis. We assume that the score data is drawn i.i.d., consistent with the description of our experiment above. Through elementary considerations or following [9] we find that, under regularity conditions - see Appendix A.4- to first order and in the sense of weak convergence of stochastic process on \([0,1]\) [19], if \( B_1 \) and \( B_2 \) are independent standard Brownian bridges on \([0,1]\), and the population ROC is \( ROC(t) = 1 - G(F^{-1}(1-t)) \),

\[
\hat{ROC}_{m,n}(t) \overset{d}{\sim} ROC(t) + \frac{1}{\sqrt{m}} B_1(G(F^{-1}(1-t))) + \frac{1}{\sqrt{n}} \frac{g(F^{-1}(1-t))}{f(F^{-1}(1-t))} B_2(1-t).
\]

3.1 Weighted AUROC with general bounded weight \( w \)

As already noted, the AUROC puts a disproportionate amount of importance on a part of the ROC that is relatively unimportant from the point of view of the practical performance of the classifier. Hence we consider a richer metric, the weighted area under the ROC, i.e.

\[
I(w) = \int_0^1 w(t)\hat{ROC}_{m,n}(t)dt.
\]

Using the result above, we have under mild regularity conditions (see Appendix A.4.1)

\[
I(w) \overset{d}{\sim} \int_0^1 w(t)ROC(t)dt + \frac{1}{\sqrt{m}} \int_0^1 w(t)B_1(G(F^{-1}(1-t)))dt + \frac{1}{\sqrt{n}} \int_0^1 w(t)ROC'(t)B_2(1-t)dt.
\]

Standard results (see Appendix and [14]) guarantee that the integrals involving Brownian Bridge under considerations are independent Gaussian random variables and so is \( I(w) \). Let us call \( I_1(w) = \int_0^1 w(t)B_1(G(F^{-1}(1-t)))dt \) and \( I_2(w) = \int_0^1 w(t)\frac{g(G^{-1}(1-t))}{f(G^{-1}(1-t))} B_2(1-t)dt \).

Lemma 2. We call \( U \) a uniform \([0,1]\) random variable. Let \( W \) be a primitive of \( w \) and \( \gamma(u) = 1 - F(G^{-1}(u)) \). Then

\[
\var[ I_1(w) ] = \var[ W(\gamma(1-U)) ].
\]

Suppose \( w \) is differentiable in the sense of distributions and so is \( ROC \). Let \( P_2(t) = w(t)ROC(t) - \int_0^t w'(u)ROC(u)du \). Then

\[
\var[ I_2(w) ] = \var[ P_2(U) ].
\]

The limiting variance [12] of \( I(w) \) is simply \( \var[ I_1(w) ]/m + \var[ I_2(w) ]/n \).
So these are simple functions of the (population) ROC curve and its inverse, the “mirror” ROC curve, i.e. $\text{ROC}(t) = \gamma(1 - t) = 1 - F(G^{-1}(1 - t))$ and as such are fairly easy to estimate using plug-in methods. We develop connections of these results to Mann-Whitney-type statistics in Appendix B, and propose an alternate derivation there. The proof of the lemma can be found in A.6.

**Case** $w(t) = 1_{[t \leq \alpha]}$: As this case is of particular interest ($\alpha = .2$ would be reasonable in many applied situations), we provide a lemma for this specific case.

**Lemma 3** (Variance AUROC below cutoff). The limiting variance of $I(w)$ for $w(t) = 1_{[t \leq \alpha]}$ can be written as, if $U$ is uniform on $[0, 1]$,

$$\frac{1}{m} \text{var} [W(\gamma(1 - U))] + \frac{1}{n} \text{var} [P_2(U)].$$  (4)

If $\text{var} [\text{ROC}(U)1_{[U \leq \alpha]}] = \int_0^\alpha \text{ROC}^2(t)dt - \left[\int_0^\alpha \text{ROC}(t)dt\right]^2$, and $E\left(\text{ROC}(U)1_{[U \leq \alpha]}\right) = \int_0^\alpha \text{ROC}(t)dt$, we have

$$\text{var} [P_2(U)] = \text{var} [\text{ROC}(U)1_{[U \leq \alpha]}] + \alpha(1 - \alpha)[\text{ROC}(\alpha)]^2 - 2(1 - \alpha)\text{ROC}(\alpha)E\left(\text{ROC}(U)1_{[U \leq \alpha]}\right).$$

If we call $\tilde{\text{ROC}}(t) = 1 - F(G^{-1}(1 - t))$, we have

$$\text{var} [W(\gamma(1 - U))] = \int_0^{\text{ROC}(\alpha)} \tilde{\text{ROC}}^2(t)dt - \left(\int_0^{\text{ROC}(\alpha)} \tilde{\text{ROC}}(t)dt\right)^2$$

$$+ \alpha^2\text{ROC}(\alpha)(1 - \text{ROC}(\alpha)) - 2\alpha(1 - \text{ROC}(\alpha)) \int_0^{\text{ROC}(\alpha)} \tilde{\text{ROC}}(t)dt.$$

When $\alpha = 1$, we recover the variance of the Mann-Whitney statistic, as expected. Furthermore, the results above can give us conservative bounds on $\text{var} [I(w)]$ since ROC and $\tilde{\text{ROC}}$ are between 0 and 1. However when $n$ and $m$ are very large, these conservative bounds will probably be too loose to assess whether there is a statistical difference between two groups, hence the need for precise results.

### 3.2 A fast algorithm for $w(t) = 1_{[t \leq \alpha]}$

We provide a fast implementation of the results of Lemma 3, one that requires few passes over the data, an almost mandatory requirement for applications in industrial practice. This algorithm allows fast computation at multiple cutoffs, all at once. One of the main advantages of the theory and the fast algorithm is that we get confidence intervals for the parameters of interest (instead of p-values), and our work allows us to avoid resampling methods which do not scale to the data size we require (however, see the interesting paper [6]). From a scalability point of view, Algorithm 1 has the same order of complexity as computing the ROC-AUC. However, we save orders of magnitude on computing resources since we do not need to perform bootstrap simulations for computing the variance. This is crucial from a computing resources standpoint when one needs to perform such tests hundreds of times during the course of a day, in large-scale industry applications.

