Theory of Optimizing Pseudolinear Performance Measures: Application to F-measure

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Abstract

Non-linear performance measures are widely used for the evaluation of learning algorithms. For example, F-measure is a commonly used performance measure for classification problems in machine learning and information retrieval community. We study the theoretical properties of a subset of non-linear performance measures called pseudo-linear performance measures which includes F-measure, Jaccard Index, among many others. We establish that many notions of F-measures and Jaccard Index are pseudo-linear functions of the per-class false negatives and false positives for binary, multiclass and multilabel classification. Based on this observation, we present a general reduction of such performance measure optimization problem to cost-sensitive classification problem with unknown costs. We then propose an algorithm with provable guarantees to obtain an approximately optimal classifier for the F-measure by solving a series of cost-sensitive classification problems. The strength of our analysis is to be valid on any dataset and any class of classifiers, extending the existing theoretical results on pseudo-linear measures, which are asymptotic in nature. We also establish the multi-objective nature of the F-score maximization problem by linking the algorithm with the weighted-sum approach used in multi-objective optimization. We present numerical experiments to illustrate the relative importance of cost asymmetry and thresholding when learning linear classifiers on various F-measure optimization tasks.

Keywords: machine learning, cost-sensitive classification, pseudo-linear performance measures, F-score, Jaccard Index

1. Introduction

Different performance measures exist to assess the efficiency of learning algorithms. Accuracy is the most commonly used performance measure in classification systems. Like many other measures; which we will investigate in this paper, it is defined over the set of classification outcomes. The four possible outcomes of a classifier are True Positive($tp$), True Negative($tn$), False Negative($fn$) and False Positive($fp$). Given a binary dataset and classifier, $tp$ corresponds to the correct prediction of a positive label, $tn$ corresponds to the correct prediction of a negative label, $fn$ corresponds to the incorrect prediction of a negative label, and $fp$ corresponds to the incorrect prediction of the positive label as positive. In general, these outcomes are depicted using a confusion matrix, also called contingency table (See Table 2). Accuracy is a linear function of these outcomes, defined
as the sum of $tp$ and $tn$. Theoretically, classification algorithms are optimization problems where we optimize a loss function corresponding to the performance measure (see Devroye et al. [1996] Anthony and Bartlett [2009]). For example, the loss function that corresponds to accuracy is 0-1 loss. In practice, due to the algorithmic complexity of optimizing 0-1 loss, we use convex surrogates of the 0-1 loss (eg: hinge loss, logistic loss etc) (see Bartlett et al. [2006]; Anthony and Bartlett [2009]).

As mentioned, accuracy is a commonly used performance measure, albeit unsuitable for specific class of problems. For example, consider the classification (binary) of an imbalanced dataset of size 100 with 95 being samples of one specific class (let us say negative) and 5 being other class (say positive). A trivial classifier of the form ‘always predict negative’ results in a high accuracy albeit useless classifier. In this specific example, $F_3$ (Rijsbergen 1979) or Jaccard Index (see Waegeman et al. [2014]), can be considered as a more meaningful performance measure than accuracy. In general, non-accuracy performance measures, like $F$-score, are extensively used in practical problems (Cheng et al. 2012; Kim et al. 2013). As the name indicates, one of the striking characteristics of these performance measures is the non-linearity with respect to the in-class false negatives and false positives; whereas accuracy is a linear function of false negatives and false positives. Moreover, there is no convex surrogate loss function that exists for such non-linear measures; specifically, there is no surrogate loss function that exists for $F$-score or Jaccard Index. Another interesting property specific to $F$-measure and Jaccard Index is: it is a sample level measure and does not decompose over individual examples. These three aspects makes the optimization problem a difficult and interesting one.

In the current paper we study theoretical and algorithmic aspects of a subset of non-linear performance measures called pseudo-linear performance measures. A pseudo-linear measure is a pseudo-linear function of in-class false positives and false negatives. The commonly used performance measure $F_1$ is an example of pseudo-linear performance measure. Less commonly used measures like Jaccard Index also come under this title; among many others. Here, we focus primarily on pseudo-linear notions of $F$-score. We consider the setting in which a dataset, given as a set of feature vectors, is to be classified such that the $F$-score (restricted to pseudolinear functions) of the resulting classification is optimal (approximately). We call such a classifier as "Optimal $F$ Classifier". We use the term $F$-score and $F$-measure interchangeably to denote the same metric. Unless otherwise explicitly stated, all the discussion in this paper refers to $F$-score optimization. At a later point, we generalize the results to other pseudo-linear measures.

Our principle goal is to study the empirical optimality of pseudo-linear $F$-scores. Given a training set, our analysis proves that "Optimal $F$ Classifier" for pseudo-linear $F$-measures can be found by minimizing the total cost of classification. This theory can be linked to the weighted-sum approach used in multi-objective optimization. Furthermore, our experimental results suggest that minimizing the total cost classification is same as selecting the optimal $F$-score a posteriori in case of binary $F_3$ and multilabel-macro-$F_3$. Our experiments also reveals the importance of thresholding classification scores to optimize $F$-scores.

This article is an extended version of an already published conference paper (Puthiya Parambath et al. [2014]). The article is organized as follows. Section 2 introduces basic definitions and notations used throughout the paper. It also present earlier works in $F$-measure optimization. Section 3 presents the theoretical analysis, where we establish the pseudo-linearity
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of different practical $F$-scores, and prove that "Optimal $F$ Classifier" can be found by minimizing the total cost. We derive the values for the cost vector for many pseudo-linear $F$-measures. We establish the multi-objective view of the $F$-measure optimization problem and link our cost-minimization approach to the popular weighted-sum approach for solving multi-objective optimization problems. Section [5 presents the experimental results. We study the importance of thresholding for finding optimal solutions. We conclude the paper in Section [6]. The proofs for all the propositions in Section [3 can be found in the appendix.

2. Background and Related Work

Here we give a brief review of the state-of-the-art methods for $F$-score maximization. We start by introducing the notations used throughout in the paper; we also give the definitions of some basic quantities like $F_\beta$-score.

2.1 Notation and Basic Definitions

We are given (i) a measurable space $X \times Y$, where $X$ is the feature space and $Y$ is the (finite) prediction set, (ii) a probability measure $\mu$ over $X \times Y$, and (iii) a set of (measurable) classifiers $\mathcal{H}$ from the feature space $X$ to $Y$. We distinguish here the prediction set $Y$ from the label space $L = \{1, \ldots, L\}$: in binary or single-label multiclass classification, the prediction set $Y$ is the label set $L$, but in multilabel classification, $Y = 2^L$ is the powerset of the set of possible labels. In that framework, we assume that we have an i.i.d. sample drawn from an underlying data distribution $P$ on $X \times Y$. The empirical distribution of this finite training (or test) sample will be denoted by $\hat{P}$. Then, we may take $\mu = P$ to get results at the population level (concerning expected errors), or we may take $\mu = \hat{P}$ to get results on a finite sample. Similarly, we denote estimated values over a finite sample using a hat(\hat{)} over the variable, wherever required. Likewise, $\mathcal{H}$ can be a restricted set of functions such as linear classifiers if $X$ is a finite-dimensional vector space, or may be the set of all measurable classifiers from $X$ to $Y$ to get results in terms of Bayes-Optimal Predictors. Finally, when required, we will use bold characters for vectors and normal font with subscript for indexing.

Most of the previous work on pseudo-linear metric is centered around $F_\beta$-score in binary settings. $F_\beta$-score is defined as the weighted harmonic mean of precision and recall. Precision is defined as the fraction of predicted positive instances that are indeed positive and recall is defined as the fraction of positive instances that are correctly predicted as positive. In terms of the classification outcomes ($tp$, $tn$, $fn$, $fp$), we formally define precision, recall and $F_\beta$ associated with a binary classifier $h \in \mathcal{H}$, given a sample $(x, y) \in X \times Y$ of size $n$ as

\[
\begin{align*}
(precision) \quad \text{Precision}(h(x), y) &= \frac{\sum_{i=1}^n tp(h(x_i))}{\sum_{i=1}^n [tp(h(x_i)) + fp(h(x_i))]} \\
(recall) \quad \text{Recall}(h(x), y) &= \frac{\sum_{i=1}^n tp(h(x_i))}{\sum_{i=1}^n [tp(h(x_i)) + fn(h(x_i))]} \\
(binary-F_\beta) \quad F_\beta(h(x), y) &= \frac{(1 + \beta^2) \sum_{i=1}^n tp(h(x_i))}{\sum_{i=1}^n [(1 + \beta^2) tp(h(x_i)) + \beta^2 fn(h(x_i)) + fp(h(x_i))]} \end{align*}
\]
In the above, dependence of label vector \( y \) on classification outcome is omitted for convenience. \( \beta \) is the weighting factor of \( F \)-score. Specifically, \( F_0 \) corresponds to precision and \( F_\infty \) corresponds to recall. The \( F_1 \)-measure, the most widely used, corresponds to the case \( \beta = 1 \). In case of the example mentioned in the introduction, classifying a sample of 100 instances, the trivial classifier gives precision, recall and \( F_1 \) values to 0. Precision does not consider false negatives, and recall does not consider false positives. So in practical problems, \( F_\beta \) is preferred. One thing to note: unlike accuracy, \( F \)-measure is not invariant under label switching i.e. if we change the positive label to negative, we get a different \( F \)-score. Hence it is used in problems where correct classification of minority label is of vital importance. In multilabel and multiclass settings, three different definitions of \( F \)-score can be found; namely instance-wise, macro and micro \( F \)-scores. We will give formal definition of these in Section 3 in connection with our theoretical framework.

2.2 Related Work

\( F \)-score optimization had been studied on a limited basis in the past (Musicant et al., 2003; Jansche, 2005; Joachims, 2005; Jansche, 2007; Fujino et al., 2008). Last couple of years witnessed an increasing interest in this domain (Dembczynski et al., 2011; Nan et al., 2012; Pillai et al., 2012; Dembczynski et al., 2013; Cheng et al., 2012; Lipton et al., 2014; Koyejo et al., 2014; Narasimhan et al., 2014; Waegeman et al., 2014). Majority of the work was confined to \( F \)-score maximization in binary classification settings, whereas very little work was done on multilabel and multiclass \( F \)-score maximization tasks (Pillai et al., 2012; Dembczynski et al., 2011). (Jansche, 2005) suggested an algorithm for finding locally maximal \( F_1 \)-score for binary classification problems by approximating the classification outcomes using logistic models. Since the objective function used is non-convex, the algorithm does not guarantee optimality. This issue is addressed by running the procedure multiple times and selecting the best in hand. The orthogonal problem of inferring the hypothesis with optimal \( F_1 \) from a probabilistic model is discussed in (Jansche, 2007). In the scientific literature, the two problem formulation has been referred to as empirical utility maximization (EUM) and decision-theoretic aproach (DTA) respectively (Nan et al., 2012).

