Refinement revisited with connections to Bayes error, conditional entropy and calibrated classifiers

Hamed Masnadi-Shirazi HMASNADI@SHIRAZU.AC.IR
School of Electrical and Computer Engineering, Shiraz University, Shiraz, Iran

Abstract

The concept of refinement from probability elicitation is considered for proper scoring rules. Taking directions from the axioms of probability, refinement is further clarified using a Hilbert space interpretation and reformulated into the underlying data distribution setting where connections to maximal marginal diversity and conditional entropy are considered and used to derive measures that provide arbitrarily tight bounds on the Bayes error. Refinement is also reformulated into the classifier output setting and its connections to calibrated classifiers and proper margin losses are established.

Keywords: Refinement Score, Probability Elicitation, Calibrated Classifier, Bayes Error Bound, Conditional Entropy, Proper Loss

1. Introduction

The concept of refinement can be traced back to a well known partition of the Brier (or quadratic) score in early works by Murphy (1972) but was explicitly defined and generalized for all proper scoring rules in a series of seminal papers by DeGroot and Fienberg (1982, 1983). This concept is also well known under different names depending on the literature. In the forecasting and meteorology literature it is known as sharpness Sanders (1963); Gneiting et al. (2007) or resolution Brcker (2009) and in the probability elicitation literature Savage (1971); Schervish (1989). This concept has also been studied most recently in the meteorology and forecasting literature in papers such as Gneiting et al. (2005); Wilks (2006); Gneiting et al. (2007); Brcker (2009).

Despite the fact that refinement is closely related to proper scoring rules and calibrated loss functions it has remained largely restricted to the probability elicitation and forecasting literature. In this paper we initially briefly review the concepts of calibration and refinement. The concept of refinement will be emphasized and explained using the original works of DeGroot and Fienberg (1982). We will then proceed to bring three different yet closely interlocked arguments that will each initially seem to refute the validity of the refinement concept, but will instead after a subtle clarification, lead to the generalization of the refinement concept and establish its connections to Bayes error, maximum margin diversity and conditional entropy in feature selection Vasconcelos (2002); Fleuret and Guyon (2004); Pene et al. (2005); Vasconcelos and Vasconcelos (2003); and classification with Bayes calibrated loss functions Friedman et al. (2000); Zhang (2004); Reid and Williamson (2010) among

©2013 Hamed Masnadi-Shirazi.
others. Specifically, the original refinement definition on the probability elicitation setting will be extended to the classifier output setting and underlying data distribution setting.

A series of results are presented by extending refinement to the underlying data distribution setting which show that conditional entropy and maximum margin diversity used in feature selection are a special case of refinement using the logistic score function. A number of other novel refinement measures based on other score functions are derived along with conditional refinement which can be used for feature selection and ranking. Refinement is also related to the Bayes error. A number of well known bounds on the Bayes error such as the Bhatnagarry bound [1990], the asymptotic nearest neighbor bound [1990], Cover and Hart (1967) and the Jensen-Shannon divergence [1991] are shown to be special cases of refinement measures. Other novel bounds on the Bayes error are derived using the refinement interpretation along with a method for deriving arbitrarily tight bounds on the Bayes error.

Extending refinement to the classifier output setting allows for a statistically rigorous parallel to the classifier margin which we call classifier marginal density which allows for the ranking of calibrated classifiers simply based on their outputs. We also show how each calibrated loss function has a corresponding refinement measure and derive a number of such novel measures. Refinement is also further studied in its original probability elicitation setting and a Hilbert space and inner product interpretation is provided. The inner product interpretation leads to further insight into refinement using different symmetric scoring rules.

The paper is organized as follows. In Section-2 a review of the refinement concept in probability elicitation is provided. In Section-3 the refinement concept is further analyzed from the perspective of the axioms of probability which leads to a novel refinement formulation in the underlying data distribution setting and connections to the Bayes error. In Section-4 refinement and its connections to maximal marginal diversity and conditional entropy are considered. Connections to calibrated classifiers are considered in Section-5. In Sections-6,7, and 8 refinement is further studied in its original setting, the proposed classifier output and underlying data distribution settings, respectively. Finally, in Section-9 refinement in the underlying data distribution setting is used to derive measures that provide arbitrarily tighter bounds on the Bayes error. Summary and conclusions are provided in Section-10.

2. Refinement In Probability Elicitation

In probability elicitation [1971] a forecaster produces a probability estimate \( \hat{\eta} \) of the occurrence of event \( y = 1 \) where \( y \in \{1, -1\} \), such as a weatherman predicting that it will rain \( (y = 1) \) tomorrow. \( \eta = P(1|\hat{\eta}) \) is the actual relative frequency of event \( y = 1 \) (rain) among those days which the forecaster’s prediction was \( \hat{\eta} \). A forecaster is said to be calibrated if \( \eta = \hat{\eta} \) for all \( \hat{\eta} \), meaning that the weatherman is skilled and trustworthy. In other words it actually rains \( \eta = \hat{\eta} \) percent of the time when he predicts the chance of rain is \( \hat{\eta} \).

It has been argued in [1979], [1982], [1982] that a calibrated forecaster is not necessarily a good forecaster or an informative and useful one and that another concept called refinement is also needed to evaluate forecasters. Intuitively, let \( s(\hat{\eta}) \) denote the probability density function of the forecaster’s predictions, then the more concentrated the probability density function \( s(\hat{\eta}) \) is around the values \( \hat{\eta} = 0 \) and \( \hat{\eta} = 1 \) the more refined the forecaster is. To further demonstrate the concept of refinement, it is useful to consider the following slightly modified example taken from [1982]. Consider two calibrated weather fore-
casters $A$ and $B$ working at a location where the expected probability of rain is $\mu = 0.5$ on any given day. Weatherman $A$ is such that
\begin{align}
s_A(\mu) &= 1 \\
s_A(\hat{\eta}) &= 0 \quad \text{for} \quad \hat{\eta} \neq \mu
\end{align}
and weatherman $B$ is such that
\begin{align}
s_B(1) &= \mu \\
s_B(0) &= 1 - \mu \\
s_B(\hat{\eta}) &= 0 \quad \text{for} \quad \hat{\eta} \neq 0, 1.
\end{align}
Both forecasters can be calibrated. To demonstrate this, assume that both weathermen make 100 predictions. Weatherman $A$ predicts that the chance of rain is $\hat{\eta} = 0.5$ all the time. If it actually rains as expected on 50 days we have $\eta = \frac{50}{100} = 0.5$ so $\hat{\eta} = \eta$ and $A$ is calibrated. In the case of weatherman $B$ the predictions are 1) chance of rain is $\hat{\eta} = 1$ on 50 days and 2) chance of rain is $\hat{\eta} = 0$ on the other 50 days. If it actually rains on the 50 days $B$ predicted rain then $\eta = \frac{50}{50} = 1$ and if it actually does not rain when $B$ predicted no rain then $\eta = \frac{0}{50} = 0$. In either case $\hat{\eta} = \eta$ and $B$ is also calibrated.

Although we have shown that both $A$ and $B$ are calibrated forecasters, it is acceptable to say that the forecasts made by $A$ are useless while forecaster $B$ is the ideal weatherman in the sense that he only makes definite predictions of chance of rain is 0 or chance of rain is 1 and is always correct. On the other hand, forecaster $A$ always makes the conservative but useless prediction that chance of rain is 0.5. We say that weatherman $A$ is the least-refined forecaster and that weatherman $B$ is the most-refined forecaster [DeGroot and Fienberg (1982)]. This leads to the argument that well calibrated forecasters can be compared based on their refinement [DeGroot and Fienberg (1983)].

