Abstract

This paper investigates the properties of the widely-utilized F1 metric as used to evaluate the performance of multi-label classifiers. We show that given an un-informative binary classifier, F1-optimal thresholding is to predict all instances positive. More surprisingly, we prove a relationship between the optimal threshold and the best achievable F1 score over all thresholds. We demonstrate that macro-averaged F1, a commonly used multi-label performance metric, can conceal this extreme thresholding behavior. Finally, based on these properties of F1, we suggest average skill score as an alternative to macro-averaged F1 for multi-label classification.

1 Introduction

Performance metrics are useful for comparing the quality of predictions across systems. Some commonly used metrics for binary classification are accuracy, precision, recall, F1 score, and Jaccard index (Marina Sokolova (2009)). Multi-label classification is an extension of binary classification that is currently an area of active research in supervised machine learning (Tsoumakas & Katakis (2007)). Micro-averaging, macro-averaging, and per instance averaging are three approaches to extend F1 score to the multi-label setting. In general, macro-averaging increases the impact on final score of performance on rare labels, while per instance averaging increases the importance of performing well on each example (Tan (2005)).

Two approaches exist for optimizing performance on F1. Structured loss minimization incorporates the performance metric into the loss function and then optimizes
during training. In contrast, plug-in rules convert the output of a probabilistic classifier into optimal predictions (Dembczynski et al. (2013)). In this paper, we highlight the latter scenario to differentiate between the beliefs of a system and the predictions selected to optimize alternative metrics. We show that the same beliefs can produce markedly dissimilar optimally thresholded predictions depending upon the choice of metric.

While F1 is widely used, some of its properties are not widely recognized. For example, when choosing optimal predictions to maximize the expectation of F1 for a batch of examples, each prediction depends not only on the probability that the label applies to that example but also the distribution of probabilities for all other examples in the batch. We quantify this dependence in Theorem 5.1 where we derive an expression for the optimal threshold. This dependence obfuscates the interpretation of optimally thresholded predictions for F1, i.e. it can be difficult to relate predictions to a system’s true beliefs. We term this the “batch observation.”

Additionally, F1 is an asymmetric classifier, insofar as it regards the “positive” and “negative” classes differently. Given complemented predictions and gold standard, F1 may award a different score. We can demonstrate this asymmetry by considering the case when the classes are perfectly balanced. Predicting all positive has an expected F1 of .67, while predicting all negative always achieves a score of 0. By contrast, both predictions achieve an accuracy of .5. While this basic bias is well-known, we prove that F1’s positive bias is so extreme that given an uninformative classifier, optimal thresholding to maximize F1 requires predicting all instances positive for any base rate\(^1\).

We show that the difference in F1 score between a perfect prediction and the optimal thresholding of an uninformative classifier depends strongly on the base rate. As a result, macro-averaging emphasizes performance on rare labels and can be optimized with inaccurate predictions when the classifier for a label is uninformative and the base rate is low. We also demonstrate via the “batch observation” that predictions made to optimize micro and macro-F1 can be quite dissimilar even given the same underlying probabilistic classifiers.

As a case study, we consider tagging articles in the biomedical literature with MeSH terms, a controlled vocabulary of 26,853 labels. These labels have heterogeneously distributed base rates. We show that if the predictive features for rare labels are lost (because of feature selection or another cause) then the optimal threshold to maximize macro-F1 leads to predicting these rare labels frequently. For the case study application, and likely for related ones, this behavior is not desirable.

### 2 Definitions of Performance Metrics

Consider binary classification in the single or multi-label setting. Given training data of the form \(\{(x_1, y_1), ..., (x_n, y_n)\}\), where each \(x_i\) is a feature vector of dimension \(d\) and each \(y_i\) is a binary vector of true labels of dimension \(m\), a probabilistic classifier outputs a model which specifies the conditional probabilities of each label applying to

\(^1\) For concreteness, the results of this paper are given specifically for the F1 metric and its multi-label extensions. However, the results can be generalized to F/\(\beta\) metrics for \(\beta \neq 1\).
each instance given the feature vector. For a batch of data of dimension $n \times d$, the model outputs an $n \times m$ matrix $C$ of probabilities. In the single-label setting, $m = 1$ and $C$ is an $n \times 1$ matrix, i.e. a column vector.