Let $\{(s_1, y_1), \ldots, (s_N, y_N)\}$ be an ordered dataset where $s_i$ is the score of the $i$-th sample and $y_i \in \{0, 1\}$ is the corresponding response and $s_{(1)} \leq \cdots \leq s_{(N)}$ is an ordering of the scores. Let $m = \sum_i 1_{\{y_i = 1\}}$, $n = \sum_i 1_{\{y_i = 0\}}$, true positive rate $TPR(i) = \frac{1}{m} \sum_{j=1}^{i} 1_{\{y_{(N+1-j)} = 1\}}$ and false positive rate $FPR(i) = \frac{1}{n} \sum_{j=1}^{i} 1_{\{y_{(N+1-j)} = 0\}}$ denote the number of true positives and the number of false positives when top-$i$ samples are classified as 1 and the rest are classified as 0.

The empirical ROC curve is a non-decreasing step function in $[0, 1]$ where the step sizes are of the form $r/n$ for $r \in \{0, \ldots, n\}$. This observation motivates us to represent the ROC curve as $\{(0, T_0), (1/n, T_1), \ldots, (1, T_n)\}$ with $T_i := \max\{TPR(j) : FPR(j) = i/n\}$. Then the ROC-AUC is given by $\sum_{i=0}^{n-1} T_i \times (1/n)$ and the area under the squared ROC curve is given by $\sum_{i=0}^{n-1} T_i^2 \times (1/n)$. Similarly, we represent the inverse ROC curve (i.e., $\text{ROC}(t)$ above) as $\{(0, F_0), (1/m, F_1), \ldots, (1, F_n)\}$ where $F_i := \max\{FPR(j) : TPR(j) = i/m\}$. Then the inverse ROC-AUC is given by $\sum_{i=0}^{m-1} F_i \times (1/m)$ and the area under the squared inverse ROC curve is given by $\sum_{i=0}^{m-1} F_i^2 \times (1/m)$.

6
Algorithm 1 Truncated AUCs with estimated variances for multiple cutoffs

Require: \{\{(s_1, y_1), \ldots, (s_N, y_N)\}\}, Cutoffs \(0 < \alpha_1 < \cdots < \alpha_k \leq 1\).
Ensure: \{\{(\alpha_r, auc_r, var_r) : r = 1, \ldots, k\}\}

1: Sort the data in ascending order based on the score \(s_i\)'s to obtain \((s_{(1)}, y_{(1)}), \ldots, (s_{(N)}, y_{(N)})\);
2: Compute \(m = \sum_{i=1}^N 1\{y_i=1\}\) and \(n = \sum_{i=1}^N 1\{y_i=0\}\);
3: Initialize \(r = 1\), \(tpr = fpr = auc = sqauc = \tilde{auc} = sq\tilde{auc} = 0\);
4: for \(i = 1, \ldots, n\) do:
5: \hspace{1em} if \(fpr + 1/n > \alpha_r\) then:
6: \hspace{2em} \(auc_r = auc + tpr \times (\alpha_r - fpr)\);
7: \hspace{2em} \(sqauc_r = sqauc + tpr^2 \times (\alpha_r - fpr)\);
8: \hspace{2em} \(var_r = \frac{1}{n} \{sqauc_r - auc_r^2 + \alpha(1-\alpha)(tpr)^2 - 2(1-\alpha) \times tpr \times auc_r\} + \frac{1}{m} \{sq\tilde{auc} - \tilde{auc}^2 + \alpha^2 tpr(1-tpr) - 2\alpha(1-tpr) \times \tilde{auc}\} + \frac{1}{n} \{sqauc - auc^2 + \alpha^2 tpr(1-tpr) - 2\alpha(1-tpr) \times auc\}\);
9: \hspace{1em} \(r = r + 1\);
10: \hspace{1em} end if
11: \hspace{1em} end if
12: \hspace{1em} if \(y_{(N+1-i)} = 0\) then:
13: \hspace{2em} \(fpr = fpr + 1/n, auc = auc + tpr/n, sqauc = sqauc + tpr^2/n\);
14: \hspace{2em} else:
15: \hspace{3em} \(tpr = tpr + 1/m, \tilde{auc} = \tilde{auc} + fpr/m, sq\tilde{auc} = sq\tilde{auc} + fpr^2/m\);
16: \hspace{2em} end if
17: \hspace{1em} end for

To compute the partial AUC and its variance for \(w(t) = 1_{[t \leq \alpha]}\), we need to stop at \(FPR(i) = \alpha\) (see line 5 in Algorithm 1). Note that various normalizations can be done “at the last step” to avoid dividing small numbers by very large ones and encountering floating-point precision arithmetic errors. Furthermore, having now understood how the variance of the statistics of interest scale with \(n\) and \(m\), we could potentially subsample the data to estimate the variance of the statistics of interest, effectively using the above algorithm on a subsample of the data, while properly normalizing for the original size in the end.

## 4 Simple proxy-penalized methods

In many applications, we only have access to the protected characteristic at the time of training but not at the serving time (out of sample prediction). Post-processing methods require serve-time access to the protected characteristic and hence are unusable in this setup. The goal of this section is to use regularization methods based on simple penalties that result in highly scalable solutions that reduce the gap in model performance between different groups. The solution is motivated by the fact that conditional independence (hence equalized odds) can be verified by establishing that conditional mutual information between two variables is zero. Denote the predicted score for observation \(i\) by \(s(X_i; \theta)\), the label by \(Y_i\), and the protected characteristic by \(C_i\). Let \(L(Y, s(X; \theta))\) be the loss function for classification; the unconstrained problem solves \(\arg\min_{\theta} L(Y, s(X; \theta))\), for a set of parameters \(\theta\). Denote the conditional mutual information between \(s(X; \theta)\) and \(C\) given \(Y\) by \(I(s(X; \theta); C|Y)\). Then, define the fairness-constrained problem as

\[
\arg\min_{\theta} L(Y, s(X; \theta)) + 2\lambda I(s(X; \theta); C|Y),
\]