Before providing a formal measure of refinement, proper scoring functions need to be introduced. A scoring function is such that a score of $I_1'(\hat{\eta})$ is attained if the forecaster predicts $\hat{\eta}$ and event $y = 1$ actually happens and a score of $I_{-1}(\hat{\eta})$ is attained if event $y = -1$ happens. $I_1(\hat{\eta})$ is an increasing functions of $\hat{\eta}$ and $I_{-1}(\hat{\eta})$ is decreasing in $\hat{\eta}$. Since the relative frequency with which the forecaster makes the prediction $\hat{\eta}$ is $s(\hat{\eta})$, the expected score of the forecaster over all $\hat{\eta}$ and $y$ is
\begin{equation}
\int \int s(\hat{\eta})[\eta I_1(\hat{\eta}) + (1 - \eta)I_{-1}(\hat{\eta})]d(\hat{\eta}),
\end{equation}
and the expected score for a given $\hat{\eta}$ is
\begin{equation}
I(\eta, \hat{\eta}) = \eta I_1(\hat{\eta}) + (1 - \eta)I_{-1}(\hat{\eta}).
\end{equation}

The score function is denoted as strictly proper if $I_1(\hat{\eta})$ and $I_{-1}(\hat{\eta})$ are such that the expected score of (7) is maximized when $\hat{\eta} = \eta$ or in other words
\begin{equation}
I(\eta, \hat{\eta}) \leq I(\eta, \eta) = J(\eta).
\end{equation}

It can be shown [Savage (1971)] that a score function is strictly proper if and only if the maximal reward function $J(\eta)$ is strictly convex and
\begin{align}
I_1(\eta) &= J(\eta) + (1 - \eta)J'(\eta) \\
I_{-1}(\eta) &= J(\eta) - \eta J'(\eta).
\end{align}
A formal definition of refinement can be provided when considering the proper scoring function $I_y$. The expected score $S_{I_y}$ can be written as

$$S_{I_y} = \int \tilde{s}(\hat{y}) \sum_y P(y|\hat{y}) I_y(\hat{y}) d(\hat{y})$$

$$= \int \tilde{s}(\hat{y}) \left( P(1|\hat{y}) I_1(\hat{y}) + P(-1|\hat{y}) I_{-1}(\hat{y}) \right) d(\hat{y}).$$

By simply adding and subtracting $s(\hat{y}) [P(1|\hat{y}) I_1(\eta) + P(-1|\hat{y}) I_{-1}(\eta)]$, we can dissect any expected score $S_{I_y}$ of a forecaster into two parts of $S_{\text{Calibration}}$ and $S_{\text{Refinement}}$ that are measures of calibration and refinement [DeGroot and Fienberg (1983)].

$$S_{I_y} = \int \tilde{s}(\hat{y}) \sum_y P(y|\hat{y}) I_y(\hat{y}) d(\hat{y})$$

$$= \int \tilde{s}(\hat{y}) \left( P(1|\hat{y}) I_1(\hat{y}) + P(-1|\hat{y}) I_{-1}(\hat{y}) \right) d(\hat{y})$$

$$= \int \tilde{s}(\hat{y}) \left[ P(1|\hat{y}) \{ I_1(\hat{y}) - I_1(\eta) \} + P(-1|\hat{y}) \{ I_{-1}(\hat{y}) - I_{-1}(\eta) \} \right] d(\hat{y})$$

$$+ \int \tilde{s}(\hat{y}) \left[ P(1|\hat{y}) I_1(\eta) + P(-1|\hat{y}) I_{-1}(\eta) \right] d(\hat{y})$$

$$= S_{\text{Calibration}} + S_{\text{Refinement}}.$$

Recall that $I(\hat{y}, \eta) \leq I(\eta, \eta) = J(\eta)$ so that $S_{\text{Calibration}}$ has a maximum equal to zero when the forecaster is calibrated ($\hat{y} = \eta$) and is negative otherwise.

The second term $S_{\text{Refinement}}$ can be simplified to

$$S_{\text{Refinement}} = \int \tilde{s}(\hat{y}) \left[ P(1|\hat{y}) I_1(\eta) + P(-1|\hat{y}) I_{-1}(\eta) \right] d(\hat{y})$$

$$= \int \tilde{s}(\hat{y}) \left[ \eta I_1(\eta) + (1 - \eta) I_{-1}(\eta) \right] d(\hat{y})$$

$$= \int \tilde{s}(\hat{y}) J(\eta) d(\hat{y}).$$

Note that $J(\eta) = J(P(1|\eta))$ is a convex function of $\hat{y}$ over the $[0,1]$ interval. Intuitively, the more concentrated $s(\hat{y})$ is near 0 and 1 the larger the $s(\hat{y}) J(\eta)$ term will become. In other words $S_{\text{Refinement}}$ will increase as $\hat{y}(x)$ becomes more refined [DeGroot and Fienberg (1983)]. We will formalize this and present the inner product interpretation of refinement in Section 6.

As an example, the expected score of the strictly proper Brier score (BS) (or least squares) $I_{y'} = (\hat{y} - y')^2$ where $y' = \frac{\hat{y} + 1}{2}$, can be expressed as a measure of calibration and refinement [Murphy (1972), DeGroot and Fienberg (1983)]

$$S_{BS} = -\int \tilde{s}(\hat{y}) \left( P(1|\hat{y}) (\hat{y} - 1)^2 + P(-1|\hat{y}) (\hat{y} + 1)^2 \right) d(\hat{y})$$

$$= -\int \tilde{s}(\hat{y}) (\hat{y} - P(1|\hat{y}))^2 d(\hat{y}) + \int \tilde{s}(\hat{y}) P(1|\hat{y}) (P(1|\hat{y}) - 1) d(\hat{y})$$

$$= S_{\text{Calibration}} + S_{\text{Refinement}}.$$
The expected score $S_{I_y}$ is maximized when the forecaster is calibrated $\hat{\eta} = P(1|\hat{\eta}) = \eta$ and the distribution of predictions $s(\hat{\eta})$ are mostly concentrated around 0 and 1 since $P(1|\hat{\eta})(P(1|\hat{\eta})-1) = \eta(\eta-1)$ is a symmetric convex function of $\eta$ on this interval with minimum at $\eta = \frac{1}{2}$ and maximums at $\eta = 0$ and $\eta = 1$ (DeGroot and Fienberg 1983).

3. Further Analysis Of The Refinement Concept

In this section we present a series of three arguments from different angles that further clarify and extend the concept of refinement. The first is an argument based on Cox’s theorem on subjective probability that basically points out a subtle yet important flaw in the assumptions that might be made in understanding the refinement concept.

3.1 Argument based on the basic desiderata of probability

A forecaster is simply producing subjective probabilities. It is well understood that subjective probabilities are based on the axioms of Cox’s theory which are elegantly presented as the desiderata of probability in the form of three logical statements in Jaynes and Bretthorst (2003). It is the failure to strictly follow these requisites that has led to many unnecessary errors, paradoxes and controversies in probability. Here we show that the concept of refinement might seem to contradict the third desiderata of probability if not presented correctly, namely that of consistency. This requires that 1) if a conclusion can be reasoned out in more than one way, then every possible way must lead to the same result, 2) the forecaster always takes into account all the evidence it has relevant to the question and does not arbitrarily ignore some of the information and 3) if in two problems the forecasters state of knowledge is the same, then it must assign the same probabilities in both. It is also important to note that subjective probability and their logic does not depend on the person or machine making them. Anyone who has the same information but comes to a different probability assignment is necessarily violating one of the desiderata of probability Jaynes and Bretthorst (2003).

Ignoring the above requisites can lead to a misunderstanding or contradiction when considering the concept of refinement. This can best be presented with an example similar to that in Section-2. Assume that two calibrated forecasters A and B have access to the same information, for the sake of argument we assume this to be data $x$ in the form of air pressure readings which is a good indicator for predicting rain. Also assume that the actual probability of rain given air pressure $x$ is known to be $P(1|x) = 0.7$. In terms of forecasters, the consistency property requires that each $x$ lead to a corresponding forecast $\hat{\eta}$ (and $\eta$) and that no $x$ lead to more than one forecast $\hat{\eta}$ (and $\eta$). In other words $\hat{\eta}$ and $\eta$ are functions of the information $x$ such that we can write $\hat{\eta}(x)$ and $\eta(x)$.

Let Forecaster A make the prediction that chance of rain is $\hat{\eta}_A(x) = 1$ and forecaster B make the prediction that chance of rain is $\hat{\eta}_B(x) = 0.7$. It might initially seem that forecaster A is more refined than forecaster B, but in fact the consistency principle of probability elicitation is being violated. In other words, since both forecasters are basing their forecasts on the same information $x$, they should both make identical predictions.

We extend the concept of forecasters and require two more reasonable properties from a forecaster. First, a forecaster should be responsive. In other words different information must lead to a different forecast. Formally, we require that if the information $x_1 \neq x_2$ then $\hat{\eta}(x_1) \neq \hat{\eta}(x_2)$ and $\eta(x_1) \neq \eta(x_2)$. This is equivalent by definition to requiring that $\hat{\eta}(x)$ and $\eta(x)$ be one-to-one func-
tions. Second, a forecaster should be encompassing and any forecast should be possible. Formally, their exists a corresponding \( x \) for any \( \hat{\eta} \) and \( \eta \). This is equivalent by definition to requiring that \( \hat{\eta}(x) \) and \( \eta(x) \) be onto functions. Both required properties can be summarized by equivalently requiring that \( \hat{\eta}(x) \) and \( \eta(x) \) be invertible functions. The immediate consequence of invertibility is that

\[
\eta(x) = P(1|\hat{\eta}(x)) = P(1|x). \tag{15}
\]

This in turn leads to another contradiction in the example above meaning that forecaster A is not actually calibrated. If as stated \( P(1|x) = 0.7 \) then \( \eta(x) = P(1|\hat{\eta}(x)) = P(1|x) = 0.7 \) while forecaster A predicted \( \hat{\eta}_A(x) = 1 \neq \eta(x) \) i.e. forecaster A is not calibrated as initially claimed. Forecaster B, on the other hand, is verifiably calibrated.