The two formulations differ in the way expected \( F \)-score is defined. In case of EUM based approach, population \( F \)-score is defined as the \( F \)-score of the expected \( tp, fp \) and \( fn \). Formally, In EUM, expected \( F \)-score is defined as,

\[
F^\text{EUM}_\beta(h(x), y) = \frac{(1 + \beta^2)\mathbb{E}[tp(h(x), y)]}{(1 + \beta^2)\mathbb{E}[\hat{tp}(h(x), y)] + \beta^2\mathbb{E}[\hat{fn}(h(x), y)] + \mathbb{E}[\hat{fp}(h(x), y)]}
\]

An optimal EUM classifier can be defined as,

\[
h^* = \arg\max_{h \in \mathcal{H}} F^\text{EUM}_\beta(h(x), y)
\]

In DTA, expected \( F \)-score can be formally defined as,

\[
F^\text{DTA}_\beta(h(x), y) = \mathbb{E}[\hat{F}_\beta(h(x), y)]
\]

An optimal DTA classifier is of the form

\[
h^* = \arg\max_{h \in \mathcal{H}} \sum_{y \in Y} \hat{F}_\beta(h(x), y) P(y)
\]
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From an algorithmic point of view, DTA based algorithms are computationally more expensive than EUM algorithms. DTA based algorithms require an efficient method to estimate the joint probability and iterate over exponentially many combinations of $h$ and $y$; and the problem of estimating exact probabilities is as hard as the original problem. But assuming i.i.d samples and considering the functional properties of $F$-score (it is a function of integer counts($tp, fp, fn$)), the above problem can be solved more efficiently. The algorithm given by (Jansche, 2007) runs in $O(n^4)$, where $n$ is the number of examples. (Nan et al., 2012) improved this algorithm with a complexity of $O(n^3)$ using dynamic programming methodology. They also argued that Optimal Classifier for binary $F_1$ is of the form $\text{sign}(p(y = 1|x) - \delta^*)$, where $\delta^*$ is a threshold score dependent on the underlying distribution. (Dembczynski et al. (2011)) extended the algorithm given by (Jansche (2007)) with dependence assumption and given a method to calculate optimal $F_1$ classifier with $O(n^3)$ complexity in time, given $n^2 + 1$ parameters of the joint distribution $p(y)$. This algorithm was used in a multilabel setting for instance-wise $F$-measure (see Remark 1). In addition to the high computational footprint, there is no optimality guarantee on finite samples. In general, optimality in DTA algorithms are asymptotic in nature.

On the other hand, EUM based approaches are computationally less demanding, and are based on structured risk minimization (SRM) principle. Here we minimize an approximate surrogate loss function, and select the hypothesis with minimal error on the validation set. The most commonly employed EUM approach is to threshold the score obtained using linear classifiers like logistic regression (LR) (Bishop, 2006) or support vector machines (SVM) (Cortes and Vapnik, 1995) such that $F_1$ is maximized. An approximate surrogate function based approach named SVM$^\text{perf}$ is given by (Joachims, 2005), based on the observation that $F_1$ is a sample level measure. In the suggested method, the discriminant function is defined over the linear combination of the feature vectors, where the scalar multiplier is the label associated with each feature vector in the training sample. Even though the reported experimental results were promising, the method does not offer any theoretical optimality guarantee. Moreover, our experiments establish that SVM$^\text{perf}$ is a sub-optimal method. (Musicant et al., 2003) observed that cost-sensitive SVM can be used to find optimal $F_1$ classifier by selecting sample specific values for false negative and false positive costs. But the results were specific to SVMs and no empirical proof was given. In case of multilabel classification, (Pillai et al., 2012) argued that Optimal Classifier for multilabel-micro-$F$-score can be found by thresholding on the class confidence score, one label at a time. (Pillai et al., 2012) used $k$-nearest neighbours and SVM to generate the scores. In general, thresholding cost-insensitive SVM scores does not guarantee empirical optimality, and the paper does not address the issue of hyperparameter selection of the backend algorithm ($k$ of $k$-nearest neighbor and regularization co-efficient of SVM).

(Fujino et al., 2008) tackle the problem by combining different classification models. They combined two logistic models, (i) maximum likelihood logistic regression and (ii) approximate logistic approximation (see Jansche, 2005) to maximize multilabel micro,macro and instance-wise $F$-score. This line of work comes under multiple classifier systems. Multiple classifier systems are not widely used for $F$-measure maximization, and are still in nascent stages. No proper statistical study regarding the optimality of the multiple classifier systems for $F$-measure maximization is found.
Apart from $F$-measure, some of the most recent work discusses non-linear performance measures like Jaccard Index [Koyejo et al., 2014; Narasimhan et al., 2014; Waegeman et al., 2014]. Following the footsteps of [Nan et al., 2012], [Koyejo et al., 2014; Narasimhan et al., 2014] proposed algorithms to maximize linear-fractional performance performance measure by thresholding on the class confidence score. But as mentioned earlier, results hold only asymptotically.

In this work, we aim to perform empirical risk minimization-type learning, that is, to find a classifier with highest population level $F$-score by maximizing its empirical counterpart. In that sense, we follow the EUM framework. Nonetheless, regardless of how we define the generalization performance, our results can be used to maximize the empirical value of the $F_\beta$-score.

3. Theoretical Framework and Analysis

In this section, we present the theoretical framework which is at the heart of this work. Our results are mainly motivated by the maximization of $F$-measures for binary and multilabel classification. They are based on a general property of these performance measures, namely their pseudo-linearity with respect to the false negative and false positive probabilities. For binary classification, the results we prove in this section are that in order to optimize the $F$-measure, it is sufficient to solve a binary classification problem with different costs allocated to false positive and false negative errors (Proposition 2). However, these costs are not known a priori, so in practice we need to learn several classifiers with different costs, and choose the best one (according to the $F$-measure) in a second step. Propositions 3 and 4 provide approximation guarantees on the $F_\beta$-score we can obtain by following this principle depending on the granularity of the search in the cost space. We establish the results for the $F_\beta$-score in binary classification, and extend to other cases of $F$-measures with similar functional forms used in multilabel and multiclass classification. We also briefly describe pseudo-linear notions of Jaccard Index, which can also be solved using our framework. For that reason, we present the results and proofs for the binary case, succeeded by multilabel/multiclass $F$-measures.

3.1 Error Profiles and Pseudo-Linearity

3.1.1 Error Profiles

The performance of a classifier $h$ on distribution $\mu$ can be summarized by the elements of the contingency table (See Table 2) which contains the summary of errors. For all classification tasks (binary, multiclass and multilabel), the $F$-measures we consider here are functions of this non-diagonal elements of contingency table, which themselves are defined in terms of the marginal probabilities of classes and the per-class false negative/false positive probabilities. The marginal probabilities of label $k$ will be denoted by $P_k$, and the per-class false negative/false positive probabilities of a classifier $h$ are denoted by $\text{FN}_k(h)$ and $\text{FP}_k(h)$. Their definitions are given below:

\[
\begin{align*}
    (\text{binary/multiclass}) \quad P_k &= \mu(\{(x, y) | y = k\}), \\
    \text{FN}_k(h) &= \mu(\{(x, y) | y = k \text{ and } h(x) \neq k\}), \\
    \text{FP}_k(h) &= \mu(\{(x, y) | y \neq k \text{ and } h(x) = k\}).
\end{align*}
\]
(multilabel) \[ P_k = \mu(\{(x, y) | y \in k\}), \quad \text{FN}_k(h) = \mu(\{(x, y) | k \in y \text{ and } k \not\in h(x)\}), \]
\[ \text{FP}_k(h) = \mu(\{(x, y) | y \not\in k \text{ and } k \in h(x)\}). \]

These probabilities of a classifier \( h \) are then summarized by the error profile \( E(h) \):
\[ E(h) = (\text{FN}_1(h), \text{FP}_1(h), ..., \text{FN}_L(h), \text{FP}_L(h)) \in \mathbb{R}^{2L}. \]

### 3.1.2 Pseudo-Linear Functions

Throughout the paper, we need the notion of pseudo-linearity of a function, which itself is defined from the notion of pseudo-convexity (See Cambini and Martein 2009, Definition 3.2.1): a differentiable function \( F: \mathcal{D} \subset \mathbb{R}^d \rightarrow \mathbb{R} \), defined on a convex open subset of \( \mathbb{R}^d \), is pseudo-convex if
\[ \forall e, e' \in \mathcal{D}, \quad F(e) > F(e') \Rightarrow \langle \nabla F(e), e' - e \rangle < 0, \]
where \( \langle ., . \rangle \) is the canonical dot product on \( \mathbb{R}^d \).

Moreover, \( F \) is pseudo-linear if both \( F \) and \( -F \) are pseudo-convex. In practice, working with gradients of non-linear functions may be cumbersome, so we will use the following characterization, which is a rephrasing of (Cambini and Martein 2009, Theorem 3.3.9):

**Theorem 1** (Cambini and Martein 2009) A non-constant function \( F: \mathcal{D} \rightarrow \mathbb{R} \), defined and differentiable on the open convex set \( \mathcal{D} \subseteq \mathbb{R}^d \), is pseudo-linear on \( \mathcal{D} \) if and only if \( \forall e \in \mathcal{D}, \ \nabla F(e) \neq 0 \), and: \( \exists a: \mathbb{R} \rightarrow \mathbb{R}^d \) and \( \exists b: \mathbb{R} \rightarrow \mathbb{R} \) such that, for any \( t \) in the image of \( F \):
\[ F(e) \geq t \iff \langle a(t), e \rangle + b(t) \leq 0 \quad \text{and} \quad F(e) \leq t \iff \langle a(t), e \rangle + b(t) \geq 0. \]

That is, level sets of pseudo-linear functions are hyperplanes. Pseudo-linearity is the main property of fractional-linear functions (ratios of linear functions) with positive denominator. Proposition 1 proves this result.