where \(\lambda\) is a tuning parameter. \(I(s(X; \theta); C|Y)\) is data-dependent and can be estimated in various non-parametric and parametric ways. [13] use a kernel density estimate to estimate the \(\chi^2\) divergence at the mini-batch level and use it with DNNs. In this work, we suggest using very scalable parametric estimators of \(I(s(X; \theta); C|Y)\) at the population level and use it with gradient-based methods to solve the constrained optimization problem. We obtain a parametric estimate of \(I(s(X; \theta); C|Y)\), by approximating the scores for each combination of \((C, Y)\), as well as for each \(Y\), by a normal distribution. Although these approximations are not necessarily accurate on real data, the point is that they yield a (proxy-)penalty that can be computed very fast and scalably, along with its gradients. This is crucial in real-world applications since we usually work with enormous datasets and these estimates have to be computed at every step of the gradient-based algorithms. Non-parametric estimates on the other hand are expensive to compute and it is computationally prohibitive to compute them on the entire dataset at every step of the optimization algorithm.
Under the normality “assumption”, the penalty term can be “estimated” by the proxy

\[
2I(s(X; \theta); C|Y) = \frac{n_+}{n} \left( \log \hat{\sigma}_+^2 - \sum_{j=1}^M p_j \log \hat{\sigma}_j^2 \right) + \frac{n_-}{n} \left( \log \hat{\sigma}_-^2 - \sum_{j=1}^M p_j \log \hat{\sigma}_j^2 \right),
\]

where \( n_+ = |\{i : Y_i = 1\}|, n = n_+ + n_-, n_{j+} = |\{i : C_i = j, Y_i = 1\}|, p_{j+} = n_{j+}/n_+, \)

\[
\hat{\mu}_{j+} = \frac{1}{n_{j+}} \sum_{\{i : C_i = j, Y_i = 1\}} s(X_i; \theta) \quad \text{and} \quad \hat{\sigma}_{j+}^2 = \frac{1}{n_{j+}} \sum_{\{i : C_i = j, Y_i = 1\}} s(X_i; \theta)^2 - \hat{\mu}_{j+}^2,
\]

and similarly for \( \hat{\mu}_{j-} \) and \( \hat{\sigma}_{j-}^2 \) (see Section C). Since the \( \hat{\sigma}_j^2 \)s are smooth functions of \( \theta \), it is easy to differentiate the regularizer during our optimization. In particular, the time complexity of this computation is of the order of the computation of the gradient of the loss function. In real world applications on hundreds of features and millions of observations, the penalized logistic regression takes between two to three times longer than the non-penalized logistic regression, both using ADAGRAD.

### 4.1 Application to real-world data

We now analyze two benchmark open-source dataset and the fairness as measure through partial AUC for different groups. Most of the existing methods in the literature have been showcased on these datasets. However, since there are no scalable solutions that do not require access to the protected characteristic at the prediction time, further comparisons have not been conducted in this work.

**COMPAS dataset:** COMPAS is a commercial tool used by judges and parole officers to assess the risk of reoffending (recidivism). It has come under scrutiny due to analyses showing that it may misclassify black defendants.\(^1\) It includes data on criminal history, jail and prison time, demographics, and COMPAS risk scores for defendants from Broward County from 2013 and 2014. We trained a logistic regression to predict the likelihood of recidivism within two years of release and compared the performance of the model for White and African-American defendants. The AUC (and partial AUC at different cutoffs) is not significantly different between the two groups, as shown in Figure 2a.

**Adult Income dataset:** The dataset includes census data for adults and the task is to predict whether an individual’s income exceeds $50K. After restricting to the US population and one-hot-encoding the categorical features, we have 29170 observations of 65 features. The protected characteristic is gender. We fit a penalized logistic regression with different values of \( \lambda \). The vanilla models perform significantly better for females than males and the difference disappears by adding enough penalty. Figure 2b shows the partial AUCs for various values of \( \lambda \) and two score cutoffs. The plots for other values of the cutoff are similar. The regularization closes the gap between females and males at a slight cost in performance.

![COMPAS data across racial groups](image1)

![Adult Income data across different genders](image2)

**Figure 2:** Performance of real-world datasets

### 5 Conclusion

We have proposed tools for handling three central tasks in fairness in ML at scale: 1) post-processing methods for handling Equality of Opportunity in rankings; 2) fast uncertainty assessment tools for assessing fair model performance and 3) new penalties that act as scalable fairness proxies in classification. They should be very useful in several Internet-industry applications.

\(^1\)https://www.propublica.org/article/how-we-analyzed-the-compas-recidivism-algorithm
Broader impact

Machine Learning (ML) systems may contain implicit biases and reproduce or reinforce them. It is hence crucial to develop tools for assessment and mitigations of potential implicit biases in large scale ML systems, since they increasingly power decisions affecting larger and larger portions of society.

In this paper, we develop tools for those exact purposes that are theoretically sound and practically applicable at the Internet-data scale. We hope that these tools will be broadly applicable where they matter crucially, in real-life applications. Our methods try to measure and mitigate unfairness with respect to classic ethical principles rooted in the Rawlsian tradition of fairness in moral and political Philosophy, epitomized by the concept of equality of opportunity, for instance.

This research should benefit groups that are currently disadvantaged in large-scale automatic decision systems and should yield positive outcomes for those groups. The consequences of the failure of the system might be the perpetuation of the status quo in terms of performance (broadly construed) of those systems. While we do not see immediately clear negative outcomes of this work, we remind mindful that fairness is in practice a dynamic problem, and we have mostly addressed it from a static standpoint in this paper (though see comments in Appendix A.1). This work has also not addressed intersectionality issues explicitly, though the framework is rich enough to handle some intersectional questions. Hence good practice will require not only monitoring the fairness performance of the tools we have developed but also whether they have unintended intersectional consequences.

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A Appendix

A.1 Variants of EO algorithm, Lemma 1

This approach could also allow to maintain EO between retraining of the models by updating $F_c,1$'s online, as indeed fairness problems are dynamic [7]. If keeping these CDFs in memory is too costly, they can be discretized (for instance, at every percentile or every $10^{-3}$) and create a linear or higher-order interpolation increasing between the points.

Furthermore, one could relax the strict EO constraint, by considering the following modification to the transformation of the scores:

$$\tilde{s}_c(\alpha) = (1 - \alpha)s_c + \alpha F^{-1}_c(F_{c,1}(s_c))$$

where $s_c$ denote the score restricted to $C = c$ and $0 \leq \alpha \leq 1$. We can tune $\alpha$ to achieve a desirable performance-fairness trade-off, where larger values of $\alpha$ would bring more fairness (in terms of EO), possibly at the expense of a lower performance. In Figure 3, we demonstrate this trade-off with the simulation setting (and the weighed CDF transformations) described in Section 2.2.