### 3.2 Extending refinement to the underlying data distribution setting

The discussion and example presented in Section 3.1 suggest that a forecaster and its measure of refinement depend on the underlying data distribution \( P(1|x) \) from which the forecasts are established. This can be formally presented by writing the expected score as

\[
E_{\hat{\eta},Y}[I_y(\hat{\eta})] = \int_{\hat{\eta}} s(\hat{\eta}) \sum_y P(y|\hat{\eta}) I_y(\hat{\eta}) d(\hat{\eta}) \tag{16}
\]

\[
= \int_{\hat{\eta}} s(\hat{\eta}) \sum_y \frac{P(\hat{\eta}|y)P(y)}{s(\hat{\eta})} I_y(\hat{\eta}) d(\hat{\eta})
\]

\[
= \int_{\hat{\eta}} \left[ P(\hat{\eta}|1)P(1)I_1(\hat{\eta}) + P(\hat{\eta}|\overline{1})P(\overline{1})I_{\overline{1}}(\hat{\eta}) \right] d(\hat{\eta})
\]

\[
= \int_{X} \left[ \frac{P(x|1)}{\hat{\eta}'} P(1)I_1(\hat{\eta}) + \frac{P(x|\overline{1})}{\hat{\eta}'} P(\overline{1})I_{\overline{1}}(\hat{\eta}) \right] (\hat{\eta}' dx)
\]

\[
= \int_{X} \left[ P(x|1)P(1)I_1(\hat{\eta}) + P(x|\overline{1})P(\overline{1})I_{\overline{1}}(\hat{\eta}) \right] dx
\]

\[
= \int_{X} P_X(x) \sum_y P(y|x) I_y(\hat{\eta}) dx
\]

where \( \hat{\eta}' = \hat{\eta}'(x) = \frac{d\hat{\eta}(x)}{dx} \) and we have made use of the change of variable theory from calculus and function of random variable theory from probability theory. Using this theory demands that \( \hat{\eta}(x) \) be an invertible function as previously required for a forecaster.
REFINEMENT REVISITED

The refinement term \( S_{\text{Refinement}} \) can also be similarly reduced to

\[
S_{\text{Refinement}} = \int s(\hat{\eta}) \left[ P(1|\hat{\eta})I_1(\eta) + P(-1|\hat{\eta})I_{-1}(\eta) \right] d(\hat{\eta})
\]

\[
= \int_X \left[ \frac{P(x|1)}{\hat{\eta}'} P(1|\eta) + \frac{P(x|-1)}{\hat{\eta}'} P(-1|\eta) \right] (\hat{\eta}' dx)
\]

\[
= \int_X \left[ P(x|1)P(1|\eta) + P(x|-1)P(-1|\eta) \right] dx
\]

\[
= \int_X P_X(x) \sum_y P(y|x)I_y(\eta) dx
\]

\[
= \int_X P_X(x)J(\eta) dx
\]

\[
= \int_X P_X(x)J(P(1|x)) dx.
\]

The above formulation shows that the distribution of forecasts \( s(\hat{\eta}) \) in the original refinement formulation (13) reduces to \( P_X(x) \) which is the distribution of the data. This means that the refinement of a forecaster has nothing to do with how good the forecaster is but depends on the distribution of the underlying data itself which is outside the control of the forecaster. Given observations \( x \) the best a forecaster can do is be calibrated. This can also be seen by noting that refinement is a constant term independent of the forecaster predictions \( \hat{\eta} \) and only depends on the distribution of the data. This observation leads us to make a connection with the Bayes rule in decision theory which we explore in the next section.

3.3 Refinement and the Bayes rule

We can think of a forecaster as a kind of classifier that tries to classify days into rainy or sunny. We again assume that the forecaster/classifier has access to a set of observations \( x \), for example air pressure. What is the optimal decision a forecaster can make? The Bayes rule tells us that the optimal decision is to choose rainy if \( P(1|x) > P(-1|x) \) and sunny otherwise; or equivalently the forecaster’s predictions should be chance of rain is \( \hat{\eta} = P(1|x) \). This, by definition, is simply the requirement of a calibrated forecaster \( \hat{\eta} = P(1|x) = \eta \).

This can also be written as choose rainy if \( \frac{P(x|1)P(1)}{P(x)} > \frac{P(x|-1)P(-1)}{P(x)} \). Assuming no prior knowledge of the chance of rain on any given day we can write choose rainy if \( P(x|1) > P(x|-1) \).

We see that the optimal decision rule depends only on the distribution of the data \( P(x|y) \). Given that two forecasters have access to the same air pressure readings, the best forecast they can each give on any given day depends on the distributions of \( P(x|1) \) and \( P(x|-1) \) and is simply \( \hat{\eta} = P(x|1) \).

Given equal access to data \( x \), both forecasters will make identical predictions. A central part of Bayes decision theory is the Bayes error. We will return to the subject of Bayes error and its connections to refinement in Section 8.

3.4 Clarifying the refinement concept

At this point, given the three arguments above, it is evident that the concept of refinement can only be meaningful when comparing forecasters that use different types of evidence or data to form their predictions. For example, it could be such that one forecaster uses \( x_1 \) air pressure and another uses...
with the highest refinement using the logistic leads to a set of maximally diverse marginal densities where the marginal diversity for each feature is defined as 

\[ I_i = \log(1 - P_i) + \log(P_i) \]

Choosing a feature \( x_i \) with maximally diverse marginal density is equivalent to choosing a feature

In other words the best feature to use for classification is the one that has the highest

In summary, for a fixed data type \( x_1 \) with distribution \( P(x_1) \), the best forecaster possible is the calibrated forecaster and all other forecasters that base their predictions on this type of data \( x_1 \) can at best be identical to the calibrated forecaster. The only way to improve on the forecaster’s predictions is to use a different type of data or feature \( x_2 \) with a different distribution of \( P(x_2) \) resulting in a calibrated forecaster that has higher refinement. This brings us to the notion of feature selection and its connections to refinement which we explore in the next section.

4. Refinement, Maximum Marginal Diversity And Conditional Entropy

In this section we show that conditional entropy and maximum margin diversity Vasconcelos (2002, 2003) are both special cases of the extended concept of refinement in the underlying data distribution setting when considering the logistic maximal reward function \( J(\eta) = \eta \log(\eta) + (1 - \eta) \log(1 - \eta) \).

4.1 Refinement and Maximum Marginal Diversity

The principal of maximum marginal diversity Vasconcelos (2002, 2003) is studied in feature selection and states that for a classification problem with observations drawn from a random variable \( Z \in \mathbb{Z} \) and a feature transformation \( T_i : \mathbb{Z} \rightarrow \mathbb{X} \), the best feature transformation is the one that leads to a set of maximally diverse marginal densities where the marginal diversity for each feature is defined as

\[ \text{md}(X_i) = \sum_{y=1, -1} P_Y(y) D_{KL}(P(x_i | 1) || P(x_i)) \] (18)

In other words the best feature to use for classification is the one that has the highest \( \text{md}(X_i) \). Choosing a feature \( x_i \) with maximally diverse marginal density is equivalent to choosing a feature with the highest refinement using the logistic \( J(\eta) \) function. This can be shown by writing (17) as

\[
S_{\text{Refinement}} = \\
= \int_X \left[ P(x|1)P_Y(1)I_1(P(1|x)) + P(x|1)P_Y(-1)I_{-1}(P(1|x)) \right] dx \\
= \int_X \left[ P(x|1)P_Y(1)I_1(P(1|x)) + P(x|1)P_Y(-1)I_{-1}(P(1|x)) \right] dx. 
\]

For the special case where \( J(\eta) = \eta \log(\eta) + (1 - \eta) \log(1 - \eta) \) such that \( I_1(\eta) = \log(\eta) \) and \( I_{-1}(\eta) = \log(1 - \eta) \) we have

\[
S_{\text{Refinement}} = \\
= \int_X \left[ P(x|1)P_Y(1) \log \left( \frac{P(x|1)P_Y(1)}{P(x)} \right) + P(x|1)P_Y(-1) \log \left( 1 - \frac{P(x|1)P_Y(1)}{P(x)} \right) \right] dx \\
= P_Y(1)D_{KL}(P(x|1) || P(x)) + P_Y(-1)D_{KL}(P(x|1) || P(x)) + P_Y(1) \log(P_Y(1)) + P_Y(-1) \log(P_Y(-1)). 
\]
Assuming that $P_Y(1) = \gamma$ we can write

$$
S_{\text{Refinement}} = P_Y(1)KL(P(x|1)||P(x)) + P_Y(-1)KL(P(x|-1)||P(x))
$$

(21)

and maximum marginal diversity is equivalent, up to a constant, to the refinement formula for the special case of when $J(\eta) = \eta \log(\eta) + (1 - \eta) \log(1 - \eta)$. The consequences of realizing such an equivalence is that in the case of probability elicitation one realizes that the best a forecaster can do using a certain feature such as $x = $ air pressure is to be calibrated, increased refinement can only come from using better features such as maybe $x = $ air humidity. The insight gained in terms of feature selection is that the KL-divergence is not unique and that other valid $J(\eta)$ functions such as those in Table-4 and plotted in Figure-4 and Figure-5 can be used to find refinement formulations as seen in Table-3 and Table-5. The question that still remains is how different convex $J(\eta)$ differ in terms of their feature selection properties. We consider this problem in Sections-8 and 9.