A decision rule $D(C) : \mathbb{R}^{n \times m} \to \{0, 1\}^{n \times m}$ converts a matrix of probabilities $C$ to binary predictions $P$. The gold standard $G \in \mathbb{R}^{n \times m}$ represents the true values of all labels for all instances in a given batch.

A performance metric $M$ assigns scores to a prediction given a gold standard:

$$M(P|G) : \{0, 1\}^{n \times m}, \{0, 1\}^{n \times m} \to \mathbb{R} \in [0, 1].$$

The counts of true positives $tp$, false positives $fp$, false negatives $fn$, and true negatives $tn$ are represented via a confusion matrix.

| Predicted Pos. | Actual Pos. | Actual Neg. |
|----------------|-------------|-------------|
| $tp$           | $fp$        |             |
| $fn$           |             | $tn$        |

Figure 1: Confusion Matrix

Precision $p = tp/(tp + fp)$ is the fraction of all positive predictions that are true positives, while recall $r = tp/(tp + fn)$ is the fraction of all actual positives that are predicted positive. By definition the F1 score is the harmonic mean of precision and recall: $F1 = 2/(1/r + 1/p)$. By substitution, F1 can be expressed as a function of counts of true positives, false positives and false negatives:

$$F1 = \frac{2tp}{2tp + fp + fn}$$

The harmonic mean expression for F1 is undefined when $tp = 0$, but the translated expression is defined. This difference does not impact the results below.

### 2.1 Multi-label Variations of F1

While F1 was developed for single-label information retrieval, there are a few extensions to adapt F1 to the multi-label setting. Micro-F1 treats the entire set of predictions on all labels as one vector and calculates the F1. In particular, $tp = 2 \sum_{i=1}^{n} \sum_{j=1}^{m} \mathbb{1}(P_{ij} = 1) \mathbb{1}(G_{ij} = 1)$. We define $fp$ and $fn$ analogously and calculate the final score using (1). Macro-F1, which can also be called per label F1, calculates the F1 for each label and averages them:

$$F1_{Macro}(P|G) = \left(\frac{\sum_{j=1}^{m} F1(P_{j}, G_{j})}{m}\right).$$

Per-instance F1 is similar but averages F1 over all examples rather than over each label:

$$F1_{Instance}(P|G) = \left(\frac{\sum_{i=1}^{n} F1(P_{i}, G_{i})}{n}\right).$$
2.2 Alternative Metrics

Accuracy evaluates the fraction of all instances that are predicted correctly:

\[
\text{Accuracy} = \frac{tp + tn}{tp + tn + fp + fn}
\]  

(2)

Accuracy is adapted to the multi-label setting by summing \(tp\) and \(tn\) for all labels and then dividing by the total number of predictions:

\[
\text{Accuracy}(P|G) = \frac{1}{nm} \left( \sum_{i=1}^{n} \sum_{j=1}^{m} 1(P_{ij} = G_{ij}) \right).
\]

Jaccard Index, a monotonically increasing function of F1, calculates the ratio of the intersection to the union between predictions and gold standard:

\[
\text{Jaccard} = \frac{tp}{tp + fn + fp}.
\]

Skill scores are a less frequently used family of metrics. We define a skill score as the improvement in performance with respect to a baseline that could be achieved by a trivial system. We construct a skill score from accuracy by letting the baseline be the score achieved by guessing the majority class on each instance:

\[
\text{Skill}(P|G) = \max \left( \frac{\text{Acc}(P|G) - \text{Acc}(V|G)}{1 - \text{Acc}(V|G)}, 0 \right).
\]

where \(V\) is the predictor that guesses the majority class.

We adapt skill score to the multi-label setting by averaging the skill scores across all labels. We call this macro-skill score. In the next section, we show that unlike F1, accuracy is a linear function of its inputs. As skill score is a linear function of accuracy, it too is a linear function. We explain the importance of skill score in the multi-label setting after discussing the potentially undesirable consequences of macro-averaging F1.

3 Prior Work

Motivated by F1’s widespread use for information retrieval and in single and multi-label binary classification, researchers have published extensively on its optimization. (Jansche (2007)) proposed an outer-inner maximization technique for F1 maximization. (José del Coz & Bahamonde (2009)) study extensions to the multi-label setting, and show simple threshold search strategies are sufficient when individual probabilistic classifiers are independent. Finally, (Dembczyński et al. (2011)) describe how the method of Jansche can be extended to efficiently label data points even when classifier outputs are dependent. More recent work in this direction can be found in (Ye et al. (2012)). However, none of this work directly identified the relationship of optimal thresholds to the Jaccard index or the maximum achievable F1 score over all thresholds, as we do here.

