Extrapolating expected accuracies for multi-class classification

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Abstract

The difficulty of multi-class classification generally increases with the number of classes. Using data from a subset of the classes, can we predict how well a classifier will scale with an increased number of classes? Under the assumption that the classes are sampled exchangeably, and under the assumption that the classifier is generative (e.g. QDA or Naive Bayes), we show that the expected accuracy when the classifier is trained on k classes is the $k-1$st moment of a *conditional accuracy distribution*, which can be estimated from data. This provides the theoretical foundation for performance extrapolation based on pseudolikelihood, unbiased estimation, and high-dimensional asymptotics. We investigate the robustness of our methods to non-generative classifiers in simulations and one optical character recognition example.

1 Introduction

An algorithm that can use sensory information to automatically distinguish between multiple scenarios has increasingly many applications in modern life. Examples include detecting the speaker from his voice patterns, identifying the author from her written text, or labeling the object category from its image. All these examples can be described as multi-class classification problems: the algorithm observes an input x, and uses the classifier function f to guess the label y from a discrete set $\mathcal{Y}$ of possible labels. In all applications described above, the space of potential labels is practically infinite.

But in any particular experiment, the number of different labels k used would be finite. A natural question, then, is how changing the number of possible labels affects the classification accuracy.

More technically, we consider a sequence of classification problems on finite label subsets $\mathcal{S}_1 \subset \cdots \subset \mathcal{S}_K \subset \mathcal{Y}$, where in the i-th problem, one constructs the classification rule $f^{(i)} : \mathcal{X} \to \mathcal{S}_i$. Supposing that (X, Y) have a joint distribution, define the misclassification error for the i-th problem as

$$\text{Err}^{(i)} = \Pr[f^{(i)}(X) \neq Y | Y \in \mathcal{S}_i].$$

The problem of *performance extrapolation* is the following: using data from only $\mathcal{S}_k$, can one predict the misclassification error on the larger label set $\mathcal{S}_K$, with $K > k$? Note that unlike other extrapolations from a smaller sample to a larger population, the classification problem becomes harder as the number of distractor classes increases.

Accurate answers to this problem are not only of theoretical interest, but also have practical implications:

- Example 1: A researcher develops a classifier for the purpose of labelling images in 10,000 classes. However, for a pilot study, her resources are sufficient to tag only a smaller subset of these classes, perhaps 100. Can she estimate how well the algorithm work on the full set of classes based on an initial ”pilot” subsample of class labels?

- Example 2: A neuroscientist is interested in how well the brain activity in various regions of the brain can discriminate between different classes of stimuli. Kay et al. [1] obtained fMRI brain scans which record how a single subject's visual cortex responds to natural images. They wanted to know how well the brain signals could discriminate between different images. For a set of 1750 photographs, they constructed a classifier which achieved over 0.75 accuracy of classification. Based on exponential extrapolation, they estimate that it would take on the order of $10^{9.5}$ classes before the accuracy of the model drops below 0.10! A theory of performance extrapolation could be useful for the purpose of making such extrapolations in a more principled way.

- The stories just described can be viewed as a metaphor for typical paradigm of machine learning research, where academic researchers, working under limited resources, develop novel algorithms and apply

> them to relatively small-scale datasets. Those same algorithms may then be adopted by companies and applied to much larger datasets with many more classes. In this scenario, it would be convenient if one could simply assume that performance on the smaller-scale classification problems was highly representative of performance on larger-scale problems.

Previous works have shown that generalizing from a small set of classes to a larger one is not straightforward. In a paper titled "What does classifying more than 10,000 Image Categories Tell Us," Deng and co-authors compared the performance of four different classifiers on three different scales: a small-scale (1,000-class) problem, medium-scale (7,404-class) problem, and large-scale (10,184-class) problem (all from ImageNet.) They found that while the nearest-neighbor classifier outperformed the support vector machine classifier (SVM) in the small and medium scale, the ranking switched in the large scale, where the SVM classifier outperformed nearest-neighbor. As they write in their conclusion, "we cannot always rely on experiments on small datasets to predict performance at large scale." Theory for performance extrapolation may therefore reveal models with bad scaling properties in the pilot stages of development.