**Proposition 1** A linear fractional function \( F: e \in \mathbb{R}^d \rightarrow \frac{\alpha_0 + \langle \gamma, e \rangle}{\alpha_1 + \langle \delta, e \rangle} \), \( \alpha_1 + \langle \delta, e \rangle > 0 \) is pseudo-linear.

### 3.2 Pseudo-Linearity of F-measures

Different notions of F-measures used in practical problems are pseudo-linear. We establish that binary \( F_\beta \) and multilabel/multiclass macro/micro \( F \)-scores are pseudo-linear functions using Proposition 1.

#### 3.2.1 Binary Classification

In binary classification, we have \( \text{FN}_2 = \text{FP}_1 \) and we write \( F \)-measures only by reference to class 1. Then, for any \( \beta > 0 \) and any binary classifier \( h \), the \( F_\beta \)-measure is
\[ F_\beta(h) = \frac{(1 + \beta^2)(P_1 - \text{FN}_1(h))}{(1 + \beta^2)P_1 - \text{FN}_1(h) + \text{FP}_1(h)}. \]
We can immediately notice that $F_\beta$ is fractional-linear and hence by Proposition 1 it is pseudo-linear with respect to $F_{N_1}$ and $F_{P_1}$. Thus, with a slight (yet convenient) abuse of notation, we write the $F_\beta$-measure for binary classification as a function of vectors in $\mathbb{R}^4 = \mathbb{R}^{2L}$:

\[
\forall e \in \mathbb{R}^4, F_\beta(e) = \frac{(1 + \beta^2)(P_1 - e_1)}{(1 + \beta^2)P_1 - e_1 + e_2}
\]

In the above, $e_i$ represents the $i^{th}$ element of the error profile $e$. A surface plot of $F_1$ as a function of $F_{N_1}$ and $F_{P_1}$ with level sets is given in Figure 1. As the Theorem 1 states, it can be easily verified from the plot that level sets are hyperplanes.

### 3.2.2 Multilabel Classification

In multilabel classification, there are several definitions of $F$-measures. For those based on the error profiles, we first have the macro-$F$-score (denoted by $MF_\beta$), which is the average over class labels of the $F_\beta$-score of each binary classification problem associated to the prediction of the presence/absence of a given class:

\[
MF_\beta(e) = \frac{1}{L} \sum_{k=1}^{L} \frac{(1 + \beta^2)(P_1 - e_{2k-1})}{(1 + \beta^2)P_1 - e_{2k-1} + e_{2k}}.
\]

$MF_\beta$ is not a pseudo-linear function of an error profile $e$. However, if the multilabel classification algorithm learns independent binary classifiers for each class (a method known as one-vs-rest or binary relevance (Tsoumakas and Katakis, 2007)), then each binary problem becomes independent and optimizing the macro-$F$-score boils down to independently maximizing the $F_\beta$-score for $L$ binary classification problems, so that optimizing $MF_\beta$ is similar to optimizing $F_\beta$ in binary classification.

There are also micro-$F$-scores for multilabel classification. They correspond to $F_\beta$-measures for a new binary classification problem over $X \times L$, in which one maps a multilabel classifier $h : X \rightarrow \mathcal{Y}$ ($\mathcal{Y}$ is here the power set of $L$) to the following binary classifier.
\[ \tilde{h} : \mathcal{X} \times \mathcal{L} \rightarrow \{0, 1\} : \text{we have } \tilde{h}(x, k) = 1 \text{ if } k \in h(x), \text{ and } 0 \text{ otherwise.} \]

The micro-\(F_\beta\)-score, written as a function of an error profile \(\mathbf{e}\) and denoted by \(mF_\beta(\mathbf{e})\), is the \(F_\beta\)-score of \(\tilde{h}\) and can be written as:

\[
(multilabel\text{-}micro) \quad mF_\beta(\mathbf{e}) = \frac{(1 + \beta^2) \sum_{k=1}^{L} (P_k - \mathbf{e}_{2k-1})}{(1 + \beta^2) \sum_{k=1}^{L} P_k + \sum_{k=1}^{L} (\mathbf{e}_{2k} - \mathbf{e}_{2k-1})}.
\]

This function is also fractional-linear, and thus pseudo-linear as a function of \(\mathbf{e}\).

3.2.3 Multiclass Classification

The last example we take is from multiclass classification. It differs from multilabel classification in that a single class must be predicted for each example. This restriction imposes strong global constraints that make the task significantly harder. As for the multilabel case, there are many definitions of \(F\)-measures for multiclass classification, and in fact several definitions for the micro-\(F\)-measure itself. We will focus on the following one, which is used in information extraction (e.g. in the BioNLP Challenge [Kim et al., 2013]). Given \(L\) class labels, we will assume that label 1 corresponds to a "default" class, the prediction of which is considered as not important. In information extraction, the "default" class corresponds to the (majority) case where no information should be extracted. Then, a false negative is an example \((x, y)\) such that \(y \neq 1\) and \(h(x) \neq y\), while a false positive is an example \((x, y)\) such that \(y = 1\) and \(h(x) \neq y\). This micro-\(F\)-score, denoted \(mcF_\beta\), can be written as:

\[
(multiclass\text{-}micro) \quad mcF_\beta(\mathbf{e}) = \frac{(1 + \beta^2)(1 - P_1 - \sum_{k=2}^{L} \mathbf{e}_{2k-1})}{(1 + \beta^2)(1 - P_1) - \sum_{k=2}^{L} \mathbf{e}_{2k-1} + \mathbf{e}_1}.
\]

Once again, this kind of micro-\(F_\beta\)-score is fractional-linear and hence pseudo-linear with respect to \(\mathbf{e}\).

**Remark 1 (Non-pseudolinear F-scores)** In multilabel settings, notion of instance-wise \(F_\beta\) has been used in the past [Fujino et al., 2008; Dembczynski et al., 2011; Petterson and Caetano, 2010, 2011; Cheng et al., 2012; Dembczynski et al., 2013]. It is similar to the micro-\(F\)-measure for multilabel case defined above (\(mF_\beta\)), but defined over samples (instances) instead of the labels. It is defined as the average of the per-instance \(F\)-score. Hence, we calculate the \(F\)-scores for each instance independently (i.e. calculate \(mF_\beta\) assuming single instance) and take the average (arithmetic mean) over the number of samples. This measure can not be written as a fractional-linear function of "error profile" terms, hence it can not be solved using our framework.

3.3 Optimizing \(F\)-Measure by Reduction to Cost-Sensitive Classification

The \(F_\beta\)-scores presented above are non-linear aggregations of false negative/positive probabilities that can not be written in the usual expected loss minimization framework; usual learning algorithms are thus, intrinsically, not designed to optimize this kind of performance measures. We show in Proposition 2 that the optimal classifier for a cost-sensitive classification problem with label dependent costs ([Elkan, 2001; Zhou and Liu, 2010]) is also an optimal classifier for the pseudo-linear \(F\)-measures (within a specific, yet arbitrary classifier set \(\mathcal{H}\)).
In cost-sensitive classification, each entry of the error profile is weighted asymmetrically by a non-negative cost, and the goal is to minimize the weighted average error. Efficient, consistent algorithms exist for such cost-sensitive problems (Abe et al., 2004; Steinwart, 2007; Scott, 2012). Even though the costs corresponding to the optimal $F$-measure are not known a priori, we show in Proposition 3 that we can approximate the optimal classifier with approximate costs. These costs, explicitly expressed in terms of the optimal $F$-score, motivate a practical algorithm. Even though the discussion in this section is more general and applies to any pseudo-linear functions, we start with the discussion of the $F_\beta$-score in binary settings. We give the proofs and results for binary $F_\beta$ and in later section we extend the results to multilabel and multiclass $F$-scores defined in Section 3.2.2 and 3.2.3.

### 3.3.1 Reduction to Cost-Sensitive Classification

Let $F : \mathcal{D} \subset \mathbb{R}^d \rightarrow \mathbb{R}$ be a fixed pseudo-linear function. We denote by $a : \mathbb{R} \rightarrow \mathbb{R}^d$ the function mapping values of $F$ to the corresponding hyperplane of Theorem 1. We assume that the distribution $\mu$ is fixed, as well as the (arbitrary) set of classifier $\mathcal{H}$. We denote by $\mathcal{E}(\mathcal{H})$ the closure of the image of $\mathcal{H}$ under $e$, i.e. $\mathcal{E}(\mathcal{H}) = cl(\{E(h), h \in \mathcal{H}\})$ (the closure ensures that $\mathcal{E}(\mathcal{H})$ is compact and that minima/maxima are well-defined), and we assume $\mathcal{E}(\mathcal{H}) \subseteq D$. Finally, for the sake of discussion with cost-sensitive classification, we assume that $a(t) \in \mathbb{R}_+^d$ for any $e \in \mathcal{E}(\mathcal{H})$, that is, lower values of errors entail higher values of $F$.

**Proposition 2** Let $F^* = \max_{e \in \mathcal{E}(\mathcal{H})} F(e)$. We have: $e^* \in \arg\min_{e \in \mathcal{E}(\mathcal{H})} \langle a(F^*), e \rangle \iff F(e^*) = F^*$.

This proposition shows that $a(F^*)$ are the cost vectors (which do not need to be unique and lies orthogonal to the level set) that should be assigned to the error profile in order to find the optimal $F$ classifier in $\mathcal{H}$. Hence maximizing $F$ amounts to minimizing $\langle a(F^*), E(h) \rangle$ with respect to $h$, that is, amounts to solving a cost-sensitive classification problem. This observation suggests that the optimization of pseudo-linear measures could be a wrapper of cost-sensitive classification algorithms. The costs $a(F^*)$ are, however, not known a priori. The following result shows that having only approximate costs is sufficient to have an approximately optimal solution, which gives us the main step towards a practical solution.