While there has been some work on applying general constrained optimization techniques to related metrics (Mozer et al. (2001)), research often focuses on specific
Figure 2: For fixed base rate, F1 is a non-linear function with only two degrees of freedom.

classification methods. For example, (Suzuki et al. (2006)) study F1 optimization for conditional random fields and (Musicant et al. (2003)) perform the same optimization for SVMs. In our work, we study the consequences of such optimization on the resultant probabilistic classifiers, particularly in the multi-label setting.

4 Properties of F1 in the Single-Label Setting

Before explaining optimal thresholding to maximize F1, we first point out some properties of F1. First, for any fixed number of actual positives in the gold standard, only two of the four entries in the confusion matrix (Figure 1) vary independently. This is because the number of actual positives is equal to the sum \( tp + fn \) while the number of actual negatives is equal to the sum \( tn + fp \). A second basic property of F1 is that it is non-linear in its inputs. Specifically, fixing the number \( fp \), F1 is concave as a function of \( tp \) (Figure 3). By contrast, accuracy is a linear function of \( tp \) and \( tn \) (Figure 4).

As mentioned in the introduction, F1 is asymmetric. By this, we mean that the
Figure 3: Holding base rate and $f_p$ constant, $F1$ is concave, i.e. offers diminishing marginal returns with respect to $tp$. Each line is a different value of $f_p$.

score assigned to a prediction $P$ given gold standard $G$ can be arbitrarily different from the score assigned to a complementary prediction $P^c$ given complementary gold standard $G^c$. This can be seen by comparing Figure 3 with Figure 5. This asymmetry is problematic when both false positives and false negatives are costly. For example, $F1$ has been used to evaluate the classification of tumors as benign or malignant (Akay (2009)), a domain where both false positives and false negatives have considerable costs.

5 Optimal Thresholds for F1

In this section, we provide a characterization of the optimal thresholds to maximize $F1$ and present a relationship between the optimal threshold and the maximum achievable $F1$ score.

We first describe our framework, depicted in Figure 6. We assume that the classifier outputs scores $s \in [0, S]$ and that there exist two distributions, $p_{t=1}(s)$ and $p_{t=0}(s)$,
Figure 4: Accuracy for fixed base rate and \( tp \). Unlike F1, accuracy offers linearly increasing returns as a function of \( tp \). Each line is a fixed value of \( fp \).

which represent the conditional distribution of seeing a score \( s \) when the true label \( t \) is 1 and 0, respectively. We assume that these distributions, which represent the power of our learned model, are known and discuss an empirical version of our result in the next section.

Given \( p_{t=1}(s) \) and \( p_{t=0}(s) \), we seek a decision rule \( D : s \rightarrow \{0, 1\} \) mapping scores to class labels that maximizes F1. Given this decision rule, and the base rate
Figure 5: F1 for fixed base rate and \( fn \). An asymmetric classifier, F1 offers increasing marginal returns as a function of \( tn \) holding \( fn \) constant. Each line is a fixed value of \( fn \).

\[
P(t = 0) = b, \quad \text{we can calculate the entries of the confusion matrix as}
\]

\[
\begin{align*}
    tp &= b \int_{D(s)=1} p_{t=1}(s) \\
    tn &= (1 - b) \int_{D(s)=0} p_{t=0}(s) \\
    fp &= (1 - b) \int_{D(s)=1} p_{t=0}(s) \\
    fn &= b \int_{D(s)=0} p_{t=1}(s).
\end{align*}
\]

Given these distributions, our theorem prescribes optimal decision rules for F1 maximizing classifiers.

**Theorem 5.1.** A score \( s \) will be assigned to the positive class in the optimal F1 maxi-
Figure 6: The complicated landscape of cost-sensitive decision making.

**mizing classifier if**

\[
\frac{b \cdot p_{t=1}(s)}{(1 - b) \cdot p_{t=0}(s)} \geq J
\]

where \( J = \frac{tp}{fn + tp + fp} \) is the Jaccard Index.