Our primary goal in this paper is to formulate this question, and identify scenarios where answers are possible. The most important condition is that the smaller problem would be representative of the larger one. For simplicity, we assume that in both $\mathcal{S}_K$ and $\mathcal{S}_k$ are iid samples from a population (or distribution) of labels. (Other sampling mechanisms would require some modification). The condition of i.i.d. sampling of labels ensures that the separation of labels in a random set $\mathcal{S}_K$ can be inferred by looking at the empirical separation in $\mathcal{S}_k$, and therefore that some estimate of the achievable accuracy on $\mathcal{S}_K$ can be obtained.

Our analysis considers a restricted set of classifiers, *marginal classifiers*, which train a separate model for each class. This convenient property allows us to characterize the accuracy of the classifier by selectively conditioning on one class at a time. In section **??**, we use this technique to reveal that the expected risk for classifying on the label set $\mathcal{Y}_k$, for all k, is governed by a specific function - the *conditional risk* - that depends on the true distributions and the classifier. As long as one can recover the conditional risk function $\bar{D}(u)$, one can compute the average risk for any number of classes. In section 5, we empirically study the performance curves of classifiers on sequences of classification tasks. Since marginal classifiers only comprise a minority of the classifiers used in practice, we applied our methods to a variety of marginal and non-marginal classifiers in simulations and in one OCR dataset. Our methods have varying success on marginal and non-marginal classifiers, but seem to work badly for neural networks.

Our contribution.

To our knowledge, we are the first to formalize the problem of prediction extrapolation. We develop a general theory for prediction extrapolation under *general class priors* and under bounded cost functions. [[TODO: mention estimation results, theory]]

2 Framework

2.1 Problem Formulation

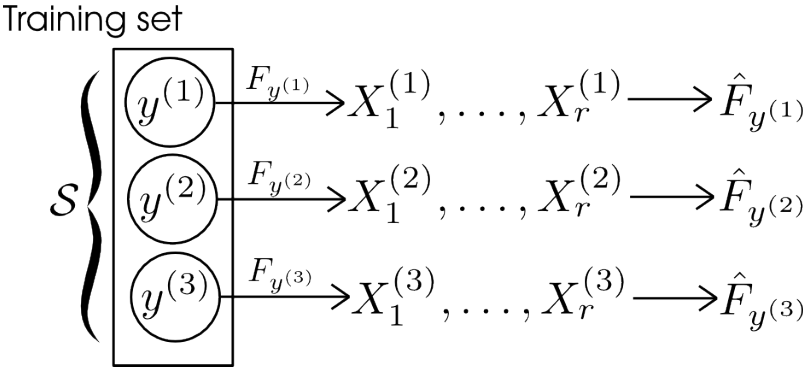


Figure 1: Training set

A *classification task* consists of a subset of labels, $\mathcal{S} \subset \mathcal{Y}$. Write $\mathcal{S} = \{y_1, \dots, y_k\}$, where k is the number of classes. It is convenient to decouple the joint distribution of (X, Y) into a prior distribution over the k labels $\mathcal{S}_k$, and the conditional distribution of elements, or feature vectors describing them, within a label class $X|Y = y \sim F_y$.

We would like to identify the sources of randomness in evaluating a classifier. First, there is the specific choice of k classes for the label set. Second, there is randomness in training the classifier for these classes, which comes