**Proposition 3** Let $\varepsilon_0 \geq 0$ and $\varepsilon_1 \geq 0$, and assume that there exists $\Phi > 0$ such that for all $e, e' \in \mathcal{E}(\mathcal{H})$ satisfying $F(e') > F(e)$, we have:

$$F(e') - F(e) \leq \Phi \langle a(F(e')), e - e' \rangle.$$  

Then, let us take $e^* \in \arg\max_{e' \in \mathcal{E}(\mathcal{H})} F(e')$, and denote $a^* = a(F(e^*))$. Let furthermore $g \in \mathbb{R}_+^d$ and $h \in \mathcal{H}$ satisfying the following conditions:

$$\text{(i)} \quad \|g - a^*\|_2 \leq \varepsilon_0, \quad \text{(ii)} \quad \langle g, e \rangle \leq \min_{e' \in \mathcal{E}(\mathcal{H})} \langle g, e' \rangle + \varepsilon_1.$$

We have: $\forall e \in \mathcal{E}(\mathcal{H}), \quad F(e) \geq F(e^*) - \Phi \cdot (2\varepsilon_0 M + \varepsilon_1), \quad$ where $M = \max_{e' \in \mathcal{E}(\mathcal{H})} \|e'\|_2.$
The above proposition suggests that in order to optimize of pseudo-linear measures the cost-sensitive classification algorithm should be wrapped inside an inner loop with an outer loop setting the appropriate costs. This proposition also gives an upper bound on the achievable optimal value. This value depends on the size of the maximum error associated with the hypothesis, $M$, measured in $\ell_2$ sense and the constant $\Phi$. The value of $M$ depends on the hypothesis class ($\mathcal{E}(\mathcal{H})$), and without loss of generality we can assume it to be constant for any set of non-trivial classifier class (for example, linear classifiers). $\Phi$ is called the discretization factor and it depends on the specific form of $F$-measure and training sample. We can find an approximately optimal classifier using a procedure, where we search for the optimal cost (approximate) and associated error profile by iterating through the cost space in small steps. Thus searching for a cost such that $\varepsilon_0$ is close to zero, we can find an optimal $F$ classifier. $\varepsilon_1$ is the approximation guarantee provided by the cost-sensitive classification algorithm. It upper bounds the difference between the convex loss used by the tractable algorithm and the actual $0$-$1$ loss. A discussion on convex approximation of $0$-$1$ loss can be found in (Rosasco et al., 2004). $\Phi$, the discretization factor gives the magnitude of the step size. A larger value of $\Phi$ indicates more fine-grained discretization (very small step size), and a smaller value of $\Phi$ indicates coarse-grained discretization. Later, we will derive the exact values of $\Phi$ and the range of cost space for specific $F$-scores.

3.3.2 Discretization Factor and Cost Vector for $F_\beta$

Here, we derive the values of the discretization factor ($\Phi$) and the range of the cost space ($a$) for binary $F_\beta$-score.

**Proposition 4** $F_\beta$ defined in Section 3.2.1 satisfy the conditions of Proposition 3 with:

(binary) $F_\beta$: $\Phi = \frac{1}{\beta^2 P_1}$ and $a : t \in [0,1] \mapsto (1+\beta^2 - t, t, 0, 0)$.

This proposition gives the exact values of $\Phi$ and $a$ in binary settings. Here the discretization factor depends on the marginal probability of the positive class (assume label 1 represents positive class). Even though, it is not evident from the equations; this value depends on the size of sample also. Intuitively, we can think of this as follows. The equation representing the level set corresponds to the optimal $F$-score (Proposition 2) can be normalized with no harm (The hyperplane remains the same). Here the normalization constant is the size of the sample. In this case, higher values of $\Phi$ indicates a highly imbalanced data with very few positive examples, hence we need smaller step size to discretize the cost space. Given the error profile (in the form of contingency table) and associated costs as a matrix, as shown in in Figure 2 corresponding $F_\beta$-score is the sum of the elements of the Hadamard product of the two matrices.

**Proposition 5** For the $F_1$-measure, the optimal classifier is the solution to the cost-sensitive binary classifier with costs $(1 - \frac{F^*}{2}, \frac{F^*}{2})$.

Proposition 5 extends the result obtained by Lipton et al. (2014) to the non-asymptotic regime. If we take $\mathcal{H}$ as the set of all measurable functions, the Bayes-optimal classifier for
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| Actual Label | Predicted Label | \( \beta \) |
|--------------|-----------------|-------------|
| P’           | True Positive \( (tp) \) | 0           |
| P’           | False Negative \( (fn) \) | 1 + \( \beta^2 - t \) |
| N’           | False Positive \( (fp) \) | \( t \)     |
| N’           | True Negative \( (tn) \) | 0           |

(a) Contingency Table  
(b) Cost Matrix

Figure 2: Binary Classification

this cost is to predict class 1 when \( \mu(y = 1|x) \geq \frac{F_\beta^*}{2} \). The maximum \( F_1 \)-score achievable can not be more than the double of the associated cost (see Lipton et al. 2014; Steinwart 2007).

3.3.3 Algorithm for \( F_\beta \) Maximization

Based on the above results, we will give a practical algorithm to find optimal \( F_\beta \). In case of \( F_\beta \), the cost function \( a : [0, 1] \rightarrow \mathbb{R}^d \), which assigns costs to probabilities of error, is Lipschitz-continuous with constant \( \phi = \max(1, \beta^2) \). Hence it is sufficient to discretize the interval \([0, 1]\) to have a set of evenly spaced values \( \{t_1, ..., t_C\} \) (say, \( t_{j+1} - t_j = \varepsilon_0/\phi \)) to obtain an \( \varepsilon_0 \)-cover \( \{a(t_1), ..., a(t_C)\} \) of the possible costs. Using the approximate guarantee of Proposition 3, learning a cost-sensitive classifier \( h_i \) for each \( a(t_i) \) and selecting the one with minimum total cost(\( \langle a(t_i), h_i(e) \rangle \)) on a validation set is sufficient to obtain a \( \Phi(2\varepsilon_0 M + \varepsilon_1) \)-optimal solution. Since the practical cost-sensitive algorithms are based on convex surrogate loss optimization, the 0-1 cost we presented in Proposition 3 will not hold in general. Hence in practical implementation, we have to iterate over the convex surrogate loss for each value of 0-1 cost. Our experimental results suggest that, in binary classification choosing a classifier with minimum total cost (0-1 cost) is same as selecting a classifier with optimal \( F \)-measure a posteriori. Also, in practice we have to discretize the interval \([0, 1 + \beta^2]\) rather than \([0, 1]\) as given by Proposition 4. Our suggested algorithm is given in Algorithm 1.

The cost-sensitive classification algorithms that are used in the inner loop (step 5) returns the trained model. The \texttt{predict.score} method in the meta-algorithm simply returns the scores (score can be posterior probability, or functional margin etc) on the validation set and \texttt{computeF_\beta} returns the optimal \( F \)-score and corresponding threshold on the validation data. Even though our theoretical results do not suggest thresholding the scores \texttt{a posteriori}, experimental results indicate the need for thresholding. We will elaborate on this point in Section 5. This meta-algorithm can be instantiated with any cost-sensitive learning algorithm. The actual algorithm may simply consist of adjusting the hyper-parameters of a cost-insensitive classifier so as to optimize cost-sensitive classification, as in many practical implementation of cost-sensitive algorithm. This rudimentary approach results in considerable savings in computation time.
F-measure Optimization

Algorithm 1 Find Optimal $F_\beta$

1: \textbf{procedure} OPTIMAL-$F_\beta$(D, $\beta$) \hspace{1cm} $\triangleright$ D = Data, $\beta = \beta$ in $F_\beta$
2: \hspace{0.5cm} $bF = 0$
3: \hspace{0.5cm} Split Training Data into two $D_{tra}$, $D_{val}$
4: \hspace{0.5cm} for $\delta = (0 \ldots 1 + \beta^2)$ do \hspace{1cm} $\triangleright$ approximate cost
5: \hspace{1cm} $\phi = \text{cost-sensitive learner}(D_{tra}, \delta)$; \hspace{1cm} $\triangleright$ learn model on the training data
6: \hspace{1cm} $S = \text{predict_score}(\phi, D_{val})$ \hspace{1cm} $\triangleright$ predict score on the validation data
7: \hspace{1cm} $\theta, F = \text{computeF}_\beta(S, D_{val}, \beta)$ \hspace{1cm} $\triangleright$ get optimal threshold and $F_\beta$
8: \hspace{1cm} if $F > bF$ then
9: \hspace{1.5cm} $bF = F$, $\Phi = \phi$, $\Theta = \theta$;
10: \hspace{1cm} end if
11: \hspace{0.5cm} end for
12: \hspace{0.5cm} return ($\Phi, \Theta$)
13: \textbf{end procedure}

3.4 Beyond Binary $F$-score

As mentioned earlier, many notions of $F$-measures in multilabel and multiclass problems are pseudo-linear and can be solved using our framework. Here, we derive the values of cost vector ($a$) and discretization factor ($\Phi$), and give optimal $F$-measure algorithm for pseudo-linear $F$-measures described in Sections 3.2.2 and 3.2.3.

3.4.1 Multilabel micro-$F$-score

Proposition 6 multilabel micro-$F$($mF_\beta$) defined in Section 3.2.2 satisfy the conditions of Proposition 3 with:

\[
(multilabel-micro) \quad \Phi = \frac{1}{\beta^2 \sum_{k=1}^{L} P_k} \quad \text{and} \quad a_i(t) = \begin{cases} 
1 + \beta^2 - t & \text{if } i \text{ is odd} \\
t & \text{if } i \text{ is even}
\end{cases}
\]

Here the discretization factor depends on the sum of marginal probabilities of each label. As in the binary $F_\beta$ case, we take the size of the samples as the normalization factor. A large value of $\Phi$ indicates that majority of the labels are rare, and smaller value of $\Phi$ indicates that few labels are rare. Since the impact of misclassifications of rare labels does not affect the micro-$F$-score (number of positive labels are less), we have to discretize in a smaller step only if the majority of the classes are rare. This interesting property is already discussed in [Fan and Lin 2007]. Given the above result on cost vector $a$ and discretization factor $\Phi$, and following the arguments given for $F_\beta$ (here also the cost function $a$ is Lipschitz-continuous with Lipschitz constant taking value $\max(1, \beta^2)$), we can develop an algorithm for finding optimal classifier for $mF_\beta$. Unlike in binary case, here we run cost-sensitive learner with discretized cost values to find the classifier with lowest total cost($\langle a(t_i), h_i(e) \rangle$). Our proposed algorithm is given in Algorithm 2. The algorithm is similar to the $F_\beta$ algorithm given in Algorithm 1 except for the outer loop and optimal threshold selection. Here the outer loop calculates the approximate cost($a(t)$) for each value.
of $t$. Optimal threshold is the one which minimizes the total cost ($\langle a(t), e \rangle$) over all possible values of $a(t)$ and $e$.