Before we describe the proof of this theorem, we note the difference between the rule in (3) and conventional cost-sensitive decision making (Elkan (2001)) or Neyman-Pearson detection where the right hand side \( J \) is replaced by a constant \( \lambda \) that depends only on the costs of \( 0 - 1 \) and \( 1 - 0 \) classification and not on the performance of the classifier on the given batch. We describe how this relationship leads to potentially undesirable thresholding behavior for many applications in the multi-label setting.

**Proof.** We divide the range of \( s \) into regions of size \( \Delta \). Suppose the decision rule \( D(\bullet) \) has been fixed for all regions except a particular region around a point (with some abuse of notation) \( s \) which we denote with \( \Delta s \). We write \( P_1(\Delta s) = \int_{\Delta s} p_{t=1}(s) \, ds \) and define \( P_2(\Delta(s)) \) similarly.

Suppose that the F1 achieved with decision rule \( D \) for all scores besides \( D(\Delta s) \) is \( F1 = \frac{2tp}{2tp + fn + fp} \). Now, if we add \( \Delta s \) to the positive part of our decision rule, \( D(\Delta s) = 1 \), then the new F1 score will be

\[
F1' = \frac{2tp + 2bP_1(\Delta s)}{2tp + 2bP_1(\Delta s) + fn + (1 - b)P_0(\Delta s) + fp}
\]

On the other hand, if we add \( \Delta s \) to the negative part of our decision rule, \( D(\Delta s) = 0 \), then the new F1 score will be

\[
F1'' = \frac{2tp}{2tp + fn + bP_1(\Delta s) + fp}
\]
Thus, we will add $\Delta s$ to the positive class only if $F_1' \geq F_1''$. With some algebraic simplification, this condition becomes

$$\frac{bP_1(\Delta s)}{(1-b)P_2(\Delta s)} \geq \frac{tp}{tp + fn + fp + bP_1(\Delta s)}$$

Taking the limit $\Delta \to 0$ gives the claimed result.

If a model outputs calibrated probabilities, where $p_{t=1}(s) = s$ and $p_{t=0}(s) = 1-s$, then we have the following corollary.

**Corollary 5.2.** An instance with predicted probability $s$ will be assigned to the positive class by the decision rule that maximizes $F_1$ if and only if

$$s \geq \frac{F_1}{2}$$

where $F_1 = \frac{2tp}{2tp + fn + fp}$ is the maximum $F_1$ achievable.

### 5.1 An Algorithm to Calculate the Maximum Expected $F_1$ Given Output from a Probabilistic Classifier

The above result can be extended to the multi-label setting with dependence. We give a different proof that confirms the optimal threshold for empirical maximization of $F_1$.

We first present an algorithm from [Dembczyński et al. (2011)]. Let $s$ be the output vector of scores from a model. Let $y \in \{0, 1\}^n$ be the gold standard and let $h \in \{0, 1\}^n$ be the thresholded output. In addition, define $a = y^T 1$, $c = h^T 1$, $z^a = \sum_{y: y^T 1 = a} y p(y)$. The maximum achievable macro-$F_1$ is

$$F_1 = \max_c \max_h c E_{p(y)} \left[ \frac{h^T y}{y^T 1 + h^T 1} \right]$$

Algorithm: Loop over the number of predicted positives $c$. Sort the $\sum_a z^a / a+c$. This is a vector of length $n$. Proceed along its entries one by one. Adding an entry to the positive class increases the numerator by $z^a$, which is always positive. Stop after entry number $c$. Pick the $c$ value and corresponding threshold which give the largest $F_1$.

Some algebra gives the following interpretation:

$$\max_c \mathbb{E}(F_1) = \max_c \left( \sum_a \frac{\mathbb{E}(tp|c)}{a+c} p(a) \right)$$

**Theorem 5.3.** The stopping threshold will be $\max E_{p(y)} F_1 / T$. 
5.2 Consequences of Optimal Thresholding

We demonstrate two consequences of applying optimal thresholding to maximize F1. These are the “batch observation” and the “uninformative classifier observation.” We will later demonstrate with a large case study that these can combine to produce surprising and potentially undesirable optimal predictions when macro-F1 is optimized in practice.

The batch observation is that a label may or may not be predicted for an instance depending on the distribution of probabilities in the batch. Earlier, we observed a relationship between the optimal threshold and the maximum \( E(F1) \) and demonstrated that the maximum \( E(F1) \) is related to the distribution of probabilities for all predictions. Therefore, depending upon the distribution in which an instance is placed, it may or may not exceed the optimal threshold. Note, because F1 can never exceed 1, the optimal threshold can never exceed .5.