![Figure 3](image-url)

**Figure 3**: EO and performance for a number of values of the tuning parameter $\alpha$, where EO is measured by the Kolmogorov-Smirnov distance between the distribution of scores with positive responses, and the performance is measured by the proportion of positive responses (i.e., click-through rate when clicks are the positive responses).

A.2 Proofs of Section 2

**Proof of Lemma 1.** Let $s_{c,1}$ denote the random variable corresponding to the score $s(X)$ restricted to $C = c$ and $Y = 1$. Since $F_{c,1}$ is the CDF of $s_{c,1}$, the distribution of $F_{c,1}(s_{c,1})$ is $\text{Uniform}[0,1]$ for all $c$. Hence these transformed scores satisfy equality of opportunity across all thresholds.

**Proof of Theorem 1.** We first prove the results using the following claims and then prove the claims.

Claim 1:

$$\mathbb{P}(s(X) \leq t \mid \gamma = j, Y(j) = 1, C = c) = \mathbb{P}(s(X) \leq t \mid \gamma = j, Y(1) = 1, C = c) \text{ for all } t.$$ 

Claim 2:

$$\mathbb{P}(\gamma = j \mid Y(\gamma) = 1, C = c) = \frac{w_j \mathbb{P}(\gamma = j \mid Y(1) = 1, C = c)}{\sum_r w_r \mathbb{P}(\gamma = r \mid Y(1) = 1, C = c)}.$$
Using Claims 1 and 2, we show that the CDF of \( s(X) \) given \( Y(1) = 1 \) and \( C = c \) equals \( F_{c,1}^* \).

\[
F_{c,1}^*(t) := \sum_j \mathbb{P}(s(X) \leq t \mid \gamma = j, Y(j) = 1, C = c) \mathbb{P}(\gamma = j \mid Y(\gamma) = 1, C = c) / w_j
\]

This implies that the conditional distribution of \( \tilde{s}(X) := F_{c,1}^*(s(X)) \) given \( Y(1) = 1 \) and \( C = c \) is Uniform[0, 1] for all \( c \). Therefore, the conditional distributions of the position \( \tilde{\gamma} \) given \( Y(1) = 1 \) and \( C = c \) are identical for all \( c \). This completes the proof of the first part of the theorem.

To prove the second part, we will use Claims 1 and 2 with \( (\tilde{s}(X), \tilde{\gamma}) \) instead of \( (s(X), \gamma) \).

\[
\mathbb{P}(\tilde{s}(X) \leq t \mid C = c, Y(\gamma) = 1)
= \sum_j \mathbb{P}(\tilde{s}(X) \leq t \mid \gamma = j, Y(j) = 1, C = c) \mathbb{P}(\gamma = j \mid Y(\gamma) = 1, C = c)
= \sum_j w_j \mathbb{P}(\gamma = j \mid Y(1) = 1, C = c)
= \sum_j w_j \mathbb{P}(\gamma = j \mid Y(1) = 1, C = c).
\]

This completes the second part of the theorem, since the distributions of \( (\tilde{s}(X), \tilde{\gamma}) \) given \( Y(1) = 1 \) and \( C = c \) are identical for all \( c \).

**Proof of Claim 1:** From the second part of Assumption 1, it follows that

\[
\mathbb{P}(s(X) \leq t \mid \gamma = j, Y(j) = 1, C = c) = \mathbb{P}(s(X) \leq t \mid \gamma = j, Y(j) = 1, Y(1) = 1, C = c).
\]

Therefore, the results follows from the first part of Assumption 1 that ensures that \( Y(j) \) is independent of \( s(X), \gamma \) and \( C \) given \( Y(1) \).

**Proof of Claim 2:** Using the second part of Assumption 1 and then applying the Bayes’ theorem, we get

\[
\mathbb{P}(\gamma = j \mid Y(\gamma) = 1, C = c)
= \mathbb{P}(\gamma = j \mid Y(1) = 1, C = c)
= \mathbb{P}(Y(\gamma) = 1 \mid Y(1) = 1, C = c) \mathbb{P}(\gamma = j \mid Y(1) = 1, C = c)
= \sum_r \mathbb{P}(Y(\gamma) = 1 \mid Y(1) = 1, C = c) \mathbb{P}(\gamma = j \mid Y(1) = 1, C = c)
= w_j \mathbb{P}(\gamma = j \mid Y(1) = 1, C = c).
\]

The second last equality follows from the first part of Assumption 1, and the last equality follows from the definition of \( w_j \).

**Proof of Corollary 1.** Note that

\[
\frac{v_{obs}(c)}{M_c} = \sum_j \frac{\mathbb{P}(Y(j) = 1 \mid Y(1) = 1, \tilde{\gamma} = j, C = c) \mathbb{P}(\tilde{\gamma} = j \mid Y(1) = 1, C = c)}{\mathbb{P}(Y(1) = 1 \mid C = c)}
= \sum_j \frac{\mathbb{P}(Y(j) = 1 \mid Y(1) = 1) \mathbb{P}(Y(1) = 1, \tilde{\gamma} = j \mid C = c)}{\mathbb{P}(Y(1) = 1 \mid C = c)}
= \sum_j w_j \mathbb{P}(\tilde{\gamma} = j \mid Y(1) = 1, C = c),
\]

where \( w_j \) is as in Theorem 1 and the second equality follows from the first part of Assumption 1. Therefore, the result follows from the first part of Theorem 1. 

\[\square\]
A.3 Position bias estimation from observational data

![Figure 4: Estimating the position bias $w_j = 1/\log 2(1 + j)$ using the adjacent-pairwise importance sampling approach with the threshold $T = 30$ (see Section 2.2).]

A.4 Elementary reminders on weak convergence

For the sake of convenience, we recall some elementary empirical process results. We assume that the data is i.i.d. We call $\hat{F}_n$ the empirical distribution of the data. Recall that pointwise, if $Z$ is $N(0, 1)$, the central limit theorem guarantees that (Section 19.1)

$$\hat{F}_n(x) \stackrel{d}{\asymp} F(x) + \frac{1}{\sqrt{n}} \sqrt{F(x)(1 - F(x))} Z,$$

and as a process

$$\hat{F}_n(x) \stackrel{d}{\asymp} F(x) + \frac{1}{\sqrt{n}} B_1(F(x)),$$

where $B_1$ is standard brownian bridge (Theorem 19.3 in [19]).