4.2 Refinement, mutual information and conditional entropy

Refinement also has a close relationship with mutual information and conditional entropy. From (21) we write refinement for the special case of $J(\eta) = \eta \log(\eta) + (1 - \eta) \log(1 - \eta)$ as

$$
S_{\text{Refinement}} = 
$$

(22)

where $I(x; y)$ is the mutual information and $H(y|x)$ is the conditional entropy. This shows that conditional entropy is a special case of the refinement score when the logistic $J(\eta)$ is used. Note that a higher refinement is a number that is less negative which corresponds to a lower conditional entropy. In other words if $y$ is completely determined by $x$ then the conditional entropy will be zero, which corresponds to maximum refinement.

Refinement can be directly used for feature selection and is closely related to conditional mutual information or conditional entropy conditioned on two or more variables. Ranking all features by their refinement score is not very useful because this does not take into account the dependencies that exist between the features. Simply using the first $n$ highest ranked features is usually a bad idea since most of the first few features will be redundant, related and dependent. We would like to choose the second feature $z$ such that it not only provides information for classifying the class $y$, but is also complementary to the previously chosen feature $x$. This can be accomplished by considering the conditional refinement score defined as

$$
S_{\text{ConditionalRefinement}} = \sum_{x, z} P(x, z)J(P(1|x, z)).
$$

(23)
Conditional entropy is a special case of conditional refinement when the logistic \( J(\eta) = \eta \log(\eta) + (1 - \eta) \log(1 - \eta) \) is used

\[
S_{\text{ConditionalRefinement}} = \sum_{x,z} P(x,z) J(P(1|x,z))
\]

\[
= \sum_{x,z} P(x,z) [P(1|x,z) \log(P(1|x,z)) + (1 - P(1|x,z)) \log(1 - P(1|x,z))]
\]

\[
= \sum_{x,z} P(x,z) \sum_{y} P(y|x,z) \log(P(y|x,z))
\]

\[
= \sum_{x,z,y} P(x,z,y) \log(P(y|x,z))
\]

\[
= -H(y|x,z).
\]

A more practical formula for conditional refinement can be written as

\[
S_{\text{ConditionalRefinement}} = \sum_{x,z} P(x,z) J(P(1|x,z))
\]

\[
= \sum_{x,y,z} P(z|x,y) P(x|y) P(y) \log(P(y|x,z))
\]

\[
= \sum_{x,y,z} P(z|x,y) P(x|y) P(y) \log\left( \frac{P(z|x,y) P(x|y) P(y)}{P(z|x) P(x)} \right)
\]

where we have used the logistic \( J(\eta) \) to demonstrate. The above formula iteratively picks the best feature conditioned on the previously chosen feature. Note that all the distributions can be estimated with one dimensional histograms. Conditional entropy has been successfully used in Fleuret and Guyon (2004) as the basis of a feature selection algorithm that has been shown to outperform boosting Freund and Schapire (1997); Friedman et al. (2000) and other classifiers on the datasets considered. Finally, note that similar to refinement, different conditional refinement scores can be derived for different choices of convex \( J(\eta) \).

5. Refinement And Calibrated Classifiers

Probability elicitation and classification by way of conditional risk minimization are closely related and have been most recently studied in Friedman et al. (2000); Zhang (2004); Buja et al. (2005); Masnadi-Shirazi and Vasconcelos (2008); Reid and Williamson (2010). A classifier \( h \) maps a feature \( x \in X \) to a class label \( y \in \{-1, 1\} \). This mapping can be written as \( h(x) = \text{sign}[p(x)] \) for a classifier predictor function \( p : X \to \mathbb{R} \). A predictor function is called an optimal predictor \( p^*(x) \) if it minimizes the risk

\[
R(p) = E_{X,Y}[L(p(x), y)]
\]

for a given loss \( L(p(x), y) \). This is equivalent to minimizing the conditional risk \( E_{X|Y}[L(p(x), y)|X = x] \) for all \( x \). Classification can be related to probability elicitation by expressing the predictor as a composite of two functions

\[
p(x) = f(\hat{\eta}(x))
\]
where \( f : [0, 1] \rightarrow \mathbb{R} \) is called the \textit{link function}. The problem of finding the predictor function is now equivalent to finding the link and forecaster functions. A link function is called an optimal link function \( f^*(\eta) \) if it is a one-to-one mapping and also implements the Bayes decision rule, meaning that it must be such that

\[
\begin{cases} 
  f^* > 0 & \text{if } \eta(x) > \frac{1}{2} \\
  f^* = 0 & \text{if } \eta(x) = \frac{1}{2} \\
  f^* < 0 & \text{if } \eta(x) < \frac{1}{2}.
\end{cases}
\] (28)

Examples of optimal link functions include \( f^* = 2\eta - 1 \) and \( f^* = \log\frac{\eta}{1-\eta} \), where we have omitted the dependence on \( x \) for simplicity.

A predictor is denoted \textit{calibrated} if it is optimal, i.e. minimizes the risk of (26), and an optimal link function exists such that

\[
\eta(x) = (f^*)^{-1}(p^*(x)) = \hat{\eta}(x).
\] (29)

The loss \( L(p(x), y) \) associated with a calibrated predictor is called a \textit{proper} loss function.

In a classification algorithm a proper loss function is usually fixed beforehand. The associated conditional risk is

\[
C_L(\eta, f) = \eta L(f, 1) + (1 - \eta)L(f, -1),
\] (30)

the optimal link function is typically found from

\[
f^*_L(\eta) = \arg\min_f C_L(\eta, f)
\] (31)

and the minimum conditional risk is

\[
C^*_L(\eta) = C_L(\eta, f^*_L).
\] (32)

For example, in the case of the zero-one loss

\[
L_{0/1}(f, y) = \begin{cases} 
  0, & \text{if } y = \text{sign}(f) \\
  1, & \text{if } y \neq \text{sign}(f)
\end{cases}
\] (33)

the associated conditional risk is

\[
C_{0/1}(\eta, f) = \begin{cases} 
  1 - \eta, & \text{if } f \geq 0 \\
  \eta, & \text{if } f < 0
\end{cases}
\] (34)

the optimal link can be \( f^* = 2\eta - 1 \) or \( f^* = \log\frac{\eta}{1-\eta} \) and the minimum conditional risk is

\[
C^*_{0/1}(\eta) = \min\{\eta, 1 - \eta\}.
\] (35)

Margin losses are a special class of loss functions commonly used in classification algorithms which are in the form of

\[
L_\phi(f, y) = \phi(yf).
\] (36)
Margin loss functions assign a non zero penalty to positive $yf$ called the margin. Algorithms such as boosting [Freund and Schapire (1997), Friedman et al. (2000)] are based on proper margin loss functions and have not surprisingly demonstrated superior performance given their consistency with the Bayes optimal decision rule [Friedman et al. (2000), Buja et al. (2005), Masnadi-Shirazi and Vasconcelos (2008)]. Table 1 includes some examples of proper margin losses along with their associated optimal links and minimum conditional risks.

The score functions $I_1$, $I_{-1}$ and maximal reward function $J(\eta)$ can be related to proper margin losses and the minimum conditional risk by considering the following theorem Masnadi-Shirazi and Vasconcelos (2008) which states that if $J(\eta)$ defined as in (8) is such that

$$J(\eta) = J(1 - \eta)$$

and a continuous function $f^*_\phi(\eta)$ is invertible with symmetry

$$(f^*_\phi)^{-1}(-v) = 1 - (f^*_\phi)^{-1}(v),$$

then the functions $I_1$ and $I_{-1}$ derived from (9) and (10) satisfy the following equalities

$$I_1(\eta) = -\phi(f^*_\phi(\eta))$$

$$I_{-1}(\eta) = -\phi(-f^*_\phi(\eta)),$$

with

$$\phi(v) = -J\{((f^*_\phi)^{-1}(v)) - (1 - (f^*_\phi)^{-1}(v))J'((f^*_\phi)^{-1}(v))\}.$$

An important direct result of the above theorem is that $J(\eta) = -C^*_\phi(\eta)$.