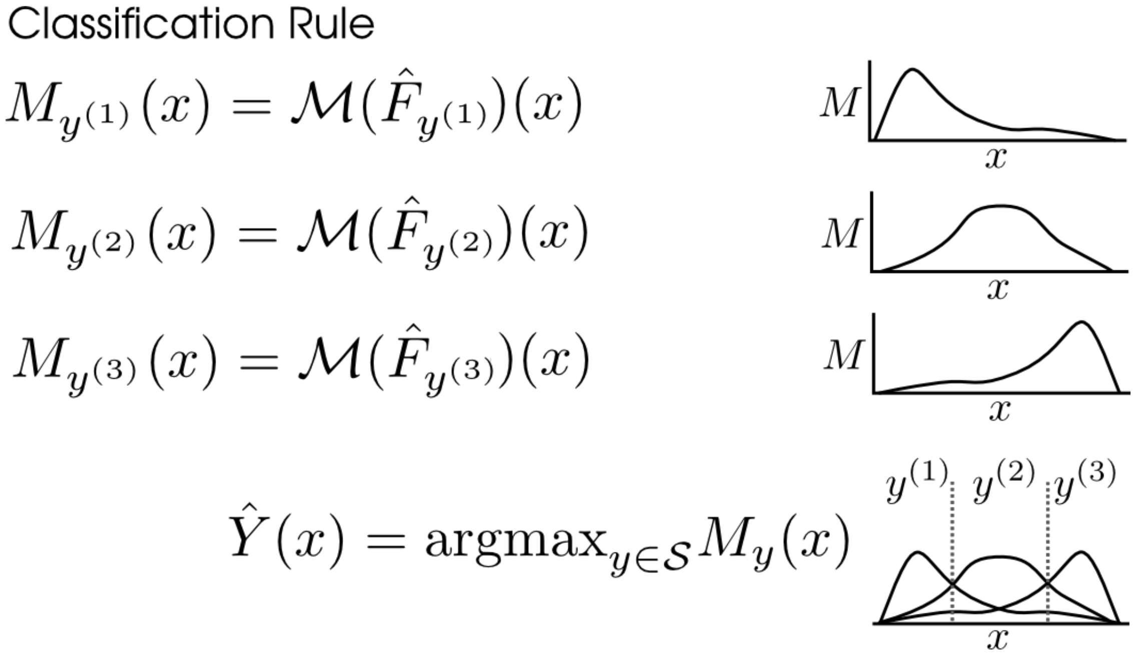

Classification Rule
$M_{y^{(1)}}(x) = \mathcal{M}(\hat{F}_{y^{(1)}})(x)$
M
x
$M_{y^{(2)}}(x) = \mathcal{M}(\hat{F}_{y^{(2)}})(x)$
M
x
$M_{y^{(3)}}(x) = \mathcal{M}(\hat{F}_{y^{(3)}})(x)$
M
x
$\hat{Y}(x) = \text{argmax}_{y \in \mathcal{S}} M_y(x)$
$y^{(1)}$
$y^{(2)}$
$y^{(3)}$
x

Figure 2: Classification rule

from the use of a finite training set. Third, there is the randomness in the observed accuracy when testing the classifier on a test set. In order to separate these three sources, we need to clarify some terms used ambiguously in the classification literature.

We call a *classification rule* a function f which maps feature vectors $x \in \mathcal{X}$ to the set of labels $\mathcal{S}$:

$$f : \mathcal{X} \to \mathcal{S}.$$

For a random class Y drawn according to the uniform distribution[1] on $\mathcal{S}$ and a feature vector drawn under F_Y, the loss of $\ell(f(X), Y)$ is obtained. The *risk*, or expected loss, of the classification rule is

$$\text{Risk}(f; \pi, \ell) = \int \ell(f(X), Y) dF_Y d\pi.$$

For now, we will assume a 0–1 loss and a uniform prior over the labels in $\mathcal{S}$.

[1] See the discussion for extensions to non-uniform priors.