The $\stackrel{d}{\asymp}$ signs here should be formally understood as weak convergence results, i.e. $\hat{F}_n(x) \stackrel{d}{\asymp} F(x) + \frac{1}{\sqrt{n}} \sqrt{F(x)(1 - F(x))} Z$ means that, if $\Rightarrow$ denotes weak convergence,

$$\sqrt{n}(\hat{F}_n(x) - F(x)) \Rightarrow \sqrt{F(x)(1 - F(x))} Z.$$

However, they are easier to manipulate in this paper as we do not have to do the cumbersome renormalizations that would appear in our paper and this notation conveys all the information needed without the awkwardness of renormalization.

Also, when the density of $F$, $f$, is non-zero at $F^{-1}(t)$, Corollary 21.5 in [19] gives for each fixed $t$

$$\hat{F}^{-1}_n(t) \stackrel{d}{\asymp} F^{-1}(t) + \frac{1}{\sqrt{n}} \frac{\sqrt{t(1 - t)}}{f(F^{-1}(t))} Z,$$

and as a process

$$\hat{F}^{-1}_n(t) \stackrel{d}{\asymp} F^{-1}(t) + \frac{1}{\sqrt{n}} \frac{1}{f(F^{-1}(t))} B_2(t),$$

where $B_2$ is standard brownian bridge, under the mild conditions of Lemma 21.4 in [19].

A.4.1 Technical requirements

We work under the same assumptions as [9], which in the notations of the current paper mean that we assume that $n/m$ and $m/n$ have a finite non-zero limit. We also assume that $F$ and $G$ have continuous densities $f$ and $g$ and that $f(G^{-1}(t))/g(G^{-1}(t))$ as well as $g(F^{-1}(t))/f(F^{-1}(t))$ are bounded on any subinterval $(c, d)$ of $(0, 1)$. $\hat{F}^{-1}_n$ and $\hat{G}^{-1}_m$ are defined using the standard definition.
of the quantile function \[19\], Chapter 21. Note that under these assumptions \(ROC(t)\) and \(\widehat{ROC}(t)\) are differentiable.

Under these assumptions, Theorem 2.2 in \[9\] applies and the same techniques as those used to prove Theorem 2.3 in that paper also apply so our arguments can be made rigorous. In particular the integration results we use hold for bounded \(w\) from Theorem 2.2 in \[9\]. And they guarantee that \(I(w)\) is asymptotically normal with variance computed from the variance of the Brownian Bridge integrals we work on.

The connection to Mann-Whitney type statistics we make in Section B suggest that these technical requirements could be weakened considerably though that is secondary in the context of this paper.

A.5 A brownian bridge computation

**Lemma 4.** We have, if \(B_1(t)\) is standard Brownian Bridge on \([0, 1]\),

\[
\int_0^1 \pi(t)B_1(t)dt \quad \text{is } N(0, \sigma^2), \quad \text{with } \sigma^2 = \text{var} [\Pi(U)] = \int_0^1 \Pi^2(t)dt - \left(\int_0^1 \Pi(t)dt\right)^2. \quad (6)
\]

**Proof.** The normality is obvious from Itô calculus (see \[14\]). We deal with the variance computation here.

Since \(B(t) = W(t) - tW(1)\), where \(W(t)\) is standard Brownian motion, we can use integration by parts. Note that using independence of Brownian increments, we have, using standard results in Itô calculus (see \[14\])

\[
\text{cov} \left( \int_0^1 f_1(t)dW_t, \int_0^1 f_2(t)dW_t \right) = \int_0^1 f_1(t)f_2(t)dt. \quad (7)
\]

Hence,

\[
\text{cov} \left( \int f(t)dW_t, W(1) \right) = \int_0^1 f(t)dt.
\]

Hence, using, for instance, Itô calculus to justify the integration by parts, we get

\[
\int_0^1 \pi(t)[W(t) - tW(1)]dt = \left[ \Pi(1) - \int_0^1 t\pi(t)dt \right] W(1) - \int_0^1 \Pi(t)dW_t.
\]

Now using deterministic integration by parts

\[
\int_0^1 t\pi(t)dt = \left. t\Pi(t) \right|_0^1 - \int_0^1 \Pi(t)dt.
\]

Hence,

\[
\int_0^1 \pi(t)[W(t) - tW(1)]dt = \int_0^1 \Pi(t)dtW(1) - \int_0^1 \Pi(t)dW_t.
\]

The covariance between the two terms is \(- \left(\int_0^1 \Pi(t)dt\right)^2\), using Equation (7) and the fact that \(W(1) = \int_0^1 dW_t\).

Hence,

\[
\text{var} \left( \int_0^1 \pi(t)B_1(t)dt \right) = \int_0^1 \Pi^2(t)dt - \left(\int_0^1 \Pi(t)dt\right)^2 = \text{var} [\Pi(U)].
\]

\[\Box\]
A.6 Proofs of Lemma 2 and 3

Proof of Lemma 2. In $I_1(w)$, calling $u = G(F^{-1}(1 - t))$, we have $t = 1 - F(G^{-1}(u)) = \gamma(u)$, the integral becomes

$$I_1(w) = \int_0^1 w(t) B_1(G(F^{-1}(1 - t))) dt = \int_0^1 w(\gamma(u)) \gamma(u) B_1(u) du .$$

Let us call $W$ a primitive of $w$. Appealing to Equation (6), since $(W(\gamma(u)))' = \gamma'(u)w(\gamma(u))$, we have

$$\text{var}[I_1(w)] = \int W^2(\gamma(t)) dt - \left[ \int W(\gamma(t)) dt \right]^2 = \text{var}[W(\gamma(U))] = \text{var}[W(\gamma(1 - U))] .$$

The last equality holds because $U = (1 - U)$ in distribution, since $U$ is Uniform[0,1].