The above discussion connects refinement to the classification setting and we can write refinement in terms of the calibrated classifier outputs $v = f(\eta)$. Specifically, assuming a calibrated classifier based on a proper loss function we have

$$v = p(x) = f(\eta(x)) = f^*(\eta(x))$$

and

$$\hat{\eta}(x) = \eta(x) = (f^*)^{-1}(v),$$

Table 1: Proper margin loss $\phi(v)$, optimal link $f^*_\phi(\eta)$, optimal inverse link $(f^*_\phi)^{-1}(v)$ and maximal reward $J(\eta)$.

| Loss | $\phi(v)$ | $f^*_\phi(\eta)$ | $(f^*_\phi)^{-1}(v)$ | $J(\eta)$ |
|------|-----------|------------------|----------------------|-----------|
| LSZhang (2004) | $\frac{1}{2}(1 - v)^2$ | $2\eta - 1$ | $\frac{1}{2} + \frac{1}{v^2}$ | $-2\eta(1 - \eta)$ |
| ExpZhang (2004) | $\exp(-v)$ | $\frac{1}{2} \log \eta$ | $\frac{1}{2} - \frac{1}{v^2}$ | $-2\sqrt{\eta(1 - \eta)}$ |
| LogZhang (2004) | $\log(1 + e^{-v})$ | $\log \eta$ | $\frac{1}{2} + \frac{1}{v^2}$ | $-4\eta(1 - \eta)$ |
| Savage-Masnadi-Shirazi and Vasconcelos (2008) | $(2 \arctan(v) - 1)^2$ | $\arctan(v) + \frac{1}{2}$ | $\arctan(v) - \frac{1}{2}$ | $-4\eta(1 - \eta)$ |
| TangentMasnadi-Shirazi et al. (2010) | $(2 \arctan(v) - 1)^2$ | $\arctan(v) + \frac{1}{2}$ | $\arctan(v) - \frac{1}{2}$ | $-4\eta(1 - \eta)$ |
Table 2: The $J((f^*_\phi)^{-1}(v))$, the domain of $v$ over which it is defined and the corresponding $J(\eta)$ and $(f^*_\phi)^{-1}(v)$.

| Loss       | $J((f^*_\phi)^{-1}(v))$ | $(f^*_\phi)^{-1}(v)$ | $J(\eta)$ | Domain       |
|------------|--------------------------|----------------------|------------|--------------|
| Zero-One-A | $-\min\{\frac{1}{e+e^v} 1 - \frac{1}{e+e^v}\}$ | $\frac{1}{(e^v - 1)^2}$ | $-\min\{\eta, 1 - \eta\}$ | $[-1 1]$     |
| Zero-One-B | $-\min\{\frac{1}{e+e^v} 1 - \frac{1}{e+e^v}\}$ | $\frac{1}{(e^v - 1)^2}$ | $-\min\{\eta, 1 - \eta\}$ | $[-\infty \infty]$ |
| LS         | $\frac{1}{e(v^2 - 1)}$    | $\frac{1}{e^v(v^2 - 1)}$ | $-2\eta(1 - \eta)$ | $[-1 1]$     |
| Exp        | $\sqrt{\frac{1}{e^v+e^v}}$ | $\sqrt{\frac{1}{e^v+e^v}}$ | $-\sqrt{\eta(1 - \eta)}$ | $[-\infty \infty]$ |
| Log        | $0.7213[\frac{1}{e^v} - \log(1 + e^v)]$ | $\frac{e^v}{e^v}$ | $0.7213[\eta \log(\eta) + (1 - \eta) \log(1 - \eta)]$ | $[-\infty \infty]$ |
| Savage     | $\frac{1}{e^v} - \frac{1}{e^v} \frac{1}{e^v}$ | $\frac{1}{e^v}$ | $-2\eta(1 - \eta)$ | $[-\infty \infty]$ |
| Tangent    | $2(\arctan(v))^2 - \frac{1}{1}$ | $\arctan(v) + \frac{1}{1}$ | $-2\eta(1 - \eta)$ | $[-\tan(\frac{1}{4}) \tan(\frac{1}{4})]$ |

and the refinement term can be written as

$$S_{\text{Refinement}} = \int \hat{\eta} s(\hat{\eta}) J(\hat{\eta}) d(\hat{\eta})$$

$$= \int_\eta s(\eta) J(\eta) d(\eta)$$

$$= \int_{(f^*_\phi)^{-1}(v)} s((f^*_\phi)^{-1}(v)) J((f^*_\phi)^{-1}(v)) d((f^*_\phi)^{-1}(v))$$

$$= \int_v s(v) \left((f^*_\phi)^{-1}(v)\right)' J((f^*_\phi)^{-1}(v)) (f^*_\phi)^{-1}(v)' dv$$

$$= \int_v s(v) J((f^*_\phi)^{-1}(v)) dv$$

For the special case of the proper margin Log loss of Table 1 we have

$$J(\eta) = 0.7213[\eta \log(\eta) + (1 - \eta) \log(1 - \eta)]$$

and

$$(f^*_\phi)^{-1}(v) = \frac{e^v}{1 + e^v} = \eta$$

so $J((f^*_\phi)^{-1}(v)) = J(\eta)$ can be simplified to

$$J((f^*_\phi)^{-1}(v)) = 0.7213 \left[ \frac{ve^v}{1 + e^v} - \log(1 + e^v) \right]$$

and is plotted in Figure 1. The $J((f^*_\phi)^{-1}(v))$ functions associated with the proper margin losses of Table 1 are presented in Table 2 and plotted in Figure 1. Refinement for the log loss can be written as

$$S_{\text{Refinement}} = \int_v s(v) J((f^*_\phi)^{-1}(v)) dv = 0.7213 \int_v s(v) \left[ \frac{ve^v}{1 + e^v} - \log(1 + e^v) \right] dv$$

where we reiterate that $s(v)$ is the distribution of the classifier’s predictions.

All of the plotted $J((f^*_\phi)^{-1}(v))$ functions in Figure 1 are quasi convex. This is shown to be always the case by considering the derivative

$$\frac{\partial J((f^*_\phi)^{-1}(v))}{\partial v} = \frac{\partial J((f^*_\phi)^{-1}(v))}{\partial (f^*_\phi)^{-1}(v)} \frac{\partial (f^*_\phi)^{-1}(v)}{\partial v}$$

$$= J'(((f^*_\phi)^{-1}(v)) \frac{\partial (f^*_\phi)^{-1}(v)}{\partial v}$$
and the fact that $(f_\phi)^{-1}(v)$ is a nondecreasing invertible function and $J(\eta)$ is convex. Since \( \frac{\partial (f_\phi)^{-1}(v)}{\partial \eta} > 0 \) and $J'((f_\phi)^{-1}(v))$ changes sign only once, the derivative of $J((f_\phi)^{-1}(v))$ also changes sign only once proving that $J((f_\phi)^{-1}(v))$ is quasi convex.

Given the quasi convex shape of $J((f_\phi)^{-1}(v))$, the refinement of a classifier increases when the distribution of the classifier predictions $s(\hat{\eta})$ is concentrated away from the decision boundary. A classifier with predictions that are concentrated further away from the boundary is preferable and the refinement of a classifier can be thought of as a measure of the classifier’s marginal density. This observation is formally considered in Section-7 and allows for the comparison of calibrated classifiers based solely on the distribution of their predictions.

We note that although the concept of classifier marginal density seems to be related to maximum margin theory Vapnik (1998) in classifier design, there are a few key differences. 1) Calibrated classifiers that are built from the same underlying data distribution will have the same classifier marginal density but can have different margins. The notion of margins is thus in contradiction to the axioms of probability theory, while the concept of classifier marginal density is not. 2) Margins are only defined for completely separable data, while classifier marginal density does not have such restrictions. 3) While the margin of a classifier considers only the data that lie on the margin, the notion of classifier marginal density considers the entire spread and distribution of the data.

6. Further Insight Into refinement In The Original Probability Elicitation Setting

The original refinement formulation is in the probability elicitation setting and was formulated as

$$ S_{Refinement} = \int_{\hat{\eta}} s(\hat{\eta}) J(\eta) d(\hat{\eta}) $$

in Section-2. As mentioned previously, it is intuitive that refinement increases as the distribution of the predictions $s(\hat{\eta})$ concentrates around $\hat{\eta} = 0$ and $\hat{\eta} = 1$. We formalize this intuition in this section and derive the maximum and minimum refinement scores using an inner product Hilbert space interpretation.
Real continuous functions $f(x)$ and $g(x)$ that are also square integrable form an inner product Hilbert space [David G (1969)] where the inner product is defined as

$$< f, g > = \int f(x)g(x)d(x)$$

with induced norm of

$$||f||^2 = \int (f(x))^2 d(x).$$

Let $\int |J(\eta)|^2 d(\eta) < \infty$ and $\int |s(\hat{\eta})|^2 d(\hat{\eta}) < \infty$ then $J(\eta)$ and $s(\hat{\eta})$ are square integrable functions. The inner product associated with this inner product Hilbert space is

$$< s, J > = \int_{\hat{\eta}} s(\hat{\eta})J(\eta)d(\hat{\eta}).$$

which is equal to the original refinement formulation of (50). In other words refinement computes the inner product between the two functions $J(\eta)$ and $s(\hat{\eta})$. As seen in Table-1 $J(\eta) \leq 0$ and $s(\hat{\eta}) \geq 0$ since $s(\hat{\eta})$ is a probability distribution function. This constrains the refinement score to $< s, J > \leq 0$. The maximum and minimum refinement scores for a fixed $J(\eta)$ can now be computed by considering the inner product between a fixed $J(\eta)$ and a distribution of prediction functions $s(\hat{\eta})$. Specifically the minimum refinement score is

$$S_{Min}^{Refinement} = < s, J > = ||s| | \cdot ||J| | \cdot \cos(\theta) = \alpha||J| | \cdot ||J| | \cdot (-1) = -\alpha||J| |^2$$

and corresponds to when $s = -\alpha J$ for some multiple $\alpha$. The maximum refinement score is

$$S_{Max}^{Refinement} = < s, J > = ||s| | \cdot ||J| | \cdot \cos(\theta) = ||s| | \cdot ||J| | \cdot (0) = 0$$

and corresponds to when $s \perp J$.