**Algorithm 2** Find Optimal $mF_\beta$

```
1: procedure OPTIMAL_mF_\beta(D,L,\beta) \triangleright D = Data, L = no. of Labels, $\beta = \beta$ in $F_\beta$
2: \hspace{1cm} $bC = +\infty$
3: \hspace{1cm} Split Training Data into two $D_{tra}, D_{val}$
4: \hspace{1cm} for $t = (0 \ldots 1 + \beta^2)$ do \hspace{1cm} \triangleright Actual Cost
5: \hspace{2cm} $\Pi = \text{gen}_mF_\beta\text{-cost}\_vector(L,t,\beta)$
6: \hspace{1cm} for $\delta = (0 \ldots 1)$ do \hspace{1cm} \triangleright Approximate Cost
7: \hspace{2cm} $\phi = \text{cost\_sensitive\_learner}(D_{tra},\delta)$ \hspace{1cm} \triangleright learn model on the training data
8: \hspace{2cm} $S = \text{predict\_score}(\phi,D_{val})$ \hspace{1cm} \triangleright predict score on the validation data
9: \hspace{2cm} $\theta, C = \text{compute\_cost}(\phi,\Pi,S,D_{val})$ \hspace{1cm} \triangleright get the optimal threshold and cost
10: \hspace{2cm} if ($C < bC$) then
11: \hspace{3cm} $bC = C, \Phi = \phi, \Theta = \theta$;
12: \hspace{2cm} end if
13: end for
14: end for
15: return ($\Phi, \Theta$)
16: end procedure
```

**Algorithm 3** Generate Weight Vector for $mF_\beta$

```
1: procedure GEN_mF_\beta\_cost\_vector(t,L) \triangleright t = Cost, L = no. of labels
2: \hspace{1cm} for $i = \{1, \ldots, 2|L|\}$ do
3: \hspace{2cm} if $i \text{ mod} 2$ then
4: \hspace{3cm} $w[i] = t$
5: \hspace{2cm} else
6: \hspace{3cm} $w[i] = 1 + \beta^2 - t$
7: \hspace{2cm} end if
8: end for
9: return $w$
10: end procedure
```

3.4.2 Multiclass micro-$F$-score

**Proposition 7** Multiclass micro-$F$($mcF_\beta$) defined in Section 3.2.3 satisfy the conditions of Proposition 3 with:

\[
\text{(multiclass–micro) } mcF_\beta: \quad \Phi = \frac{1}{\beta^2(1 - P_1)} \quad \text{and} \quad a_i(t) = \begin{cases} 
1 + \beta^2 - t & \text{if } i \text{ is odd and } i \neq 1 \\
t & \text{if } i = 1 \\
0 & \text{otherwise} 
\end{cases}
\]

14
Following the same arguments as given for multilabel micro-$F$-score, we can use the Algorithm 2 for finding optimal $mcF_\beta$ with a small modification to the $gen_{mcF_\beta cost vector}$ method. The new cost generation method for multiclass micro-$F$-score is given in Algorithm 4.

**Algorithm 4 Generate Weight Vector for $mcF_\beta$**

1. **procedure** $gen_{mcF_\beta cost vector}(t, L)$ \> $t =$ Cost, $L =$ no. of labels
2. $w[1] = t$
3. for $i =$ {2, $\ldots$, $2|L|$} do
4. \> if $i \mod 2$ then
5. \> \> $w[i] = 0$
6. \> \> else
7. \> \> \> $w[i] = 1 + \beta^2 - t$
8. \> end if
9. end for
10. **return** $w$
11. **end procedure**

**Remark 2 (Beyond $F$-Measure)** Jaccard Index is a pseudo-linear performance measure used in popular culture [Waegeman et al., 2014; Koyejo et al., 2014]. A set based similarity measure, the Jaccard Index, being rooted in set theory, has been used in cluster analysis and co-citation analysis to name a few. Given two sets, it is defined as the ratio of intersection to union. Just like $F_1$-score, it ranges from 0 to 1, where 0 indicates distinct sets and 1 indicates identical sets (Kaufman and Rousseeuw (2009)). We can define Jaccard Index for binary, multilabel and multiclass problems discussed above in terms of the error profile entries,

\[
\begin{align*}
\text{(binary)} & \quad \forall e \in \mathbb{R}^4, \quad Jac(e) = \frac{P_1 - e_1}{P_1 + e_2} \\
\text{(multilabel–micro)} & \quad \forall e \in \mathbb{R}^{2L}, \quad mJac(e) = \frac{\sum_{k=1}^{L} (P_k - e_{2k-1})}{\sum_{k=1}^{L} P_k + \sum_{k=1}^{L} e_{2k}} \\
\text{(multiclass–micro)} & \quad \forall e \in \mathbb{R}^{2L}, \quad mcJac(e) = \frac{1 - P_1 - \sum_{k=2}^{L} e_{2k-1}}{(1 - P_1) + e_1}
\end{align*}
\]

As we can infer from the above equations, these measures are pseudo-linear and hence, we can use the methodology developed in Section 3.3.1 thresholding cost-sensitive scores, to find optimal Jaccard Index classifier. Our analysis proves the remark of [Waegeman et al., 2014] “We also see that algorithms maximizing the $F$-measure perform the best for Jaccard index”.

4. Relationship to Multi-Objective Optimization

Finding “good” classifiers amounts to find good trade-offs between the different types of errors. In any case, it is a natural requirement that the chosen classifier has an error profile that is a minimal element of $\mathcal{E}(\mathcal{H})$ according to the partial order of Pareto dominance, which is denoted by $\preceq$ and is defined as:
∀e, e′ ∈ ⃗Rd, e ≤ e′ ⇔ ∀k ∈ {1, ..., d}, e_k ≤ e_k′.

The set of optimal solutions defines the Pareto front.

error profile that is a minimal element of $\mathcal{E}(\mathcal{H})$ according to Pareto-dominance (where $e \succeq e'$ if $e_k \geq e_k'$ for all $k$). This set of optimal solutions defines the Pareto front.

Multi-objective optimization defines methods for finding the Pareto front, or approximations of it ([Ehrgott and Gandibleux (2002)], and one of the motivations is to find (approximately) optimal solutions of a vector function that is hard to optimize. The process is to generate candidate points in the Pareto front, and take the candidate with optimal value of the vector function. The advantage is generating candidate points is faster than the direct optimization of the vector function. In our case, goal is to find $h \in \mathcal{E}(\mathcal{H})$ that achieves small values of $\langle a, e(h) \rangle$ for a predefined cost vector $a$.

The reduction from pseudo-linear functions to solving a series of cost-sensitive classification problems exactly corresponds to this Pareto front method. In fact, a general way of finding Pareto-optimal solutions of a multi-objective problems is called the weighted-sum method (see e.g. [Ehrgott and Gandibleux (2002); Boyd and Vandenberghe (2004)]. Applied to error profiles, the weighted-sum method would minimize positive weighted combinations of the elements of the error profiles, which exactly corresponds to solving the the cost-sensitive classification problems, as we advocate for. In usual multi-objective optimization settings, such a Pareto set method is not useful for pseudo-linear aggregation functions, because most such functions are fractional-linear, and single-objective problems with a fractional-linear objective function can be rewritten in terms of a linear objective with linear constraints (see e.g. [Boyd and Vandenberghe (2004)]. In our context however, the linearization would not help because it would introduce constraints involving values of the error profiles, which are not linear in general. What we gain with the reduction to cost-sensitive classification (or, equivalently, with the weighted-sum method), is that efficient algorithms for cost-sensitive classification, which are known to work in practice and are asymptotically optimal, are already known. In addition, weighted-sum method require the users to know the relative preferences of the objectives in advance, which is not known in general. Hence the weight components are unbounded. Our reduction clearly defines a bound on the possible weights $(a(t))$.

The relationship between the reduction to cost-sensitive classification and the weighted-sum method allows us to discuss pseudo-linear F-measures in terms of Pareto-optimal solutions. It is well-known that in general, not all Pareto-optimal solutions can be found by the weighted-sum method; in fact, only those that are on the boundary of the convex hull of the feasible set can be reached. In general however, many classification problems have Pareto-optimal solutions that do not lie on this boundary, especially if the input space is finite (as is the case on any finite dataset). Figure 3 gives the example of the Pareto front of a binary classification problem with 3 examples. The pareto front can be depicted on a 2D plane where the axis are false positives and false negatives; up to a change of basis, this Pareto front is the "optimal" ROC curve ([Bach et al. (2006); Cléménçon and Vayatis (2009)] for the problem. In the figure, the blue points on the left plot correspond to Pareto-optimal classifiers (none of them can be improved both in terms of proportion of false positives and false negatives), while the red curve is the Pareto set of the convex hull of the error profiles of the 8 classifiers. Our result of reduction to cost-sensitive classification proves that only
the classifiers whose error profile is both Pareto-optimal and on the boundary of the convex
hull are candidates as optimal classifiers for any pseudo-linear aggregation function (here,
the candidates are $c_A, c_D, c_F$), even though all classifiers are optimal for some trade-off
rule. For instance, $c_B$ is the optimal classifier for the rule "minimize the proportion of false
negatives under the constraint that the proportion of false positives is smaller than 0.1".

5. Experiments

The goal of this section is to give illustration of the efficiency of algorithms suggested by
the theory. Due to the non-availability of proper algorithms satisfying the strict global
constraints of multiclass classification, we restrict our experiments only to binary and mul-
tilabel cases. One way to carry out multiclass classification is to follow the multilabel
classification algorithm and select the best scored label as the predicted class. But, here,
we restrict ourselves to only binary and multilabel cases. Our experimental results for binary
and multilabel-macro $F$-score (using binary relevance) shows that (i) choosing "Optimal F
Classifier" by minimizing $\langle a, e \rangle$ is same as choosing classifier with optimal $F$-score a pos-
teriori and (ii) selecting a classifier based thresholding cost-sensitive scores is preferable
to algorithms based on thresholding cost-insensitive classification scores: to maximize $F$
measure. In case of multilabel-micro $F$-score, "Optimal F Classifier" is the one with lowest
$\langle a, e \rangle$ value.