Consider for example an instance probability of .1. It will be predicted positive if it has the highest probability of all instances in a batch. However, in a different batch, where the probabilities assigned to all other elements is .5 and \( n \) is large, the maximum \( E(F1) \) would be close to .67. According to our theorem, we will only predict positive on this \( nth \) instance if it has a probability greater than .335.

5.3 Uninformative Classifiers

An uninformative classifier is one that assigns the same score to all examples. If these scores are calibrated probabilities, the base rate is assigned to every example.

Theorem 5.4. Given an uninformative classifier for a label, optimal thresholding to maximize F1 results in predicting all examples positive.

Proof. Given an uninformative classifier, we seek the optimal threshold that maximizes \( E(F1) \). We condition on the existence of some nonnegative number \( a \) of actual positives, which occur with frequency \( f = a/n \) and predict some number \( c \) of them positive. Given our uninformative classifier, our only choice is how many labels to predict. By symmetry between the instances, it doesn’t matter which instances we label positive.

Conditioning on the existence of some number \( a = tp + fn \) of actual positives, and some number \( c = tp + fp \) of positive predictions, the denominator of our expression for \( F1 \) \[ 2tp + fp + fn = a + c \], is constant. The number of true positives however, is a random variable, and its expected value is equal to the sum of the probabilities that each example predicted is actually positive.

\[
E(F1) = \frac{2 \sum_{i=1}^{C} f}{a + c} = \frac{2cf}{a + c} = \frac{2f}{a/c + 1}
\]

To maximize this expectation as a function of \( C \), we calculate the partial derivative.

\[
\frac{\partial}{\partial c} E(F1) = \frac{\partial}{\partial c} \frac{2f}{a/c + 1} = \frac{\partial}{\partial c} \frac{2f(a/c + 1)^{-1}} = 2f(A/C + 1)^{-2} C^{-2} \quad (7)
\]
Figure 7: The difference between 1 and the expected F1 of an optimally thresholded uninformative classifier is highly dependent on the base rate.

Since $C$ and $A$ are always positive numbers and $0 < f \leq 1$, this derivative is always positive. Therefore, whenever the frequency of actual positives in the test set is nonzero, expected F1 is maximized by predicting all positive.

For low base rates an optimally thresholded uninformative classifier achieves an $E(F1)$ close to 0, while for high base rates it is close to 1 (Figure 7). We revisit this point in the context of macro-F1.

6 Multi-Label Setting

Different metrics are used to measure different aspects of a system’s performance. However, by changing the loss function, this can change the optimal predictions. We relate the batch observation to discrepancies between predictions optimal for micro and macro-F1. We show that while micro-F1 is dominated by performance on common labels, macro-F1 disproportionately weighs rare labels. Additionally, we show that macro averaging over F1 can conceal extreme uninformative classifier thresholding.
6.1 Micro-F1 Emphasizes Common Label Predictions

Consider the equation for F1, and imagine \( tp, fp, \) and \( fn \) to be known for \( m - 1 \) labels with some distribution of base rates. Now consider the \( m \)th label to be rare with respect to the distribution. A perfect classifier increases \( tp \) by a small amount \( \varepsilon \) equal to the number \( b \cdot n \) of actual positives for that rare label, while contributing nothing to the counts \( fp \) or \( fn \):

\[
F_1' = \frac{2(tp + b \cdot n)}{2(tp + b \cdot n) + fp + fn}.
\]

On the other hand, a trivial prediction of all negative only increases \( fn \) by a small amount:

\[
F_1'' = \frac{2tp}{2tp + fp + (fn + b \cdot n)}.
\]

By contrast, predicting all positive for a rare label will increase \( fp \) by a large amount \( \beta = n - \varepsilon \). We have

\[
\frac{F_1'}{F_1''} = \frac{1 + \frac{b \cdot n}{tp}}{1 + \frac{nb}{a + c + b \cdot n}}.
\]

where \( a \) and \( c \) are the number of positives in the gold standard and the number of positive predictions for the first \( m - 1 \) labels. We have \( a + c \leq \sum b_i \) and so if \( b_m << \sum b_i \) this ratio is small. Thus, performance on rare labels is washed out.