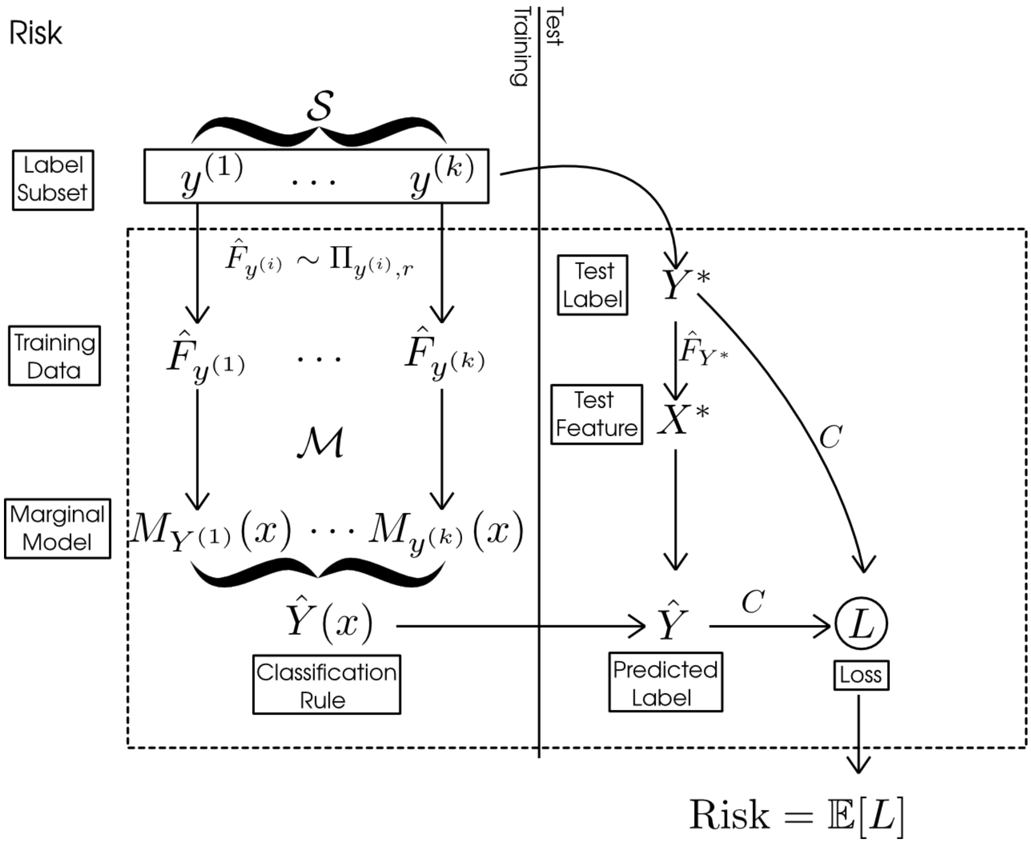


Figure 3: Classification risk

Therefore, the risk can be rewritten as

$$\text{Risk}(f; \mathcal{S}, \ell_{01}) = \frac{1}{k} \sum_{y_i \in \mathcal{S}} \Pr(f(X) \neq y_i; X \sim F_{y_i}).$$

The classification rule itself can be seen as a random function that depends on the sampling of the training set. For convenience, assume that the training set is composed of r i.i.d examples for each label $y \in \mathcal{S}$ (a total of $k \times r$). An i.i.d. sample of size r, $X_1, \ldots, X_r \sim F_y$ can also be described as an empirical distribution, using the shorthand $\hat{F}_y$. [[TODO: Should r appear in the notation for $\hat{F}_y$?]].

$$\hat{F}_y = \frac{1}{r} \sum_{i=1}^{r} \delta_{x_i^{(y)}}.$$

A *classifier* $\mathcal{F}$ is the algorithm or procedure for producing classification rules given a vector of empirical distributions $(\hat{F}_y)_{y \in \mathcal{S}}$. The classifier maps the empirical distributions to a classification rule f (Figure 2).

We can therefore describe the r-repeat risk of the model $\mathcal{F}$ as the expected risk of a classification rule $\hat{f}$ trained using a sample of size r from each of labels in $\mathcal{S}_k$. That is,

$$\text{Risk}_r(\mathcal{F}; \pi) = \int \text{Risk}(\mathcal{F}(\{\hat{F}_y\}_{y \in \mathcal{S}}; \mathcal{S}, \ell) \prod_{y \in \mathcal{S}} d\Pi_{y,r}(\hat{F}_y).$$

Figure 3 illustrates the variables involved in defining the risk.

The problem of *performance extrapolation* can now be formally defined as follows: Given a known classification task $\mathcal{S}_{k_1} = \{y_1, ..., y_{k_1}\}$ with an observed r-repeat training set and r_{test} test set per class, can we estimate the expected r-repeat risk of the classifier $\mathcal{F}$ on a second classification task with k_2 labels?

2.2 Assumptions

Implicit in our definition of performance extrapolation is that the new set of k_2 is partially or fully unknown at the time of the extrapolation. Therefore, the extrapolation must account also for the randomness in the choice of labels. We will assume that the labels in the two classification tasks are comparable.

Assumption 1 Let $\mathcal{S}_{k_1}, \mathcal{S}_{k_2}$ be the label sets for the first and second classification tasks. Then $\mathcal{S}_{k_1}, \mathcal{S}_{k_2}$ are i.i.d. samples from an infinite population π.

Comments:

1. These assumption are most easily satisfied by taking $\mathcal{Y}$ to be a continuous space and letting π be a density over $\mathcal{Y}$. However, a discrete space with a small enough probability for the classes would work well.

2. Note that here we assumed that the label subsets $\mathcal{S}_{k_1}$ and $\mathcal{S}_{k_2}$ are independent and disjoint. An alternative assumption would be that $\mathcal{S}_{k_1} \subset \mathcal{S}_{k_2}$ with $\mathcal{S}_{k_1}$ being a subsample of $\mathcal{S}_{k_2}$: this assumption can also be addressed, as we will discuss later.

3. In practice, $\mathcal{S}_{k_1}$ is often a convenience sample meant to be similar to $\mathcal{S}_{k_2}$. The theory will be relevant insofar as the assumptions approximate well the true sampling similarity between the $\mathcal{S}_{k_1}$ and $\mathcal{S}_{k_2}$.