Usually, the score functions $I_1$ and $I_{-1}$ are chosen to be symmetric such that $I_1(\eta) = I_{-1}(1-\eta)$ so that the scores attained for predicting either class $y = \{1, -1\}$ remain class insensitive. In this case the corresponding $J(\eta)$ is also symmetric such that $J(\eta) = J(1-\eta)$. This can be confirmed by noting that

$$J(1-\eta) = (1-\eta)I_1(1-\eta) + (1-1+\eta)I_{-1}(1-\eta)$$

$$= (1-\eta)I_{-1}(\eta) + \eta I_1(\eta) = J(\eta).$$

When $J(\eta) \leq 0$ is convex symmetric over $\eta \in \{0, 1\}$ then $J(\eta)$ is minimum at $\eta = \frac{1}{2}$ and $J(0) = J(1) = 0$ and the maximum refinement score verifiably corresponds to when all of the predictions are either 0 or 1 such that $s(\hat{\eta}) = \gamma \delta(\hat{\eta}) + (1-\gamma)\delta(1-\hat{\eta})$ where $0 \leq \gamma \leq 1$. The $s(\hat{\eta})$ pertaining to the cases of maximum and minimum refinement are plotted for a hypothetical symmetric $J(\eta)$ in Figure-2.
7. Further Insight Into Refinement In The Classifier Output Setting

In Section 5 we stated that when considering refinement in the classifier outputs setting under the formulation of (44), refinement increases as \( s(v) \) is concentrated away from the boundary. This can be formally addressed by letting \( s(v) \) and \( J((f_\phi^*)^{-1}(v)) \) be square integrable functions that form an inner product Hilbert space with inner product

\[
< s, J > = \int s(v)J((f_\phi^*)^{-1}(v))d(v). \tag{57}
\]

This is equal to the refinement formulation of (44) associated with the classifier output setting. An argument similar to that of Section 6 leads to the conclusion that refinement in the classifier output setting is minimum when the distribution of classifier outputs \( s(v) = -\alpha J((f_\phi^*)^{-1}(v)) \), increases as \( s(v) \) concentrates away from the decision boundary and is maximum when \( s(v) = \lim_{t \to \infty} \gamma \delta(v-t)+(1-\gamma)\delta(v+t) \) where \( 0 \leq \gamma \leq 1 \).

8. Further Insight Into Refinement In The Underlying Data Distribution Setting

In Section 3.2 we showed that the refinement score can be reduced to the underlying data distribution setting as

\[
S_{\text{Refinement}} = \int_X P_X(x)J(P(1|x))dx. \tag{58}
\]

Here we expand on this formulation and formalize its connections to the Bayes error and eventually derive novel measures that provide arbitrarily tighter bounds on the Bayes error.

First we show that refinement in the data distribution setting is also an inner product Hilbert space with inner product defined as

\[
< P_X, J > = \int_X P_X(x)J(P(1|x))dx. \tag{59}
\]

This follows directly from letting \( P_X(x) \) and \( J(P(1|x)) \) be square integrable functions which is not a stringent constraint since most probability density functions are square integrable Tang et al. (2000). We also directly show that \( J(P(1|x)) \leq 0 \) is quasi convex over \( x \). This follows from

\[
\frac{\partial J(P(1|x))}{\partial x} = \frac{\partial J(P(1|x))}{\partial P(1|x)} \frac{\partial P(1|x)}{\partial x} = J'(P(1|x)) \frac{\partial P(1|x)}{\partial x}, \tag{60}
\]
the fact that \( \eta(x) = P(1|x) \) is an invertible and hence monotonic function from \([1,1] \) and \( J(\eta) \) is convex. Since \( \frac{\partial P(1|x)}{\partial x} > 0 \) \( \forall x \) or \( \frac{\partial P(1|x)}{\partial x} < 0 \) \( \forall x \) and \( J'(P(1|x)) \) changes sign only once, the derivative of \( J(P(1|x)) \) also changes sign only once proving that \( J(P(1|x)) \) is quasi convex.

Once again, refinement in the data distribution setting \( \beta P_X, J \geq 0 \) is minimum when \( P_X(x) = -\alpha J(P(1|x)) \), and is maximum and equal to zero when \( P_X(x) \perp J(P(1|x)) \).

Assuming equal priors \( P(1) = P(-1) = \frac{1}{2} \),

\[
P(x) = \frac{P(x|1) + P(x|-1)}{2}
\]  

(61)

and

\[
P(1|x) = \frac{P(x|1)}{P(x|1) + P(x|-1)}.
\]  

(62)

We can write refinement in terms of the underlying data distributions \( P(x|1) \) and \( P(x|-1) \) as

\[
S_{\text{Refinement}} = \int_X \left( \frac{P(x|1) + P(x|-1)}{2} \right) J \left( \frac{P(x|1)}{P(x|1) + P(x|-1)} \right) dx.
\]  

(63)

For example under the least squares \( J_{LS}(P(1|x)) = 2P(1|x)(P(1|x) - 1) \), the refinement formulation simplifies to

\[
S_{\text{Refinement}}^{LS} = \int \frac{-P(x|1)P(x|-1)}{(P(x|1) + P(x|-1))} dx.
\]  

(64)

Plot 3 shows the \( P(x), J(P(1|x)) \) and \( P(x)J(P(1|x)) \) terms for three Gaussian distributions of unit variance and means of \( \mu = \pm 0.1, \mu = \pm 1.5 \) and \( \mu = \pm 4 \). In accordance with the inner product interpretation, as the means separate and the two distributions \( P(x|1) \) and \( P(x|-1) \) have less overlap, the refinement increases (is less negative) and approaches zero.

In Table 3, we have derived the refinement formulation for the different \( J(P(1|x)) \) of Table 4, which are plotted in Figure 4. Refinement for the zero-one maximum conditional score function

\[
J_{0/1}(\eta) = \begin{cases} 
-\frac{1}{2} - \frac{1}{2}, & \text{if } \eta \geq \frac{1}{2}; \\
-\eta, & \text{if } \eta < \frac{1}{2},
\end{cases}
\]  

(65)

is

\[
S_{\text{Refinement}}^{0/1} = \int P(x)J_{0/1}(P(1|x))dx =
\]

\[
\int_{P(1|x) \geq \frac{1}{2}} \left( \frac{P(x|1) + P(x|-1)}{2} \right) \left( -\frac{1}{2} - \frac{P(x|1)}{P(x|1) + P(x|-1)} \right) dx +
\]

\[
\int_{P(1|x) < \frac{1}{2}} \left( \frac{P(x|1) + P(x|-1)}{2} \right) \left( -\frac{P(x|1)}{P(x|1) + P(x|-1)} \right) dx =
\]

\[
-\frac{1}{2} \int_{P(1|x) \geq \frac{1}{2}} P(x|-1) dx - \frac{1}{2} \int_{P(1|x) < \frac{1}{2}} P(x|1) dx = -\frac{1}{2}(\epsilon_1 + \epsilon_2) = -\epsilon
\]
Figure 3: Plot of the $J_{LS}$ refinement terms for three different unit variance Gaussians.

where $\epsilon_2$ is the miss rate, $\epsilon_1$ is the false positive rate and $\epsilon$ is the Bayes error rate. In other words, refinement under the zero-one $J_{0/1}(\eta)$ is equal to minus the Bayes error. When refinement is computed under the other $J(\eta)$ of Table 4, an upper bound on the Bayes error is being computed. This can be formally written as

$$S_{0/1}^{\text{Refinement}} - S_{\text{Refinement}}^{J(\eta)} = \epsilon - S_{\text{Refinement}}^{J(\eta)}$$

$$\int_x P_X(x) J_{0/1}(P(1|x)) dx - \int_x P_X(x) J(P(1|x)) dx = \int_x P_X(x) \left( J_{0/1}(P(1|x)) - J(P(1|x)) \right) dx.$$  

In other words, the $J(\eta)$ that are closer to the $J_{0/1}(\eta)$ result in refinement formulations that provide tighter bounds on the Bayes error. Figure 4 shows that $J_{LS}$, $J_{Cosh}$, $J_{Sec}$, $J_{Log}$, $J_{Log-Cos}$ and $J_{Exp}$ are in order the closest to $J_{0/1}$ and the corresponding refinement formulations in Table 4 provide in the same order tighter bounds on the Bayes error. This can also be directly verified by noting that $S_{Exp}$ is equal to the Battacharyy bound [Fukunaga, 1990], $S_{LS}$ is equal to the asymptotic nearest neighbor bound [Fukunaga, 1990; Cover and Hart, 1967] and $S_{Log}$ is equal to the Jensen-Shannon divergence [Lin, 1991]. These three formulations have been independently studied throughout the literature and the fact that they produce upper bounds on the Bayes error have been directly verified. Here we have rederived the three measures by resorting to the concept of refinement which not only allows us to provide a unified approach to these different methods but has also led to a systematic method for deriving novel refinement measures or bounds on the Bayes error, namely the $S_{Cosh}$, $S_{Log-Cos}$ and the $S_{Sec}$. 