6.2 Macro-F1 Emphasizes Rare Label Predictions

In the single-label setting, the small range between the F1 value achieved by a trivial classifier and a perfect one may not be problematic. If a trivial system gets a score of .9, we can simply adjust our scale for what constitutes a good score. However, when averaging separately calculated F1 over all labels, this variability can skew scores to disproportionately weigh performance on rare labels.

Consider the two label case when one label has a base rate of .5 and the other has a base rate of .1. The corresponding expected F1 for trivial classifiers are .67 and .18 respectively. Thus the expected F1 for optimally thresholded trivial classifiers is .42. However, an improvement to perfect predictions on the rare label elevates the macro-F1 to .84 while such an improvement on the common label would only correspond to a macro-F1 of .59. Thus the increased variability of F1 results in outsize weight for rare labels in macro-F1.

6.3 Dissimilarity of Micro and Macro-F1 Predictions

For a rare label with an uninformative classifier, micro-F1 is optimized by predicting all negative while macro is optimized by predicting all positive. Earlier, we related the optimal threshold for predictions based on a calibrated probabilistic classifier to precisely one half the maximum F1 attainable given all possible threshold settings. In other words, which batch an example is submitted affects whether a positive prediction will be made. In practice, a system may be tasked with predicting labels.
with widely varying base rates. Additionally a classifier’s ability to make confident predictions may vary widely from label to label.

Optimizing micro-F1 as compared to macro-F1 can be thought of as choosing optimal thresholds given very different batches. If the base rate and distribution of probabilities assigned to instances vary from label to label, so will the predictions. Generally, labels with low base rates and less informative classifiers will be over-predicted to maximize macro-F1 as compared to micro-F1. We give evidence of this phenomenon in our case study.

7 Case Study

As a case study, we considered the task of assigning tags from a controlled vocabulary of 26,853 MeSH terms for articles in the biomedical literature using only titles and abstracts. We represent each abstract as a sparse bag-of-words vector over a vocabulary of 188,923 words. Our training data consists of a matrix $A$ with $n$ rows and $d$ columns, where $n$ is the number of abstracts and $d$ is the number of features in our bag of words representation. We apply a tf-idf heuristic text preprocessing step to our bag of words representation to account for word burstiness and elevate the impact of rare words.

Because linear regression models can be trained for multiple labels efficiently, we chose linear regression as a model. Further, to increase the speed of training and prevent overfitting, we approximate the training matrix $A$ by a rank restricted $A_k$ using singular value decomposition. One potential consequence of this rank restriction is that the signal of extremely rare words can be lost. This can be potentially problematic when the rare term is the only feature of predictive value for a rare label.

Given the probabilistic output of our classifier and our theory relating optimal thresholds to maximum attainable F1, we designed three different plug-in rules to maximize micro, macro and per instance F1. A manual inspection of our predictions to maximize micro-F1 revealed no irregularities. However, when inspecting the results optimized to maximize performance on macro-F1, we were surprised to discover that several terms with very low base rates were predicted for more than a third of all documents in the test data. Among these were “Platypus”, “Penicillanic Acids” and “Phosphinic Acids”.

7.1 “The Platypus Problem”: Macro-F1 Conceals Extreme Thresholding

In multi-label classification, a subset of labels can have low base rate and an uninformative classifier. In these cases, optimal thresholding requires the system to predict all positive. In the single-label case, such a system would achieve a low F1 and not be used. But in the macro-averaging multi-label case, this extreme thresholding behavior can take place on a subset of labels, while the system manages to perform well overall.
| MeSH Term         | Count | Max F1    | Threshold |
|-------------------|-------|-----------|-----------|
| Humans            | 2346  | 0.9160    | 0.458     |
| Male              | 1472  | 0.8055    | 0.403     |
| Female            | 1439  | 0.8131    | 0.407     |
| Phosphinic Acids  | 1401  | 1.5437e-04| 7.71e-05  |
| Penicillanic Acid | 1064  | 8.5342e-04| 4.27e-04  |
| Adult             | 1063  | 0.7004    | 0.350     |
| Middle Aged       | 1028  | 0.7513    | 0.376     |
| Platypus          | 980   | 4.6762e-04| 2.34e-04  |

Figure 8: Most frequently predicted MeSH Terms. When macro-F1 is optimized, extremely low thresholds are set for some rare labels with uninformative classifiers, including those in bold above.