4. We can imagine other sampling mechanisms designed to make $\mathcal{S}_{k_1}$ a representative sample from the population, e.g. by stratifying. In this paper we do not discuss these more complex sampling schemes.

Our analysis will also rely on a property of the classification model. We do not want the classifier to rely too strongly on complicated interactions between the labels in the set. We therefore propose the following property of marginal separability for classification models:

Definition 2.1 1. *The classification rule f is called a* marginal rule *if*

$$f(x) = argmax_{y \in \mathcal{S}} m_y(x),$$

where the function m_y maps $\mathcal{X}$ to $\mathbb{R}$.

2. *Define a marginal model $\mathcal{M}$ as a mapping from empirical distributions to margin functions,*

$$\mathcal{M}(\hat{F}_y) = m_y(x).$$

3. *A classifier that produces marginal classification rules*

$$f(x) = argmax_{y \in \mathcal{S}} m_y(x),$$

by use of a marginal model, i.e. such that $m_y = \mathcal{M}(\hat{F}_y)$ for some marginal model $\mathcal{M}$, is called a marginal classifier.

In words, a marginal classification rule produces a *margin*, or score, for each label, and chooses the label with the highest margin. The marginal model converts empirical distributions $\hat{F}_y$ over $\mathcal{X}$ into the margin function m_y. The *marginal* property allows us to prove strong results about the accuracy of the classifier under i.i.d. sampling assumptions.

Comments:

1. The marginal model includes several popular classifiers. A primary example for a marginal model is the estimated Bayes classifier. Let $\hat{f}_y$ be a density estimate obtained from the empirical distribution $\hat{F}_y$. Then, we can use the estimated densities of each class to produce the margin functions:

$$m_y^{EB}(x) = \log(\hat{f}_y(x)).$$

The resulting empirical approximation for the Bayes classifier (further assuming a uniform prior π) would be

$$f^{EB}(x) = \text{argmax}_{y \in \mathcal{S}}(m_y^{EB}(x)).$$

2. Both the Quadratic Discriminant Analysis and the naive Bayes classifiers can be seen as specific instances of an estimated Bayes classifier [2]. For QDA, the margin function is given by

$$m_y^{QDA}(x) = -(x - \mu(\hat{F}_y))^T \Sigma(\hat{F}_y)^{-1}(x - \mu(\hat{F}_y)) - \log\det(\Sigma(\hat{F}_y)),$$

where $\mu(F) = \int y dF(y)$ and $\Sigma(F) = \int (y - \mu(F))(y - \mu(F))^T dF(y)$. In Naive Bayes, the margin function is

$$m_y^{NB}(x) = \sum_{i=1}^{n} \log \hat{f}_{y,i}(x),$$

where $\hat{f}_{y,i}$ is a density estimate for the i-th component of $\hat{F}_y$.

3. There are also many classifiers which do not satisfy the marginal property, such as multinomial logistic regression, multilayer neural networks, decision trees, and k-nearest neighbors.

2.3 Definition of average risk

Since the classification tasks are randomly generated, the r-repeat risk becomes a *random variable* which depends on the random label subset $\mathcal{S}$.

Therefore, define the k-class, r-repeat *average risk* of classifier $\mathcal{F}$ as

$$\text{AvRisk}_{k,r}(\mathcal{F}) = \mathbf{E}[\text{Risk}_k(\mathcal{F})]$$

where the expectation is taken over the distribution of $\mathcal{S} = (Y^{(1)}, \ldots, Y^{(k)})$ when $Y^{(i)} \overset{iid}{\sim} \text{Unif}(\mathcal{S})$.

As we can see from Figure 4, the average risk is obtained by averaging over four randomizations:

A1. Drawing the label subset $\mathcal{S}$.

A2. Drawing the training dataset.

A3. Drawing Y^* uniformly at random from $\mathcal{S}$.