18
Table 3: Refinement measure for different $J(\eta)$

| $J(\eta)$ | $S_{\text{Refinement}}$ |
|-----------|-----------------|
| Zero-One  | Bayes Error     |
| LS        | $\int_x -P(x|1)P(x|-1) dx$ |
| Exp       | $-\frac{1}{2} \int_x \sqrt{P(x|1)P(x|-1)} dx$ |
| Log       | $\frac{0.7213}{2} D_{KL}(P(x|1)||P(x|1) + P(x|-1)) + \frac{0.7213}{2} D_{KL}(P(x|-1)||P(x|1) + P(x|-1))$ |
| Log-Cos   | $\int_x \frac{P(x|1)+P(x|-1)}{2} \left[ -\frac{1}{2.5854} \log \left( \frac{\cos(\frac{2.5854}{2}(\eta-1))}{\cos(\frac{2.5854}{2})} \right) \right] dx$ |
| Cosh      | $\int_x \frac{P(x|1)+P(x|-1)}{2} \left[ \cosh\left(\frac{1.9248(P(x|-1)-P(x|1))}{2(P(x|1)+P(x|-1))}\right) - \cosh\left(\frac{-1.9248}{2}\right) \right] dx$ |
| Sec       | $\int_x \frac{P(x|1)+P(x|-1)}{2} \left[ \sec\left(\frac{1.6821(P(x|-1)-P(x|1))}{2(P(x|1)+P(x|-1))}\right) - \sec\left(\frac{-1.6821}{2}\right) \right] dx$ |

Table 4: $J$ specifics used to compute the refinement score.

| Method | $J(\eta)$ |
|--------|------------|
| LS     | $2\eta(\eta - 1)$ |
| Log    | $0.7213(\eta \log(\eta) + (1 - \eta) \log(1 - \eta))$ |
| Exp    | $-\sqrt{\eta(\eta - 1)}$ |
| Log-Cos| $(\frac{-1}{2.5854}) \log\left(\frac{\cos(2.5854(\eta-1))}{\cos(2.5854)}\right)$ |
| Cosh   | $\cosh(1.9248(\frac{1}{2} - \eta)) - \cosh\left(\frac{-1.9248}{2}\right)$ |
| Sec    | $\sec(1.6821(\frac{1}{2} - \eta)) - \sec\left(\frac{-1.6821}{2}\right)$ |
9. Measures With Tighter Bounds On The Bayes Error

Although the three novel refinement score functions discussed above provide relatively tighter upper bounds on the Bayes error, they do not produce the tightest bounds. In Table 4, $J_{LS}(\eta)$ provides the closest approximation to $J_{0/1}(\eta)$, thus resulting in a tighter bound. A natural question is if the refinement approach can be used to derive formulations that provide even tighter bounds on the Bayes error. In order to do so, (67) states that we simply need to find $J(\eta)$ that are closer approximations to $J_{0/1}(\eta)$. In this section we derive polynomial functions $J_{Poly}(\eta)$ that are arbitrarily close approximations to $J_{0/1}(\eta)$ thus leading to measures that have the tightest bounds on the Bayes error.

The Weierstrass approximation theorem [Bartle 1976; Burden and Faires 2010] states that for a continuous function $f(x)$ defined on $[a, b]$ there exists a polynomial $P(x)$ that is as close to $f(x)$ as desired such that

$$|f(x) - P(x)| < \epsilon, \forall x \in [a, b].$$

With $J_{0/1}(\eta)$ as the target function, we demonstrate a general procedure for deriving a class of polynomial functions $J_{Poly-n}(\eta)$ that are as close to $J_{0/1}(\eta)$ as desired. As an example, we derive the $J_{Poly-2}(\eta)$ which leads to the $S_{Poly-2}$ bound on the Bayes error which is a tighter bound on the Bayes error than $J_{LS}(\eta)$. We also derive the $S_{Poly-4}$ bound which is an even tighter bound and show that $J_{LS} = J_{Poly-0}$.

When $J(\eta)$ is convex symmetric over $\eta \in \{0, 1\}$ then $J(\eta)$ is minimum at $\eta = \frac{1}{2}$ and so $J'(\frac{1}{2}) = 0$. The symmetry $J(\eta) = J(1-\eta)$ results in a similar constrain on the second derivative $J''(n) = J''(1-\eta)$ and convexity requires that the second derivative satisfy $J''(\eta) > 0$. The symmetry and convexity constraint can both be satisfied by considering

$$J''_{Poly-n}(\eta) = (\eta(1-\eta))^n$$

where $n$ is an even number. From this we write

$$J'_{Poly-n}(\eta) = \int (\eta(1-\eta))^n d(\eta) + K_1 = Q(\eta) + K_1.$$
Satisfying the constraint that \( J_{Poly-n}(\frac{1}{2}) = 0 \), we find \( K_1 \) as

\[
K_1 = -\int (\eta(1-\eta))^n d(\eta) \bigg|_{\eta=\frac{1}{2}} = -Q(\frac{1}{2}). \tag{71}
\]

Finally, \( J_{Poly-n}(\eta) \) is

\[
J_{Poly-n}(\eta) = K_2 \left( \int Q(\eta)d(\eta) + K_1 \eta \right) = K_2 \left( R(\eta) + K_1 \eta \right), \tag{72}
\]

where \( K_2 \) is a scaling factor such that

\[
K_2 =\frac{-0.5}{(\int Q(\eta)d(\eta) + K_1 \eta)|_{\eta=\frac{1}{2}}} \tag{73}
\]

In other words this scaling factor is set to satisfy \( J_{Poly-n}(\frac{1}{2}) = J_{0/1}(\frac{1}{2}) = -\frac{1}{2} \).

As an example, we derive \( J_{Poly-2}(\eta) \). Following the procedure above

\[
J''_{Poly-2}(\eta) = (\eta(1-\eta))^2 = \eta^2 + \eta^4 - 2\eta^3 > 0. \tag{74}
\]

From this we have

\[
J'_{Poly-2}(\eta) = \frac{1}{3} \eta^3 + \frac{1}{5} \eta^5 - \frac{2}{4} \eta^4 + K_1. \tag{75}
\]

Satisfying \( J'_{Poly-2}(\frac{1}{2}) = 0 \) we find \( K_1 = -0.0167 \). Therefore,

\[
J_{Poly-2}(\eta) = K_2 \left( \frac{1}{12} \eta^4 + \frac{1}{30} \eta^6 - \frac{1}{10} \eta^5 + (-0.0167)\eta \right). \tag{76}
\]

Satisfying \( J_{Poly-2}(\frac{1}{2}) = -\frac{1}{2} \) we find \( K_2 = 87.0196 \).

Figure 5 plots \( J_{Poly-2}(\eta) \) which shows that, as expected, it is a closer approximation to \( J_{0/1}(\eta) \) when compared to \( J_{LS}(\eta) \). Following the same steps, it is readily shown that \( J_{LS}(\eta) = J_{Poly-0}(\eta) \), meaning that \( J_{LS}(\eta) \) is derived from the special case of \( n = 0 \). As we increase \( n \), we increase the order of the resulting polynomial which provides a tighter fit to \( J_{0/1}(\eta) \). Figure 5 also plots \( J_{Poly-4}(\eta) \)

\[
J_{Poly-4}(\eta) = 1671.3(\frac{1}{90} \eta^{10} - \frac{1}{18} \eta^9 + \frac{3}{28} \eta^8 - \frac{2}{21} \eta^7 + \frac{1}{30} \eta^6 + (-7.9365 \times 10^{-4})\eta)
\]

and we see that this provides an even closer approximation to \( J_{0/1}(\eta) \). Table 5 shows the corresponding refinement measure for each of the \( J_{Poly-n}(\eta) \) functions, with \( S_{Poly-4} \) providing the tightest bound on the Bayes error. Arbitrarily tighter bounds are possible by simply using \( J_{Poly-n} \) with larger \( n \).
Figure 5: Plot of $J_{\text{Poly}-n}(\eta)$.