We compare thresholded cost-sensitive classification, as implemented by SVMs and Lo-
gistic Regression, with asymmetric costs, to thresholded linear classifiers(SVMs and Logistic
Regression). Besides, SVM$_{perf}$, the structured SVM approach to $F_1$-measure maximization
of Joachims (Joachims, 2005), provides another baseline. For completeness, we also re-

\[
\begin{array}{cccc}
\mu(x) & 0.65 & 0.30 & 0.05 \\
\mu(y = 1|x) & 0.70 & 0.40 & 0.15 \\
\text{classifier} & x_0 & x_1 & x_2 & F_1^m (\%) \\
h_A(x) & 2 & 2 & 2 & 2.22 \\
h_B(x) & 2 & 2 & 1 & 2.37 \\
h_C(x) & 2 & 1 & 2 & 27.22 \\
h_D(x) & 1 & 2 & 2 & 73.83 \\
h_E(x) & 1 & 2 & 1 & 72.12 \\
h_F(x) & 1 & 1 & 2 & 75.24 \\
h_G(x) & 1 & 1 & 1 & 73.62 \\
\end{array}
\]

Figure 3: Pareto front for a binary classification problem ($\mathcal{Y} = \{1, 2\}$, the positive class is 1), where the input space contains three points $x_1, x_2, x_3$. The table on the left describes the data distribution, and defines the 8 possible classifiers and gives their $F_1^m$-score.
port results for non-thresholded cost-sensitive SVMs, non-thresholded cost-sensitive logistic regression, and for the thresholded versions of SVM^{perf}.

SVM and LR differ in the loss they optimize (weighted hinge loss for SVMs, weighted log-loss for LR), and even though both losses are calibrated in the cost-sensitive setting (that is, converging toward a Bayes-optimal classifier as the number of examples and the capacity of the class of functions grow to infinity) (Steinwart [2007]), they behave differently on finite datasets or with restricted classes of functions. We may also note that asymptotically, the Bayes-classifier for a cost-sensitive binary classification problem is a classifier which thresholds the posterior probability of being class 1. Thus, all methods but SVM^{perf} are asymptotically equivalent, and our goal here is to analyze their non-asymptotic behavior on a restricted class of functions.

For each experiment, the training set was split at random, keeping 1/3 for the validation set used to select all hyper-parameters, based on the maximization of the $F_1$-measure on this set. For datasets that do not come with a separate test set, the data was first split to keep 1/4 for test. All results are averaged over five random splits i.e. hold-out validation with five random splits. The algorithms have from one to four hyper-parameters: (i) all algorithms are run with $L_2$ regularization, with a regularization parameter $C \in \{2^{-6}, 2^{-5}, ..., 2^6\}$; (ii) for the cost-sensitive algorithms, the cost for false negatives is chosen in $\{2^{-t}, t \in \{0.1, 0.2, ..., 1.9\}\}$ of Proposition 4 [2]; (iii) for the thresholded algorithms, the threshold is chosen among all the scores of the validation examples; (iv) for kernel based SVM, we used radial basis function (RBF) kernel with $\gamma$ (measure of influence of a single training example) value $\gamma \in \{2^{-6}, 2^{-5}, ..., 2^6\}$.

The library LIBLINEAR [Fan et al., 2008] was used to implement non-kernel SVMs [2] and Logistic Regression (LR). LIBSVM [Chang and Lin, 2011] library was used for the kernel SVM. A constant feature with value 100 (to simulate an unregularized offset) was added to each dataset. Although our theoretical developments do not indicate any need to threshold the scores of classifiers, the practical benefits of a post-hoc adjustment of these scores can be important in terms of $F_1$-measure maximization, as already noted in cost-sensitive learning scenarios (Grandvalet et al., 2005; Bach et al., 2006). This is illustrated in Figure 4 on the didactic "Galaxy" distribution, consisting in four clusters of 2D-examples, indexed by $z \in \{1, 2, 3, 4\}$, with prior probability $\mu(z = 1) = 0.01$, $\mu(z = 2) = 0.1$, $\mu(z = 3) = 0.001$, and $\mu(z = 4) = 0.889$, with respective class prior probabilities $\mu(y = 1|z = 1) = 0.9$, $\mu(y = 1|z = 2) = 0.09$, $\mu(y = 1|z = 3) = 0.9$, and $\mu(y = 1|z = 4) = 0$.

We drew a very large sample (100,000 examples) from the distribution, whose optimal $F_1$-measure is 67.5%. Without thresholding the scores of the classifiers, the best $F_1$-measure among the classifiers is 55.3%, obtained by SVM^{perf}, whereas tuning thresholds enables to reach the optimal $F_1$-measure for SVM^{perf} and weighted SVM. On the other hand, LR is severely affected by the non-linearity of the level sets of the posterior probability distribution, and does not reach this limit (best $F_1$-score of 48.9%). Note also that, even with this very large sample size, the SVM and LR classifiers are very different. The other datasets we use are Adult, RCV1, Scene, Siam and Yeast. In addition, we used a subsample from the Galaxy data to demonstrate the empirical validity of the algorithm. Adult, RCV1 and Yeast. In addition, we used a subsample from the Galaxy data to demonstrate the empirical validity of the algorithm.  

1. We take $t$ greater than 1 in case the training asymmetry would be different from the true asymmetry (Bach et al., 2006).

2. The maximum number of iteration for SVMs was set to 50,000 instead of the default 1,000.
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Figure 4: Decision boundaries for the galaxy dataset before and after thresholding the classifier scores of SVM$^{perf}$ (dotted, blue), weighted SVM (dot-dashed, cyan), un-weighted logistic regression (solid, red), and weighted logistic regression (dashed, green). The horizontal black dotted line is an optimal decision boundary.

| Name   | Type   | Labels | Train   | Test    | Features | Label Frequency (min/max) |
|--------|--------|--------|---------|---------|----------|---------------------------|
| Adult  | binary | 2      | 32,561  | 16,281  | 123      | -                         |
| Galaxy | binary | 2      | 18,000  | 7,000   | 2        | -                         |
| RCV1   | multilabel | 101    | 23,149  | 10,000  | 47,236   | 0.00008/0.466             |
| Scene  | multilabel | 6      | 1,211   | 1,196   | 294      | 0.136/0.228              |
| Siam   | multilabel | 22     | 21,519  | 7,077   | 30,438   | 0.014/0.598              |
| Yeast  | multilabel | 14     | 1,500   | 917     | 103      | 0.252/0.43               |

Table 1: Dataset Attributes

Yeast are obtained from UCI repository[^3] and remaining from Libsvm repository[^4]. Data attributes are given in Table 1.

The results for binary-$F_β$ and multilabel-macro-F ($MF_β$) are reported in Table 2 and 3 respectively. As it is evident from the experimental results, cost-sensitive learning and threshold cost-sensitive learning give optimal results, whereas other methods perform suboptimally. But the difference between methods is less extreme than on the artificial "Galaxy" dataset. The Adult dataset is an example where all methods perform nearly identical; the surrogate loss used in practice seems unimportant. On the other datasets, we observe that thresholding has relatively large impact, especially for SVM$^{perf}$; this is also true for the other classifiers. The unthresholded and cost-insensitive SVM and LR results are very poor compared to thresholded and cost-sensitive versions. The cost-sensitive classifiers

[^3]: <https://archive.ics.uci.edu/ml/datasets.html>
[^4]: <http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/multilabel.html>
Table 2: Optimal $F_1$ (in %). Options: T for thresholded, CS for cost-sensitive, CS&T for combined

| Baseline | SVM$^{\text{perf}}$ | SVM | LR |
|----------|---------------------|-----|----|
|          | Options             | T   | CS | CS&T | T | CS | CS&T |
| Adult    | 67.3 67.3           | 66.9 67.5 | **67.9** 67.8 | 65.0 67.7 67.7 | **67.9** |
| Galaxy   | 48.4 61.7           | 43.1 61.4 | 58.0 | **62.0** | 35.4 51.9 41.8 56.5 |

Table 3: Optimal $MF_{\beta,1}$ (in %). Options: T for thresholded, CS for cost-sensitive, CS&T for combined

| Baseline | SVM$^{\text{perf}}$ | SVM | LR |
|----------|---------------------|-----|----|
|          | Options             | T   | CS | CS&T | T | CS | CS&T |
| RCV1     | 44.0 52.8           | 46.6 54.2 | 50.9 | **54.5** | 40.9 52.9 48.5 | 53.3 |
| Scene    | 69.3 69.9           | 65.7 70.1 | **70.2** 68.9 | 65.2 69.7 68.0 69.1 |
| Siam     | 48.2 52.8           | 48.1 52.4 | 52.7 | **53.4** | 44.7 51.9 51.7 52.2 |
| Yeast    | 46.9 **47.6**       | 37.8 46.4 | 47.0 46.4 | 38.7 **47.6** **47.6** 47.3 |

(thresholded and unthresholded) outperforms all other methods, as suggested by the theory. The cost-sensitive SVM is probably the method of choice to optimize binary-$F_\beta$ or multilabel-macro-$F(MF_{\beta})$ when predictive performance is a must. On these datasets, thresholded LR still performs reasonably well considering its relatively low computational cost. In general, on the computational cost front, LR converges faster than SVM or SVM$^{\text{perf}}$.

Table 4 presents the optimal $MF_{\beta,1}$-score with kernel SVM.