8 Experimental Thresholding for F1 and the Winner’s Curse

In practice, thresholds to maximize F1 are often set experimentally, rather than analytically. In such situations, the optimal threshold can be subject to a winner’s curse (Capen et al. (1971)) where a sub-optimal threshold is chosen because of sampling effects or limited training data. As a result, the future performance of a classifier using this threshold is less than the empirical performance. We show that threshold optimization for F1 is particularly susceptible to this phenomenon.

We show that different thresholds have different rates of convergence of estimated F1 with number of samples $n$. As a result, comparing the empirical performance of a low and a high threshold can result in suboptimal performance. We demonstrate these ideas for a problem with an uninformative classifier, though they hold more generally. Consider an uninformative model, for a label with base rate $b$. The model is uninformative in the sense that output scores are $s_i = b + n_i \forall i$, where $n_i = N(0, \sigma^2)$. Thus, scores are uncorrelated with and independent of the true labels. The empirical accuracy for a threshold $t$ is

$$A'_{exp} = \frac{1}{n} \sum_{i \in +} 1[S_i \geq t] + \frac{1}{n} \sum_{i \in -} 1[S_i \leq t]$$

where + and − index the positive and negative class respectively. Each term in (8) is the sum of $O(n)$ i.i.d r.v.s and has exponential (in $n$) rate of convergence to the mean irrespective of the base rate $b$ and the threshold $t$. Thus, for a fixed number $T$ of threshold choices, the probability of choosing the wrong threshold $P_{err} \leq T2^{-cn}$ where $c$ depends on the distance between the optimal and next nearest threshold. Thus, even if errors occur the most likely errors are thresholds close to the true optimal threshold (a consequence of Sanov’s Theorem (Cover & Thomas 2012)).

Consider how F1-maximizing thresholds would be set experimentally, given a set of independent scores from an uninformative classifier. The scores $s_i$ can be sorted in decreasing order (w.l.o.g.). The threshold will lie between two scores that include
the value $F_1$, when the scores are calibrated, as per Theorem 5.1. The threshold $s_{\text{min}}$ that classifies all examples positive (and maximizes $F_1$ analytically as per Theorem 5.4) has an empirical $F_1$ close to its expectation of $\frac{2b}{1+b^2} = \frac{2}{1+b^2}$ since $tp$, $fp$ and $fn$ are all estimated from the entire data. Consider the threshold $s_{\text{max}}$ that classifies only the first example positive and all the others negative. With probability $b$, this has a $F_1$ of $\frac{2}{2+8b^2}$ which will be lower than that of the optimal threshold only for $b \geq \sqrt{\frac{1+5}{2} - 1}$. Thus, despite the threshold $s_{\text{max}}$ being far from optimal, it has a constant probability of having a higher $F_1$ on training data, a probability that does not decrease with $n$, for $n < \frac{1-b}{b^2}$. Thus, optimizing $F_1$ will have a sharp threshold behavior, where for $n < \frac{1-b}{b^2}$ the algorithm will identify large thresholds with constant probability, whereas for large $n \geq \frac{1-b}{b^2}$ it will identify optimal small thresholds. Note that identifying optimal thresholds for $F_1$ is still problematic since it then leads to the “Platypus Problem”. While these problems are distinct, they both arise from the non-linearity of $F_1$ score and its asymmetric treatment of 0s and 1s.

We simulate this behavior, executing 10,000 runs for each setting of the base rate, with $n = 1,000,000$ samples for each run to set the threshold (Figure 9). We then plot a histogram of percentage predicted positive by the empirically chosen threshold and observe a shift from predicting almost all positives to almost all negatives as base rate is decreased. The analytically derived optimal thresholding in all cases is to predict all positive.

9 Macro Skill Score for Multi-Label Binary Classification

Skill score is a monotonically increasing function of accuracy. As a result, the same optimal threshold (0.5 for calibrated probabilities) applies. Further, skill score has the advantage over accuracy that the variability in skill score between an optimally thresholded trivial classifier and a perfect one is equal for all labels, regardless of the base rate. For this reason, macro-averaging skill score accomplishes one “goal” of macro-$F_1$, without altering threshold incentives.