Let us now turn our attention to $I_2(w)$. We first note that $\frac{d(F^{-1}(1 - t))}{d(F^{-1}(1 - t))} = (ROC(t))'$. Also, we have, in law, $B_2(t) = B_2(1 - t)$, by standard properties of Brownian Bridge. So we have, in law,

$$I_2(w) = \int_0^1 w(t) ROC'(t)B_2(t) dt .$$

If we call

$$P_2(t) = \int_0^t w(t) ROC'(t) dt = w(t) ROC(t) - \int_0^t w'(u) ROC(u) du ,$$

we have according to Equation (6),

$$\text{var}[I_2(w)] = \text{var}[P_2(U)] .$$

Proof of Lemma 3. In case $w(t) = 1_{[t\leq \alpha]}$, we have that the variance of the AUC to the left of a cutoff $\alpha$ is from Lemma 2

$$\frac{1}{n} \text{var}[W(\gamma(1 - U))] + \frac{1}{n} \text{var}[P_2(U)] .$$

More specifically, using the argument in the proof, we have $P_2(t) = \int_0^t 1_{[t \leq \alpha]} ROC'(x) dx$, with $ROC(0) = 0$, or, integrating directly,

$$P_2(t) = ROC(t)1_{[t \leq \alpha]} + ROC(\alpha)1_{[t > \alpha]} = [ROC(t) - ROC(\alpha)]1_{[t \leq \alpha]} + ROC(\alpha) .$$

So

$$\text{var}[P_2(U)] = \text{var}[P_2(U) - ROC(\alpha)] = \int_0^\alpha (ROC(t) - ROC(\alpha))^2 dt - \left[ \int_0^\alpha (ROC(t) - ROC(\alpha)) dt \right]^2 .$$

So if $\text{var}[ROC(U)1_{[U \leq \alpha]}] = \int_0^\alpha ROC^2(t) dt - \left[ \int_0^\alpha ROC(t) dt \right]^2$, we have

$$\text{var}[P_2(U)] = \text{var}[ROC(U)1_{[U \leq \alpha]}] + \alpha(1 - \alpha)[ROC(\alpha)]^2 - 2(1 - \alpha)ROC(\alpha)E(ROC(U)1_{[U \leq \alpha]}).$$

This gives the first part of the Lemma.

For the other term, a primitive of $w$ is $W(t) = t1_{[t \leq \alpha]} + \alpha1_{[t > \alpha]}$. Let us call $\overline{ROC}$ the “reverse ROC curve” $1 - F(G^{-1}(1 - t))$. So the quantity $W(\gamma(1 - t))$ reads

$$W(\gamma(1 - t)) = \overline{ROC}(t)1_{[\overline{ROC}(t) \leq \alpha]} + \alpha1_{[\overline{ROC}(t) > \alpha]} .$$

Note that

$$1_{[\overline{ROC}(t) \leq \alpha]} = 1_{[t \leq 1 - G(F^{-1}(1 - \alpha))]} = 1_{[t \leq ROC(\alpha)]} .$$
So we can rephrase the result as

$$\text{var } [W(\gamma(1 - U))] = \int_0^{\tilde{\text{ROC}}} (\tilde{\text{ROC}}^2(t) - \left( \int_0^{\tilde{\text{ROC}}} \tilde{\text{ROC}}(t) dt \right))^2 \, dt + \alpha^2 \text{ROC}(\alpha)(1 - \text{ROC}(\alpha)) - 2\alpha(1 - \text{ROC}(\alpha)) \int_0^{\tilde{\text{ROC}}} \tilde{\text{ROC}}(t) dt.$$ 

by using

$$\int_0^{\nu} [f(t) - f(\nu)]^2 dt - \left[ \int_0^{\nu} (f(t) - f(\nu)) dt \right]^2 = \int_0^{\nu} f^2(t) dt - \left[ \int_0^{\nu} f(t) dt \right]^2 - 2f(\nu)(1 - \nu) \int_0^{\nu} f(t) dt + \nu(1 - \nu)f^2(\nu).$$

with $f = \tilde{\text{ROC}}, \nu = \text{ROC}(\alpha)$ and $f(\nu) = \alpha$.

B Weighted AUC: Mann-Whitney statistics and influence functions

For the sake of completeness, we now provide a different point of view on the variance computation for the weighted AUC based on U-statistics and influence functions. This may be interesting in its own rights. The computations are left at a Physics’ level of rigor.

B.1 ROC curve and weighted AUC

Recall from the main text -see notations there - that by definition, $\tilde{\text{ROC}}(t) = 1 - \hat{G}_m(\hat{F}_n^{-1}(1 - t))$. By extension, we call $\text{ROC}(t) = 1 - G(F^{-1}(1 - t))$. Suppose we are interested in

$$\Delta(F, G) = \int_0^1 w(t)\text{ROC}(t)dt.$$ 

By a change of variable, i.e. after calling $u = F^{-1}(1 - t)$,

$$\Delta(F, G) = \int_0^1 w(t)[1 - G(F^{-1}(1 - t))]dt = \int w(1 - F(u))(1 - G(u))dF(u).$$

B.1.1 “Warm up”: $w = 1$: plug-in estimates for variability of AUC

For illustration we compute the standard AUC. The statistic is then just the Mann-Whitney statistic (see [19]):

$$\hat{\theta} = \Delta(\hat{F}_n, \hat{G}_m) = \int (1 - \hat{G}_m)d\hat{F}_n = \frac{1}{mn} \sum_{i,j} 1_{Y_j > X_i}.$$ 

It is then natural to use influence function computations for instance. Under regularity conditions, $\hat{G}_m = G + \varepsilon_m$, where $\sqrt{m}\varepsilon_m$ converges as a process to $G - \text{Brownian Bridge}$. Similarly, $\hat{F}_n = F + \eta_n$, with $\sqrt{n}\eta_n$ converges as a process to $F$-Brownian Bridge. So we can write

$$\tilde{\theta} = \int (1 - G - \varepsilon_m)d(F + \eta_n).$$

To first order, we have

$$\hat{\theta} = \theta - \int \varepsilon_m dF + \int (1 - G)d\eta_n, \text{ where } \theta = \int (1 - G)dF.$$ 

Integrating by parts, we get, if $\hat{G} = 1 - G$,

$$\hat{\theta} - \theta = \int Fd\varepsilon_m + \int (1 - G)d\eta_n = \frac{1}{m} \sum_{j=1}^m (F(Y_j) - \mathbb{E}(F(Y_j))) + \frac{1}{n} \sum_{i=1}^n [G(X_i) - \mathbb{E}(\hat{G}(X_i))] \frac{1}{m} \sum_{j=1}^m (F(Y_j) - \mathbb{E}(F(Y_j))) - \frac{1}{n} \sum_{i=1}^n [G(X_i) - \mathbb{E}(G(X_i))].$$

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This is essentially the Hajek projection of the statistic, as seen in e.g. Van der Vaart, p.166 (U-statistics) [19].