[2] QDA is the special case of the estimated Bayes classifier when $\hat{f}_y$ is obtained as the multivariate Gaussian density with mean and covariance parameters estimated from the data. Naive Bayes is the estimated Bayes classifier when $\hat{f}_y$ is obtained as the product of estimated componentwise marginal distributions of $p(x_i|y)$

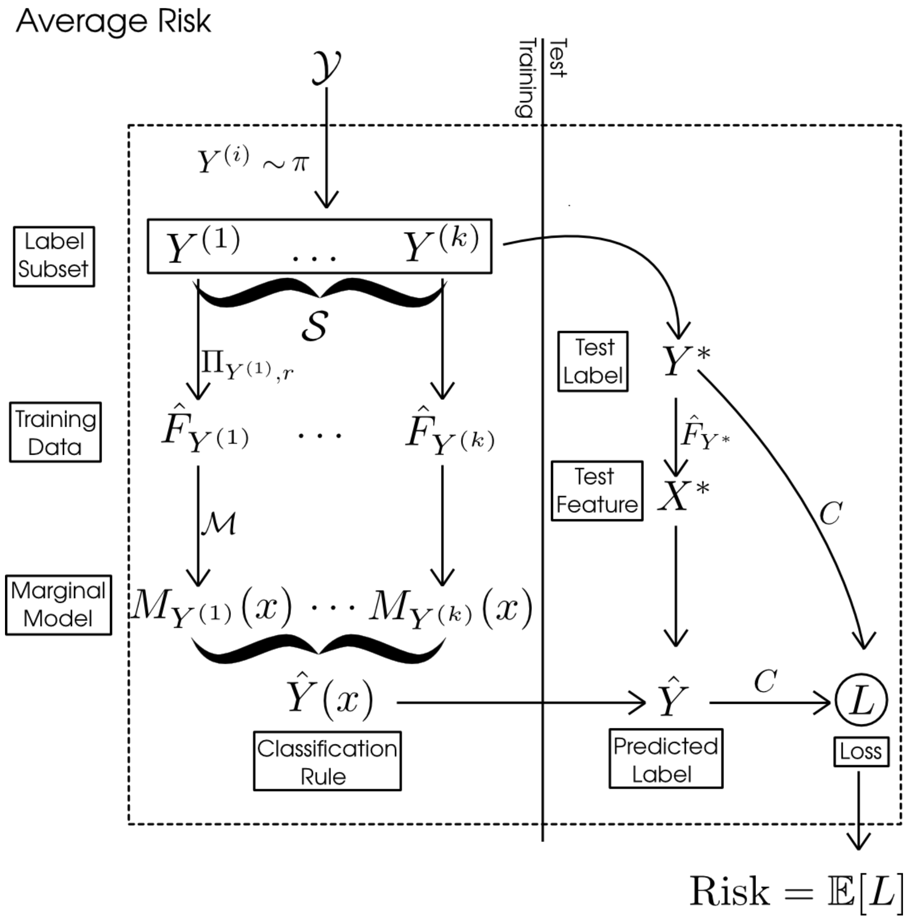


Figure 4: Average risk

A4. Drawing X^* from F_{X^*}.

For the sake of developing a better intuition of the average risk, it is helpful to define a random variable called the *loss*, which is the cost incurred by a single test instance. The loss is determined by quantities from all four randomization steps: the label subset $\mathcal{S} = \{Y^{(1)}, \dots, Y^{(k)}\}$, the training samples $\hat{F}_{Y^{(1)}}, \dots, \hat{F}_{Y^{(k)}}$, and the test point (X^*, Y^*). Formally, we write

$$L = C(\mathcal{F}(\{\hat{F}_y\}_{y \in \mathcal{S}})(X^*), Y^*).$$

Now note that the k-class, r-repeat average risk is the expected loss,

$$\text{AvRisk}_{k,r}(\mathcal{F}) = \mathbf{E}[L] = \mathbf{E}[C(\mathcal{F}(\{\hat{F}_y\}_{y \in \mathcal{S}})(X^*), Y^*)]. \tag{1}$$

where the expectation is taken over the joint distribution of all the quantities $\{Y^{(1)}, \dots, Y^{(k)}, \hat{F}_{Y^{(1)}}, \dots, \hat{F}_{Y^{(k)}}, (X^*, Y^*)\}$.

We will aim to develop a method for estimating the *average risk*. In the case where the classification tasks are independently generated, the average risk is the best predictor (in mean-squared error) for the (random) risk.

3 Performance extrapolation for marginal classifiers

Having outlined our assumption for randomized label subsets, the focus of our theory moves towards understanding the k-class average risk: that is, the expected risk of $\mathcal{F}$ when a random subset $\mathcal{S}$ of size k is drawn.

We obtain a method for estimating the risk in the second classification task using data from the first. The insight behind our estimation method is obtained via an analysis of the average risk of the classification task.

3.1 Toy example

Let us first illustrate using a toy example the computation of the average risk, and preview the theory for extrapolating the average risk.