10 Discussion

No single performance metric can capture every desirable property. For example, separately reporting precision and recall is more informative than reporting $F_1$ alone. Sometimes, however, it is practically necessary to define a single performance metric to optimize. Evaluating competing systems and objectively choosing a winner presents such a scenario. In these cases, a change of performance metric can have the consequence of altering optimal thresholding behavior.

Macro-$F_1$ is commonly used in place of micro-$F_1$ when it is desirable to increase the importance of performing well on rare labels. This, however, has the effect of radically altering the optimal thresholds for rare labels with uninformative classifiers. Potentially undesirable optimal thresholds for $F_1$ occur primarily at the extremes (low
Figure 9: The distribution of experimentally chosen thresholds changes with varying $b$. For low $b$, a low percentage of examples are predicted positive even though the optimal thresholding is to predict all positive.

base rates, uninformative classifiers). When F1 is maximized separately for each label, it is more likely that one of them hits these extremes. On the other hand, averaging the inputs to F1 can prevent the inputs from falling at the extremes. Thus, micro-F1 is less likely to result in extreme thresholding behavior than macro-F1.

To weigh the performance on each label equally, we recommend macro skill score. This metric is useful in the multi-label setting because it scales performance equally across labels, something distinct from average accuracy, without altering optimal thresholding behavior. Converting probabilistic predictions to binary classifications is lossy. Some metrics, like AUROC operate on rankings, not binary classifications. AUROC adds the property that a trivial classifier achieves a score of .5 for any base rate. When it is possible to evaluate ranks and not binary predictions, average AUROC across labels may be preferable to macro-F1.
References

Akay, Mehmet Fatih. Support vector machines combined with feature selection for breast cancer diagnosis. *Expert systems with applications*, 36(2):3240–3247, 2009.

Capen, Edward C, Clapp, Robert V, and Campbell, William M. Competitive bidding in high-risk situations. *Journal of petroleum technology*, 23(6):641–653, 1971.

Cover, Thomas M and Thomas, Joy A. *Elements of information theory*. John Wiley & Sons, 2012.

Dembczyński, Krzysztof, Waegeman, Willem, Cheng, Weiwei, and Hüllermeier, Eyke. An exact algorithm for f-measure maximization. 2011.

Dembczynski, Krzysztof, Kotłowski, Wojciech, Jachnik, Arkadiusz, Waegeman, Willem, and Hüllermeier, Eyke. Optimizing the f-measure in multi-label classification: Plug-in rule approach versus structured loss minimization. ICML, 2013.

Elkan, Charles. The foundations of cost-sensitive learning. In *International joint conference on artificial intelligence*, volume 17, pp. 973–978. Citeseer, 2001.

Jansche, Martin. A maximum expected utility framework for binary sequence labeling. In *Annual Meeting-Association For Computational Linguistics*, volume 45, pp. 736, 2007.

José del Coz, Jorge and Bahamonde, Antonio. Learning nondeterministic classifiers. *The Journal of Machine Learning Research*, 10:2273–2293, 2009.

Marina Sokolova, Guy Lapalme. A systematic analysis of performance measures for classification tasks. *Information Processing & Management*, 45:427–437, 2009.

Mozer, Michael C, Dodier, Robert H, Colagrosso, Michael D, Guerra-Salcedo, César, and Wolniewicz, Richard H. Prodding the roc curve: Constrained optimization of classifier performance. In *NIPS*, pp. 1409–1415, 2001.

Musicant, David R, Kumar, Vipin, Ozgur, Aysel, et al. Optimizing f-measure with support vector machines. In *FLAIRS Conference*, pp. 356–360, 2003.

Suzuki, Jun, McDermott, Erik, and Isozaki, Hideki. Training conditional random fields with multivariate evaluation measures. In *Proceedings of the 21st International Conference on Computational Linguistics and the 44th annual meeting of the Association for Computational Linguistics*, pp. 217–224. Association for Computational Linguistics, 2006.

Tan, Songbo. Neighbor-weighted k-nearest neighbor for unbalanced text corpus. *Expert Systems with Applications*, 28:667–671, 2005.

Tsoumakas, Grigorios and Katakis, Ioannis. Multi-label classification: An overview. *International Journal of Data Warehousing and Mining (IJDWM)*, 3(3):1–13, 2007.
Ye, Nan, Chai, Kian Ming A, Lee, Wee Sun, and Chieu, Hai Leong. Optimizing f-measures: A tale of two approaches. In Proceedings of the International Conference on Machine Learning, 2012.