Of course, since $X_i$ has distribution with cdf $F$,

$$\text{var }[G(X_i)] = \int G^2(x)dF(x) - \left(\int G(x)dF(x)\right)^2 = \int_0^1 G^2(F^{-1}(1-t))dt - \left[\int_0^1 G(F^{-1}(1-t))dt\right]^2.$$  

Since $\text{var }[G(X_i)] = \text{var }[1 - G(X_i)]$, we also have

$$\text{var }[G(X_i)] = \int_0^1 (1 - G(F^{-1}(1-t))^2dt - (AUC)^2 = \int_0^1 (\text{ROC}(t))^2 dt - (AUC)^2.$$  

The integrals involving $F$ can be computed similarly by reversing the role of $F$ and $G$ and hence using what we call $\text{ROC}(t) = 1 - F(G^{-1}(1-t))$ in the main part of the paper, with $\text{ROC}^{-1}(\text{ROC}(t)) = t$.

### B.1.2 Influence function approach for general $w$ and connection to Lemma 3

We use the representation derived above

$$\Delta_w(F,G) = \int w(1 - F(u))(1 - G(u))dF(u)$$

Assuming that $w$ is differentiable in the sense of distributions, we have to first order,

$$\Delta_w(\hat{F}_n, \hat{G}_m) = \Delta_w(F,G) - \int \epsilon_m w(1 - F)dF + \int (1 - G)w(1 - F)d\eta_n - \int \eta_n w'(1 - F)(1 - G)dF ;$$

$$= \Delta_w(F,G) + I_1(w) + I_2(w)$$

**On var $[I_1(w)]$** Note that by integration by parts, if $W$ is a primitive of $w$, i.e. $W' = w$,

$$I_1(w) = \int \epsilon_m w(1 - F)dF = \int W(1 - F)d\epsilon_m = \frac{1}{m} \sum_{i=1}^m W(1 - F(Y_i)) - \mathbb{E} \{ W(1 - F(Y_i)) \} .$$

Hence for computing the variance of this integral, all that matters is $\text{var }[W(1 - F(Y))]$. If $w_{\alpha}(t) = 1_{[t \leq \alpha]}$, $W_{\alpha}(t) = t1_{[t \leq \alpha]} + \alpha 1_{[t > \alpha]}$, so $w_{\alpha}(t) = (t - \alpha)1_{[t \leq \alpha]} + \alpha$. Of course, $Y$ is equal in law to $G^{-1}(1 - U)$, where $U$ is uniform, so this variance is just

$$\int_0^1 (1 - F(G^{-1}(1-t)) - \alpha)^2 1_{[1 - F(G^{-1}(1-t)) \leq \alpha]} - \left[\int_0^1 (1 - F(G^{-1}(1-t)) - \alpha)1_{[1 - F(G^{-1}(1-t)) \leq \alpha]} \right]^2$$

In other words, calling $1 - F(G^{-1}(1-t)) = \text{ROC}(t)$,

$$\text{var }[I_1(w)] = \int_0^1 (\text{ROC}(t) - \alpha)^2 1_{[\text{ROC}(t) \leq \alpha]} - \left[\int_0^1 (\text{ROC}(t) - \alpha)1_{[\text{ROC}(t) \leq \alpha]} \right]^2 ,$$

and we recover one of the terms in Lemma 3.

**On var $[I_2(w)]$** Recall the formula

$$\Delta_w(\hat{F}_n, \hat{G}_m) = \Delta_w(F,G) - \int \epsilon_m w(1 - F)dF + \int (1 - G)w(1 - F)d\eta_n - \int \eta_n w'(1 - F)(1 - G)dF .$$