Table 5 contains the multilabel-micro-$F$ ($mcF_\beta$) results for the datasets. The results clearly demonstrate that selecting micro-$F$ corresponds to maximal macro-$F$ (correspond to $F_{\text{max}}$ in table) always return suboptimal results. So in practice, algorithms based on per-label macro-$F$ optimization should be avoided for micro-$F$ optimization. In case of micro-$F$, effect due to thresholding is not very significant, except for RCV1 data. The unthresholded classifiers performs nearly as good as the thresholded versions. This is true for SVM$^{\text{perf}}$ also. As suggested by theory, cost-sensitive classification is the preferred method to optimize

| Baseline | SVM |
|----------|-----|
|          | Options | T | CS | CS&T |
| Scene    | 16.0 69.3 31.4 | **69.4** |
| Yeast    | 45.1 47.6 47.8 | **47.9** |

Table 4: Optimal $MF_{\beta,1}$ (using RBF Kernel). Options: T stands for thresholded, CS for cost-sensitive and CS&T for hybrid.
Table 5: Optimal \( mF_1 \) (in %). Options: T for thresholded, CS for cost-sensitive, CS&T for combined, \( C_{\text{min}} \) for optimal \( mF_1 \) by minimizing total cost \( (\langle a, e \rangle) \) and \( F_{\text{max}} \) for \( mF_1 \) corresponding to optimal \( MF_1 \)

|        | Baseline | SVMperf | SVM | LR |
|--------|----------|---------|-----|----|
|        | Options  | –      | T   | –  | T | CS | CS&T | –  | T | CS | CS&T |
| RCV1   | \( C_{\text{min}} \) | 48.2   | 49.6 | 47.6 | 49.7 | 49.9 | 50.2 | 46.3 | 49.8 | 49.9 | 49.9 |
|        | \( F_{\text{max}} \) | 42.8   | 44.7 | 47.6 | 44.1 | 49.2 | 44.2 | 46.4 | 44.3 | 49.3 | 44.5 |
| Scene  | \( C_{\text{min}} \) | 67.9   | 69.3 | 65.1 | 69.4 | 70.0 | 69.6 | 66.0 | 69.3 | 69.3 | 69.0 |
|        | \( F_{\text{max}} \) | 67.9   | 68.3 | 64.1 | 69.0 | 69.1 | 67.4 | 64.6 | 68.5 | 66.8 | 67.8 |
| Siam   | \( C_{\text{min}} \) | 59.2   | 62.5 | 60.3 | 62.2 | 62.6 | 62.5 | 60.2 | 62.4 | 62.0 | 62.3 |
|        | \( F_{\text{max}} \) | 59.2   | 62.0 | 60.1 | 62.0 | 62.3 | 62.2 | 59.0 | 61.8 | 61.9 | 62.0 |
| Yeast  | \( C_{\text{min}} \) | 62.3   | 65.3 | 64.2 | 64.8 | 65.6 | 65.3 | 63.4 | 65.3 | 65.3 | 65.1 |
|        | \( F_{\text{max}} \) | 60.5   | 61.6 | 60.6 | 61.2 | 60.6 | 61.7 | 62.8 | 61.7 | 62.8 | 61.7 |

Table 6: Optimal \( mF_1 \) (using RBF Kernel) in %. Options: T stands for thresholded, CS for cost-sensitive, CS&T for hybrid, \( C_{\text{min}} \) for optimal \( mF_1 \) by minimizing total cost \( (\langle a, e \rangle) \) and \( F_{\text{max}} \) for \( mF_1 \) corresponding to optimal \( MF_1 \)

|        | Baseline | SVM |
|--------|----------|-----|
|        | Options  | –  | T | CS | CS&T |
| Scene  | \( C_{\text{min}} \) | 26.1 | 68.2 | 31.0 | 68.4 |
|        | \( F_{\text{max}} \) | 26.0 | 68.1 | 31.1 | 68.4 |
| Yeast  | \( C_{\text{min}} \) | 65.2 | 66.2 | 67.2 | 66.9 |
|        | \( F_{\text{max}} \) | 60.6 | 61.8 | 62.0 | 63.0 |

5.1 What is the Extra Cost?

Since the 0-1 cost differs from the cost associated with surrogate loss, it introduces an extra loop in our algorithm. Hence searching for optimal cost vector in the discretized cost space might not be a good idea, especially when the value of \( \Phi \) is large. Here we do an empirical analysis of the functional dependencies between the 0-1 cost and corresponding \( F \)-measure, and devise an improved version of the algorithms discussed in Section 3.4.

Figure [5] contains the plot of micro-\( F \)-score against false negative cost. From the plot, it is evident that micro-\( F \)-score is a quasi-concave function of false negative cost. A function is quasi-concave, if every superlevel set of the function is convex [Boyd and Vandenberghe 2004]. Formally, a function \( g : D \subset \mathbb{R}^d \rightarrow \mathbb{R} \), is quasi-concave if \( \{ x \in D \mid g(x) \geq a \} \) is convex. It can be verified from the plot that superlevel sets are convex. Bracketing methods...
Figure 5: Plot of micro-$F$-score against false negative cost

[Press et al. 2007] are extensively used to find global maxima of unimodal functions like quasi-concave function. We will not be able to use the exact bracketing algorithm to find the optimal cost, since it requires the knowledge of error profile associated with each value of $F$-measure). But we can use the idea of bracketing to limit the discretization interval.

Here, we find three points $(p, q, r)$, such that $g(p) < g(q) > g(r)$, then instead of discretizing the whole interval, we can limit the discretization only to the sub-interval $(p, r)$. We start with two intervals defined by the three points: start of the interval(0), median of the interval($\frac{1+\beta^2}{2}$) and the end of the interval($1 + \beta^2$). Then we search for the triplets $(p, q, r)$ of given minimum sub-interval size inside the two intervals. In the simplest case, we find $F$-score values corresponding to five points, two start points, midpoint ($\frac{1+\beta^2}{2}$) and two midpoints of the intervals $(0, \frac{1+\beta^2}{2})$ and $(\frac{1+\beta^2}{2}, 1 + \beta^2)$. Since the function is quasi-concave, the global maxima can be either on the mid point or on left or right of the mid point. Depending up on the $F$-score values at the five points, we can limit the discretization only to one half. This way we can reduce the discretization space at least by half.

6. Conclusion

We presented an analysis of $F$-measures, leveraging the property of pseudo-linearity of specific notions of $F$-measures to obtain a strong non-asymptotic reduction to cost-sensitive classification. The results hold on any dataset, for any class of function and on any data distribution assumptions (label dependent or label independent). We suggested algorithms for $F$-measure optimization based on minimizing the 0-1 cost of the classification. We demonstrated experiments on linear functions, showing the theoretical interest of using cost-sensitive classification algorithms rather than probability thresholding. It is also shown that for $F$-measure maximization, thresholding even the cost-sensitive algorithms helps to achieve good performances.

Empirically and algorithmically, we only explored the simplest case of our result ($F_\beta$-measure in binary classification and macro-$F_\beta$-measure and micro-$F_\beta$-measure in multilabel classification), but much more remains to be done. Algorithms for the optimization of the non-pseudolinear notions of $F$-measures like instance-wise-$F_\beta$-measure in multilabel
Appendix A. Proofs of Propositions

**Proposition 1** A linear fractional function \( F : e \in \mathbb{R}^d \mapsto \frac{\alpha e + \langle \gamma, e \rangle}{\alpha_1 + \langle \delta, e \rangle}, \ \alpha_1 + \langle \delta, e \rangle > 0 \) is pseudo-linear.

**Proof** A linear fractional function \( F : e \in \mathbb{R}^d \mapsto \frac{\alpha e + \langle \gamma, e \rangle}{\alpha_1 + \langle \delta, e \rangle}, \ \alpha_1 + \langle \delta, e \rangle > 0 \) is pseudo-linear.

\[
F(e) \leq t \iff \alpha_0 + \langle \gamma, e \rangle \leq t(\alpha_1 + \langle \delta, e \rangle) \\
\Rightarrow (\alpha_0 - t\alpha_1) + \langle \gamma - t\delta, e \rangle \leq 0
\]

Now reversing the inequality, we obtain;

\[
F(e) \geq t \iff (\alpha_0 - t\alpha_1) + \langle \gamma - t\delta, e \rangle \geq 0
\]

Above equations represent open hyperplanes.

\[
\nabla F(e) = \frac{(\alpha_1 + \langle \delta, e \rangle)\delta - (\alpha_0 + \langle \gamma, e \rangle)\delta}{(\alpha_1 + \langle \delta, e \rangle)^2} \neq 0
\]

Above equations confirms the requirements for the pseudo-linearity given in Theorem 1 and hence the result.

**Proposition 2** Let \( F^* = \max_{e \in \mathcal{E}(\mathcal{H})} F(e) \), we have: \( e^* \in \arg\min_{e \in \mathcal{E}(\mathcal{H})} \langle a(F^*), e \rangle \iff F(e^*) = F^* \).

**Proof** Let \( e^* \in \arg\max_{e' \in \mathcal{E}(\mathcal{H})} F(e') \), and let \( a^* = a(F(e^*)) = a(F^*) \). We first notice that pseudo-linearity implies that the set of \( e \in \mathcal{D} \) such that \( \langle a^*, e \rangle = \langle a^*, e^* \rangle \) corresponds to the level set \( \{ e \in \mathcal{D} | F(e) = F(e') = F^* \} \). Thus, we only need to show that \( e^* \) is a minimizer of \( e' \mapsto \langle a^*, e' \rangle \) in \( \mathcal{E}(\mathcal{H}) \). To see this, we notice that pseudo-linearity of \( F \) (see Theorem 1) implies

\[
\forall e' \in \mathcal{D}, \ F(e^*) \geq F(e') \Rightarrow \langle a^*, e^* \rangle \leq \langle a^*, e' \rangle,
\]

and since \( e^* \) maximizes \( F \) in \( \mathcal{E}(\mathcal{H}) \), we get \( e^* \in \arg\min_{e' \in \mathcal{E}(\mathcal{H})} \langle a^*, e' \rangle \).