Let (Y, X) have a bivariate normal joint distribution,

$$(Y, X) \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right),$$

as illustrated in figure 5(a). Therefore, for a given randomly drawn label Y, the conditional distribution of X for that label is univariate normal with mean ρY and variance $1 - \rho^2$:

$$X|Y = y \sim N(\rho Y, 1 - \rho^2).$$

Supposing we draw $k = 3$ labels y_1, y_2, y_3, the classification problem will be to assign a test instance X^* to the correct label. The test instance would be drawn from the three-class mixture,

$$X^* \sim \frac{1}{k} \sum_{i=1}^{k} p(x|y_i),$$

as illustrated in figure 5(b, top). In this toy example, we ignore the issue of training a classifier from sampled data, and instead assume that we have access to the *Bayes classification rule*, or optimal classification rule. The Bayes rule assigns X^* to the class with the highest density $p(x|y_i)$, as illustrated by figure 5(b, bottom).

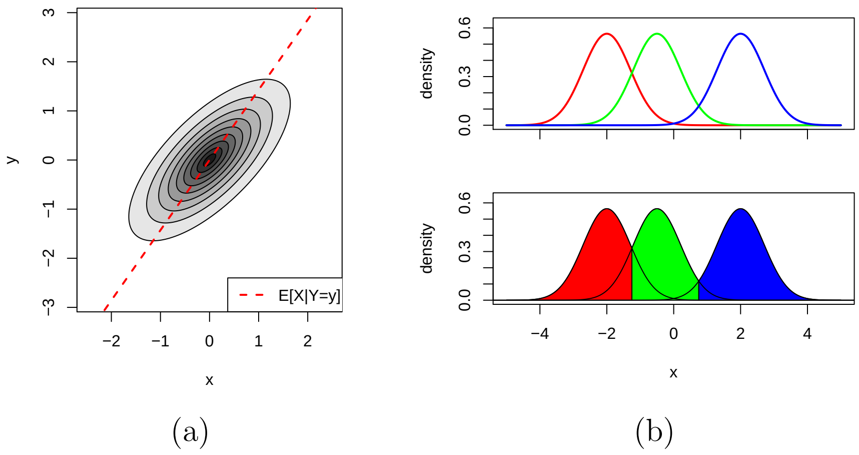


Figure 5: (a) The joint distribution of (X, Y) is bivariate normal with correlation $\rho = 0.7$. (b) A typical classification problem instance from the bivariate normal model with $k = 3$ classes. Top: the conditional density of X given label Y, for $Y = \{y_1, y_2, y_3\}$. Bottom: the Bayes classification regions for the three classes.

The risk of the Bayes rule for any label set $\{y_1, \ldots, y_k\}$ is given by

$$\text{Risk}(y_1, \ldots, y_k) = \frac{1}{k} \sum_{i=1}^{k} \Pr_{X \sim p(x|y_i)} [p(X|y_i) = \max_{j=1}^{k} p(X|y_j)].$$

We numerically computed $\text{Risk}(y_1, \ldots, y_k)$ for randomly drawn labels $Y_1, \ldots, Y_k \overset{iid}{\sim} N(0, 1)$; the distributions of $\text{Risk}(Y_1, \ldots, Y_k)$ for $k = 2, \ldots, 10$ are illustrated in figure 6. The k-class average risk, AvRisk_k, in this case, is given by

$$\text{AvRisk}_k = \mathbf{E}[\text{Risk}(Y_1, \ldots, Y_k)]$$

for $Y_1, \ldots, Y_k \overset{iid}{\sim} N(0, 1)$. The theory presented in the rest of the section deals with how to analyze the average risk AvRisk_k as a function of k. We now proceed to preview some selected aspects of the theory for the toy example.

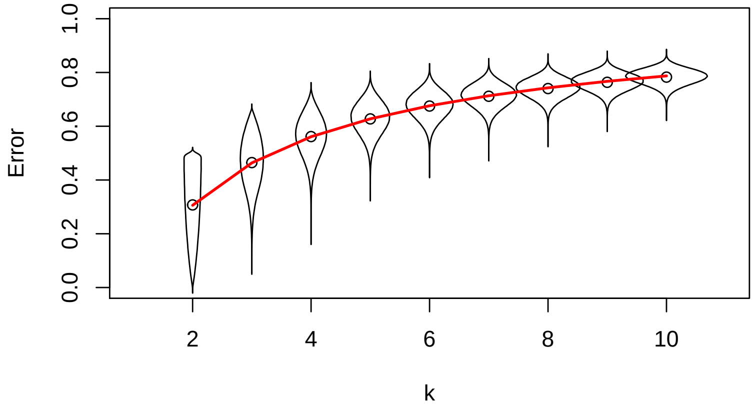


Figure 6: The distribution of the classification risk for $k = 2, 3, \ldots, 10$ for the bivariate normal model with $\rho = 0.7$. Circles indicate the average classificatin risk; the red curve is the theoretically computed average risk.