We focus here on

$$I_2(w) = \int (1 - G)w(1 - F)d\eta_n - \int \eta_n w'(1 - F)(1 - G)dF .$$

$I_1(w)$ and $I_2(w)$ are independent when $\{X_i\}_{i=1}^n$ and $\{Y_j\}_{j=1}^m$ are independent. So to understand the variance of the statistic $\Delta_w(\hat{F}_n, \hat{G}_m)$ we simply need to understand the variance of $I_2(w)$ since we already have $\text{var }[I_1(w)].$
Note that
\[ w'(1 - F)dF = -w'(1 - F)d(1 - F) = -[w(1 - F)]'. \]
In the specific case \( w(t) = 1_{[t \leq \alpha]} \), \( w(1 - F) = 1_{[1 - F(x) \leq \alpha]} = 1_{[x \geq F^{-1}(1 - \alpha)]} \). So
\[ -[w(1 - F)]' = -\delta_{x = F^{-1}(1 - \alpha)} \]
i.e. it is a Dirac mass at \( x = F^{-1}(1 - \alpha) \). Hence
\[ -\int \eta_n w'(1 - F)(1 - G)dF = \eta_n(F^{-1}(1 - \alpha))(1 - G(F^{-1}(1 - \alpha))) . \]
Since \( \eta_n(t) = \hat{F}_n(t) - F(t) \), we have
\[ \eta_n(F^{-1}(1 - \alpha))(1 - G(F^{-1}(1 - \alpha))) = (\hat{F}_n(F^{-1}(1 - \alpha)) - F(F^{-1}(1 - \alpha)))(1 - G(F^{-1}(1 - \alpha))) \]
The question that remains is correlation with the other term involving \( \eta_n \) in \( I_2(w) \). We have
\[ \int (1 - G)w(1 - F)d\eta_n = \frac{1}{n} \sum_{i=1}^{n} \left[ (1 - G(X_i))1_{[1 - F(X_i) \leq \alpha]} - \mathbb{E}((1 - G(X))1_{[1 - F(X) \leq \alpha]} \right] . \]
Similarly,
\[ (\hat{F}_n(F^{-1}(1 - \alpha)) - F(F^{-1}(1 - \alpha))) = \frac{1}{n} \sum_{i=1}^{n} [1_{[X_i \leq F^{-1}(1 - \alpha)]} - (1 - \alpha)] . \]
Note further that
\[ 1_{[1 - F(X_i) \leq \alpha]} = 1_{[X_i \geq F^{-1}(1 - \alpha)]} . \]
So if \( C_\alpha = (1 - G(F^{-1}(1 - \alpha))) = \text{ROC}(\alpha) \)
\[ \text{var} \left[ \int (1 - G)w(1 - F)d\eta_n - \int \eta_n w'(1 - F)(1 - G)dF \right] = \frac{1}{n} \left[ \text{var} \left[ (1 - G(X))1_{[1 - F(X) \leq \alpha]} \right] + \text{var} \left[ 1_{[X \leq F^{-1}(1 - \alpha)]} \right] \right] C_\alpha^2 \]
\[ + 2C_\alpha \text{cov}(1_{[X \leq F^{-1}(1 - \alpha)]}, (1 - G(X))1_{[1 - F(X) \leq \alpha]}) . \]
Now, \( \text{var} \left[ 1_{[X \leq F^{-1}(1 - \alpha)]} \right] = \alpha(1 - \alpha) \). And since \( 1_{[X \leq F^{-1}(1 - \alpha)]}1_{[1 - F(X) \leq \alpha]} = 0 \),
\[ \text{cov}(1_{[X \leq F^{-1}(1 - \alpha)]}, (1 - G(X))1_{[1 - F(X) \leq \alpha]}) = -\mathbb{E}(1_{[X \leq F^{-1}(1 - \alpha)]})\mathbb{E}((1 - G(X))1_{[1 - F(X) \leq \alpha]}) \]
\[ = -(1 - \alpha)\mathbb{E}((1 - G(X))1_{[1 - F(X) \leq \alpha]}) . \]
Note that in law, \( X = F^{-1}(1 - U) \), so that
\[ (1 - G(X))1_{[1 - F(X) \leq \alpha]} = (1 - G(F^{-1}(1 - U)))1_{[U \leq \alpha]} = \text{ROC}(U)1_{[U \leq \alpha]} . \]
So
\[ \mathbb{E}((1 - G(X))1_{[1 - F(X) \leq \alpha]}) = \int_{0}^{\alpha} (1 - G(F^{-1}(1 - t))) dt = \int_{0}^{\alpha} \text{ROC}(t) dt . \]
Hence for \( w = 1_{[t \leq \alpha]} \),
\[ n\text{var} \left[ \int (1 - G)w(1 - F)d\eta_n - \int \eta_n w'(1 - F)(1 - G)dF \right] = \text{var} \left[ (1 - G(X))1_{[1 - F(X) \leq \alpha]} \right] \]
\[ + \alpha(1 - \alpha)\text{ROC}(\alpha)^2 \]
\[ - 2(1 - \alpha)\text{ROC}(\alpha)\mathbb{E}((1 - G(X))1_{[1 - F(X) \leq \alpha]}) . \]
This is consistent with the results of Lemma 3.
We want to approximate the conditional mutual information $I(s(X; \theta); C|Y)$, using normal approximation for the scores. We have,

$$I(s(X; \theta); C|Y) = \sum_y p(Y = y) D_{KL}(p(s(X; \theta), C|y)||p(s(X; \theta)|y)p(C|y))$$

$$= p(Y = 1) (H(s(X; \theta)|Y = 1) - H(s(X; \theta)|C, Y = 1))$$
$$+ p(Y = 0) (H(s(X; \theta)|Y = 0) - H(s(X; \theta)|C, Y = 0)) ,$$
where $H(X \mid Y)$ is the conditional entropy. Moreover, if $U \sim N(\mu, \sigma^2)$, $2H(U) = (1 + \log(2\pi) + \log \sigma^2)$. Therefore, approximating $s \mid Y = y$ as $s \mid Y = y, C = c$ by normal distributions yields

$$
2I(s(X; \theta); C|Y) = \frac{n_+}{n} \left( \log \hat{\sigma}_+^2 - \sum_{j=1}^M p_{j+} \log \hat{\sigma}_{j+}^2 \right) + \frac{n_-}{n} \left( \log \hat{\sigma}_-^2 - \sum_{j=1}^M p_{j-} \log \hat{\sigma}_{j-}^2 \right),
$$

where $n_+$ denotes total number of positive examples, $n_{j+} = |\{i : C_i = j, Y_i = 1\}|$, $p_{j+} = n_{j+}/n_+$,

$$
\hat{\mu}_{j+} = \frac{1}{n_{j+}} \sum_{\{i:C_i=j,Y_i=1\}} s(X_i; \theta)
$$

and similarly for $\hat{\mu}_{j-}$ and $\hat{\sigma}_{j-}^2$.

This penalty term can be differentiated using similar computation used to differentiate the loss function. The normalized loss function is

$$
L(Y, s(X; \theta)) = \frac{1}{n} \sum_{i=1}^n L(Y_i, s(X_i; \theta)).
$$

Therefore, the gradient is

$$
\nabla_\theta L(Y, s(X; \theta)) = \frac{1}{n} \sum_{i=1}^n \nabla_\theta L(Y_i, s(X_i; \theta)) = \frac{1}{n} \sum_{i=1}^n \frac{\partial}{\partial s} L(Y_i, s(X_i; \theta)) \nabla_\theta s(X_i; \theta).
$$

The gradient of the penalty is given as

$$
2\nabla_\theta I(s(X; \theta); C|Y) = \frac{n_+}{n_0} \left( \nabla_\theta \hat{\sigma}_+^2 - \sum_{j=1}^M p_{j+} \frac{\nabla_\theta \hat{\sigma}_{j+}^2}{\hat{\sigma}_{j+}^2} \right) + \frac{n_-}{n_0} \left( \nabla_\theta \hat{\sigma}_-^2 - \sum_{j=1}^M p_{j-} \frac{\nabla_\theta \hat{\sigma}_{j-}^2}{\hat{\sigma}_{j-}^2} \right),
$$

where

$$
\nabla_\theta \hat{\sigma}_{j+}^2 = \frac{1}{n_{j+}} \sum_{\{i:C_i=j,Y_i=1\}} 2s(X_i; \theta) \nabla_\theta s(X_i; \theta) - 2\hat{\mu}_{j+} \nabla_\theta \hat{\mu}_{j+}
$$

and similarly for $\nabla_\theta \hat{\mu}_{j-}$ and $\nabla_\theta \hat{\sigma}_{j-}^2$. Therefore, all the differentiation operations required to compute the gradient of the penalty are shared with the gradient of the loss function. The difference is in how these terms are aggregated. We also need to explicitly compute the variance of the scores (therefore the scores as well) to compute the gradient of the penalty.