**Proposition 3** Let \( \varepsilon_0 \geq 0 \) and \( \varepsilon_1 > 0 \), and assume that there exists \( \Phi > 0 \) such that for all \( e, e' \in \mathcal{E}(\mathcal{H}) \) satisfying \( F(e') > F(e) \), we have:

\[
F(e') - F(e) \leq \Phi \langle a(F(e')), e - e' \rangle.
\]

Then, let us take \( e^* \in \arg\max_{e' \in \mathcal{E}(\mathcal{H})} F(e') \), and denote \( a^* = a(F(e^*)) \). Let furthermore \( g \in \mathbb{R}^d_+ \) and \( h \in \mathcal{H} \) satisfying the following conditions:

\[
(i) \| g - a^* \|_2 \leq \varepsilon_0, \quad (ii) \langle g, e \rangle \leq \min_{e' \in \mathcal{E}(\mathcal{H})} \langle g, e' \rangle + \varepsilon_1.
\]

We have: \( \forall e \in \mathcal{E}(\mathcal{H}), \ F(e) \geq F(e^*) - \Phi \cdot (2\varepsilon_0 M + \varepsilon_1), \) where \( M = \max_{e' \in \mathcal{E}(\mathcal{H})} \| e' \|_2 \).
\[ \langle g, e' \rangle = \langle a^*, e' \rangle + \langle g - a^*, e' \rangle. \]

Applying the Cauchy-Schwarz inequality and condition (i), we get

\[ \langle g, e' \rangle \leq \langle a^*, e' \rangle + \|g - a^*\|_2 \|e'\|_2 \]
\[ \leq \langle a^*, e' \rangle + \varepsilon_0 M. \]

In particular, we have:

\[ \min_{e' \in E(H)} \langle g, e' \rangle \leq \min_{e' \in E(H)} \langle a^*, e' \rangle + \varepsilon_0 M \]
\[ \leq \langle a^*, e^* \rangle + \varepsilon_0 M, \tag{2} \]

since \( e^* \in \text{argmin}_{e' \in E(H)} \langle a^*, e' \rangle \) as shown in Proposition \[ \square \]

Similarly, we have \( \langle a^*, e \rangle = \langle g, e \rangle + \langle a^* - g, e \rangle \); applying the Cauchy-Schwarz and conditions (i) and (ii), we have:

\[ \forall e \in E(H), \langle a^*, e \rangle \leq \langle g, e \rangle + \|a^* - g\|_2 \|e\|_2 \]
\[ \leq \langle g, e \rangle + \varepsilon_0 M \]
\[ \leq \min_{e' \in E(H)} \langle g, e' \rangle + \varepsilon_1 + \varepsilon_0 M. \tag{3} \]

Combining Inequalities (2) and (3), we get

\[ \forall e \in E(H), \langle a^*, e \rangle \leq \langle g, e \rangle + \varepsilon_1 + 2\varepsilon_0 M \]
\[ \forall e \in E(H), \langle a^*, e - e^* \rangle \leq \varepsilon_1 + 2\varepsilon_0 M, \]

and the final result follows from Assumption (i). \[ \square \]

**Proposition 4** \( F_\beta \) defined in Section 3.2.1 satisfy the conditions of Proposition 3 with:

\[ \text{(binary) } F_\beta: \quad \Phi = \frac{1}{\beta^2 P_1} \quad \text{and } a: t \in [0, 1] \mapsto (1 + \beta^2 - t, t, 0, 0). \]

**Proof** Since \( F_\beta \) is fractional-linear as a function of the error profile, it is pseudo-linear on the open convex set \( \{e \in \mathbb{R}^d | (1 + \beta^2)P_1 - e_1 + e_2 > 0 \} \) (i.e. when the denominator is strictly positive). Moreover, for every set of classifiers \( \mathcal{H} \), we have \( E(H) \subseteq D_0 = [O, P_1] \times [0, 1 - P_1] \times [1 - P_1] \times [1, P_1] \).

Now, by the definition of \( F_\beta \), we have

\[ \forall e \in D_0, F_\beta(e) \leq t \iff (1 + \beta^2)\varepsilon_1 + t\varepsilon_2 + (1 + \beta^2)P_1(t - 1) \geq 0, \]

and the equation still holds by reversing the inequalities. We thus have that \( a(t) = (1 + \beta^2 - t, t, 0, 0) \) satisfy the condition of Theorem \[ \square \] (with \( b(t) = (1 + \beta^2)P_1(t - 1) \)).

We now show that the condition of Equation \[ \square \] is satisfied for \( a(t) = (1 + \beta^2 - t, t, 0, 0) \) and all \( e, e' \in D_0 \) by taking \( \Phi = \frac{1}{\beta^2 P_1} \). To that end, let \( e \) and \( e' \) in \( E(H) \) and \( t \) and \( t' \) in
\[ t' = F_\beta(e') > F_\beta(e) = t. \] Denote by \( \varepsilon \) the quantity \( \langle a(t'), e - e' \rangle \). Note that \( \varepsilon > 0 \) and that:

\[
\begin{align*}
0 &= \langle a(t), e \rangle + b(t) = (1 + \beta^2 - t)e_1 + t e_2 + (1 + \beta^2)P_1(t - 1) \\
0 &= \langle a(t'), e' \rangle + b(t') = (1 + \beta^2 - t')e'_1 + t' e'_2 + (1 + \beta^2)P_1(t' - 1) \\
\varepsilon &= \langle a(t'), e - e' \rangle = (1 + \beta^2 - t')e_1 + t' e_2 + (1 + \beta^2)P_1(t' - 1)
\end{align*}
\]

where the first two equalities are given by the definition of hyperplane corresponds to \( F_\beta(e) = t \) and \( F_\beta(e') = t' \), and the last one is obtained from the definition of \( \langle a(t'), e - e' \rangle \).

Taking the difference of the third and first equality, we obtain:

\[ \varepsilon = (t - t')e_1 + (t' - t)e_2 + (1 + \beta^2)P_1(t' - t) \]

From which we get, since \( (1 + \beta^2)P_1 - e_1 + e_2 > 0 \) for \( e \in D_0 \):

\[ F_\beta(e') - F_\beta(e) = t' - t = \varepsilon ((1 + \beta^2)P_1 - e_1 + e_2)^{-1} \leq \frac{\varepsilon}{\beta^2P_1}, \]

because \( \beta^2P_1 \) the minimum of \( (1 + \beta^2)P_1 - e_1 + e_2 \) on \( D_0 \) (taking \( e_1 = P_1 \) and \( e_2 = 0 \)). We obtain the result since \( \varepsilon = \langle a(t'), e - e' \rangle \) by definition. \( \square \)

**Proposition 5** For the \( F_1 \)-measure, the optimal classifier is the solution to the cost-sensitive binary classifier with costs \( (1 - \frac{F^*}{2}, \frac{F^*}{2}) \)

**Proof** From Proposition 4, by putting \( \beta = 1 \), we have

\[ (2 - F^*)e_1 + e_2F^* + 2P_1(F^* - 1) \geq 0 \]

dividing by 2, we get

\[ (1 - \frac{F^*}{2})e_1 + e_2\frac{F^*}{2} + P_1(F^* - 1) \geq 0 \]

Cost vector, \( a(t) \), according to Theorem 4 is \( (1 - \frac{F^*}{2}, \frac{F^*}{2}) \). \( \square \)

**Proposition 6** multilabel micro-\( F(mF_\beta) \) defined in Section 3.2.2 satisfy the conditions of Proposition 3 with:

\[
(multilabel\text{-}micro) \hspace{1em} mF_\beta: \quad \Phi = \frac{1}{\beta^2 \sum_{k=1}^{L} P_k} \quad \text{and} \quad a_i(t) = \begin{cases} 1 + \beta^2 - t & \text{if } i \text{ is odd} \\ t & \text{if } i \text{ is even} \end{cases}
\]

**Proof**

\[
mF_\beta(e) \leq t \Rightarrow \frac{(1 + \beta^2) \sum_{k=1}^{L} (P_k - e_{2k-1})}{(1 + \beta^2) \sum_{k=1}^{L} P_k + \sum_{k=1}^{L} (e_{2k} - e_{2k-1})} \leq t \\
\Rightarrow (1 + \beta^2) \sum_{k=1}^{L} e_{2k-1} + t \sum_{k=1}^{L} e_{2k} + (1 + \beta^2)(t - 1) \sum_{k=1}^{L} P_k \geq 0
\]
Thus, we have that

$$a_i(t) = \begin{cases} 
1 + \beta^2 - t & \text{if } i \text{ is odd} \\
t & \text{if } i \text{ is even}
\end{cases}$$

Following the same arguments as in Proposition: 4, we get

$$mF_{\beta}(e') - mF_{\beta}(e) = t' - t = \varepsilon \left[ (1 + \beta^2) \sum_{k=1}^{L} P_k - \sum_{k=1}^{L} e_{2k-1} + \sum_{k=1}^{L} e_{2k} \right]^{-1} \leq \frac{\varepsilon}{\beta^2 \sum_{k=1}^{L} P_k},$$

because $\beta^2 \sum_{k=1}^{L} P_k$ the minimum of $(1 + \beta^2) \sum_{k=1}^{L} P_k - \sum_{k=1}^{L} e_{2k-1} + \sum_{k=1}^{L} e_{2k}$ in the respective domain (taking $e_{2k-1} = P_k$ and $e_{2k} = 0$). We obtain the result since $\varepsilon = \langle a(t'), e - e' \rangle$ by definition.

**Proposition 7** multiclass micro-$F$($mcF_{\beta}$) defined in Section 3.2.3 satisfy the conditions of Proposition 3 with:

$$\text{(multiclass-micro) } mcF_{\beta}: \Phi = \frac{1}{\beta^2 (1 - P_1)} \quad \text{and} \quad a_i(t) = \begin{cases} 
1 + \beta^2 - t & \text{if } i \text{ is odd and } i \neq 1 \\
t & \text{if } i = 1 \\
0 & \text{otherwise}
\end{cases}.$$  

**Proof**

$$\text{(multiclass-micro) } mcF_{\beta}: \Phi = \frac{1}{\beta^2 (1 - P_1)} \quad \text{and} \quad a_i(t) = \begin{cases} 
1 + \beta^2 - t & \text{if } i \text{ is odd and } i \neq 1 \\
t & \text{if } i = 1 \\
0 & \text{otherwise}
\end{cases}.$$  

Thus, we have that

$$a_i(t) = \begin{cases} 
1 + \beta^2 - t & \text{if } i \text{ is odd and } i \neq 1 \\
t & \text{if } i = 1 \\
0 & \text{otherwise}
\end{cases}.$$  

Following the same arguments as in Proposition: 4, we get

$$mcF_{\beta}(e') - mcF_{\beta}(e) = t' - t = \varepsilon \left[ (1 + \beta^2) (1 - P_1) - \sum_{k=2}^{L} e_{2k-1} + e_1 \right]^{-1} \leq \frac{\varepsilon}{\beta^2 (1 - P_1)},$$

because $\beta^2 (1 - P_1)$ the minimum of $(1 + \beta^2) (1 - P_1) - \sum_{k=2}^{L} e_{2k-1} + e_1$ in the respective domain (taking $\sum_{k=2}^{L} e_{2k-1} = 1 - P_1$ and $e_1 = 0$). We obtain the result since $\varepsilon = \langle a(t'), e - e' \rangle$ by definition. \qed
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