Table 5: Refinement measure for different $J_{\text{Poly}-n}(\eta)$

| $J(\eta)$  | $S_{\text{Refinement}}$ |
|------------|-------------------------|
| Zero-One   | $\int \frac{-P(x|1)P(x|-1)}{P(x|1)+P(x|-1)} dx$ |
| Poly-0 (LS)| $\frac{K_2}{2} \int \frac{P(x|1)^5}{12(2P(x)^8)} + \frac{P(x|1)^6}{30(2P(x)^9)} + \frac{P(x|1)^7}{10(2P(x)^8)^2} - K_1 P(x|1) dx$ $\frac{K_1 = 0.0167, K_2 = 87.0196, P(x) = \frac{P(x|1)+P(x|-1)}{2}}$ |
| Poly-2     | $\frac{K_2}{2} \int \frac{P(x|1)^6}{90(2P(x)^9)} - \frac{P(x|1)^5}{45(2P(x)^9)} + \frac{3P(x|1)^7}{45(2P(x)^9)} - 2P(x|1)^5} + \frac{P(x|1)^6}{90(2P(x)^9)^2} - K_1 P(x|1) dx$ $\frac{K_1 = 7.9365 \times 10^{-4}, K_2 = 1671.3, P(x) = \frac{P(x|1)+P(x|-1)}{2}}$ |
| Poly-4     | $\frac{K_2}{2} \int \frac{P(x|1)^7}{90(2P(x)^9)} - \frac{P(x|1)^6}{45(2P(x)^9)} + \frac{3P(x|1)^8}{45(2P(x)^9)} - 2P(x|1)^5} + \frac{P(x|1)^6}{90(2P(x)^9)^2} - K_1 P(x|1) dx$ $\frac{K_1 = 7.9365 \times 10^{-4}, K_2 = 1671.3, P(x) = \frac{P(x|1)+P(x|-1)}{2}}$ |

10. Conclusion

The concept of refinement was first established in the probability elicitation literature and despite its close connections to proper scoring functions, has largely remained restricted to the forecasting literature. In this work we have revisited this important statistical measure from the viewpoint of machine learning. In particular, this concept is first considered from a fundamental perspective with the basic axioms of probability. This deeper understanding of refinement is used as a guide to extend refinement from the original probability elicitation setting to two novel formulations namely the underlying data distribution and classifier output settings. These three refinement measures were then shown to be inner products in their respective Hilbert spaces. This unifying abstraction was then used to connect ideas such as maximum marginal diversity, conditional entropy, calibrated
classifiers and Bayes error. Specifically we showed that maximal marginal diversity and conditional entropy are special cases of refinement in the underlying data distribution setting and introduced conditional refinement. Also a number of novel refinement measures were presented for the comparison of classifiers under the classifier output setting. Finally, refinement in the underlying data distribution setting was used in a general procedure for deriving arbitrarily tight bounds on the Bayes error.

References

Robert G. Bartle. *The Elements of Real Analysis (Second Edition)*. John Wiley and Sons, New York, 1976.

Jochen Brcker. Reliability, sufficiency, and the decomposition of proper scores. *Quarterly Journal of the Royal Meteorological Society*, 135(643):1512–1519, 2009.

A. Buja, W. Stuetzle, and Y. Shen. Loss functions for binary class probability estimation and classification: Structure and applications. *(Technical Report) University of Pennsylvania*, 2005.

Richard L. Burden and J. Douglas Faires. *Numerical Analysis (Ninth Edition)*. Brooks Cole, Boston, 2010.

T. Cover and P. Hart. Nearest neighbor pattern classification. *IEEE Transactions on Information Theory*, 13(1):21–27, 1967.

Luenberger David G. *Optimization By Vector Space Methods*. John Wiley and Sons, New York, 1969.

A.P. Dawid. The well-calibrated bayesian. *Journal of the American. Statistical Association*, 77:605–610, 1982.

M.H. DeGroot. Comments on lindley, et al. *Journal of Royal Statistical Society (A)*, 142:172–173, 1979.

M.H. DeGroot and S.E. Fienberg. Assessing probability assessors: calibration and refinement. *Statistical Decision Theory and Related Topics III*, 1:291–314, 1982.

Morris H. DeGroot and Stephen E. Fienberg. The comparison and evaluation of forecasters. *The Statistician*, 32:14–22, 1983.

Francois Fleuret and Isabelle Guyon. Fast binary feature selection with conditional mutual information. *Journal of Machine Learning Research*, 5:1531–1555, 2004.

Y. Freund and R. Schapire. A decision-theoretic generalization of on-line learning and an application to boosting. *Journal of Computer and System Sciences*, 55:119139, 1997.

J. Friedman, T. Hastie, and R. Tibshirani. Additive logistic regression: A statistical view of boosting. *Annals of Statistics*, 28:337–407, 2000.

Keinosuke Fukunaga. *Introduction to Statistical Pattern Recognition, Second Edition*. Academic Press, San Diego, 1990.
T. Gneiting and A.E. Raftery. Strictly proper scoring rules, prediction, and estimation. *Journal of the American Statistical Association*, 102:359–378, 2007.

T. Gneiting, A. E. Raftery, A. H. Westveld, and T. Goldman. Calibrated probabilistic forecasting using ensemble model output statistics and minimum crps estimation. *Monthly Weather Review*, 133:1098–1118, 2005.

Tilmann Gneiting, Fadoua Balabdaoui, and Adrian E. Raftery. Probabilistic forecasts, calibration and sharpness. *Journal of the Royal Statistical Society Series B*, pages 243–268, 2007.

E. T. Jaynes and G. Larry Bretthorst. *Probability Theory: The Logic of Science*. Cambridge University Press, Cambridge, 2003.

Jianhua Lin. Divergence measures based on the shannon entropy. *IEEE Transactions on Information Theory*, 37:145–151, 1991.

Hamed Masnadi-Shirazi and Nuno Vasconcelos. On the design of loss functions for classification: theory, robustness to outliers, and savageboost. In *Advances in Neural Information Processing Systems*, pages 1049–1056. MIT Press, 2008.

Hamed Masnadi-Shirazi, Vijay Mahadevan, and Nuno Vasconcelos. On the design of robust classifiers for computer vision. In *Computer Vision and Pattern Recognition, IEEE Conference on*, pages 779–786, 2010.

A.H. Murphy. Scalar and vector partitions of the probability score: part i. two-state situation. *Journal of applied Meteorology*, 11:273–82, 1972.

A. Niculescu-Mizil and R. Caruana. Obtaining calibrated probabilities from boosting. In *Uncertainty in Artificial Intelligence*, 2005.

Hanchuan Peng, Fuhui Long, and Chris Ding. Feature selection based on mutual information: criteria of max-dependency, max-relevance, and min-redundancy. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 27:1226–1238, 2005.

J. Platt. Probabilistic outputs for support vector machines and comparison to regularized likelihood methods. In *Adv. in Large Margin Classifiers*, pages 61–74, 2000.

Mark Reid and Robert Williamson. Composite binary losses. *The Journal of Machine Learning Research*, 11:2387–2422, 2010.

F. Sanders. On subjective probability forecasting. *Journal of applied Meteorology*, 2:191–201, 1963.

Leonard J. Savage. The elicitation of personal probabilities and expectations. *Journal of The American Statistical Association*, 66:783–801, 1971.

M.J. Schervish. A general method for comparing probability assessors. *Annals of Statistics*, 17:1856–1879, 1989.

Y.Y. Tang, L.H. Yang, J. Liu, and H. Ma. *Wavelet Theory and Its Application to Pattern Recognition*. World Scientific Publishing, Singapore, 2000.
Vladimir N. Vapnik. *Statistical Learning Theory*. John Wiley Sons Inc, 1998.

Manuela Vasconcelos and Nuno Vasconcelos. Natural image statistics and low-complexity feature selection. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 31:228–244, 2009.

Nuno Vasconcelos. Feature selection by maximum marginal diversity. In *Advances in Neural Information Processing Systems*, pages 1351–1358, 2002.

Nuno Vasconcelos. Feature selection by maximum marginal diversity: optimality and implications for visual recognition. In *Computer Vision and Pattern Recognition, IEEE Computer Society Conference*, pages 762–769, 2003.

D. S. Wilks. Comparison of ensemble-mos methods in the lorenz ’96 setting. *Meteorological Applications*, 13(3):243–256, 2006.

Tong Zhang. Statistical behavior and consistency of classification methods based on convex risk minimization. *Annals of Statistics*, 32:56–85, 2004.