For a given test instance X^* drawn from the label Y^*, the closer that X^* is to the center of the correct class distribution, ρY^*, the more likely it is to be classified correctly. Based on this concept, we define the *conditional accuracy* function $U_x(y)$, which gives the conditional probability that a test instance (Y_1, X_1) will be classified correctly in the two-class classification problem. One can therefore think of $U_x(y)$ as measuring the "strength" of the pair (y, x), with stronger pairs being more likely to be classified correctly. Since in the two-class problem, there is one incorrect class label Y_2, the conditional accuracy in this case is simply the probability that ρY_2 is closer to X_1 than ρY_1. Therefore, in this toy example, we can give an explicit formula

$$\begin{aligned} U_x(y) &= \Pr[p(x|y) < p(x|Y)] \\ &= \Pr[|\rho Y - x| < |\rho y - x|] \\ &= \Phi\left(\frac{x + |\rho y - x|}{\rho}\right) - \Phi\left(\frac{x - |\rho y - x|}{\rho}\right), \end{aligned}$$

where Φ is the standard normal cumulative distribution function. Figure 7(a) illustrates the level sets of the function $U_x(y)$. The highest values of $U_x(y)$ are near the line $x = \rho y$ corresponding the to conditional mean of $X|Y$: as one moves farther from the line, $U_x(y)$ decays. Note however that large values of (y, x) (with the same sign) result in larger values of $U_x(y)$

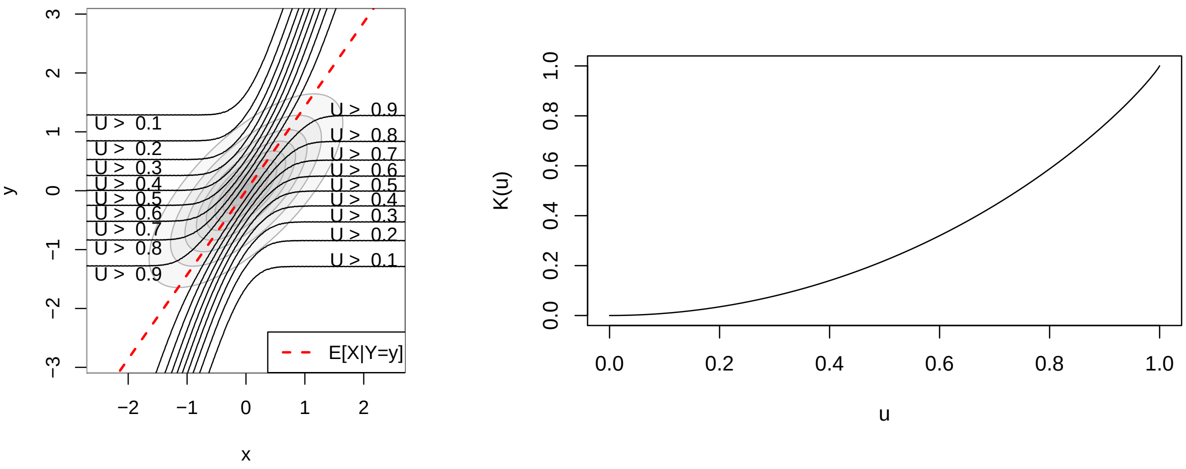
since it becomes unlikely for $Y_2 \sim N(0,1)$ to exceed $Y_1 = y$.

Now define the random variable $U = U_X(Y)$ for (X,Y) drawn from the joint distribution. An important object in our theory is the cumulative distribution function [3] of U, written as

$$\bar{D}(u) = \Pr[U \leq u].$$

The function $\bar{D}$ is illustrated in figure 7(b) for the current example with $\rho = 0.7$. The red curve in figure 6 was computed using the formula

$$\text{AvRisk}_k = (k-1)\int \bar{D}(u)u^{k-2}du.$$



(a)

(b)

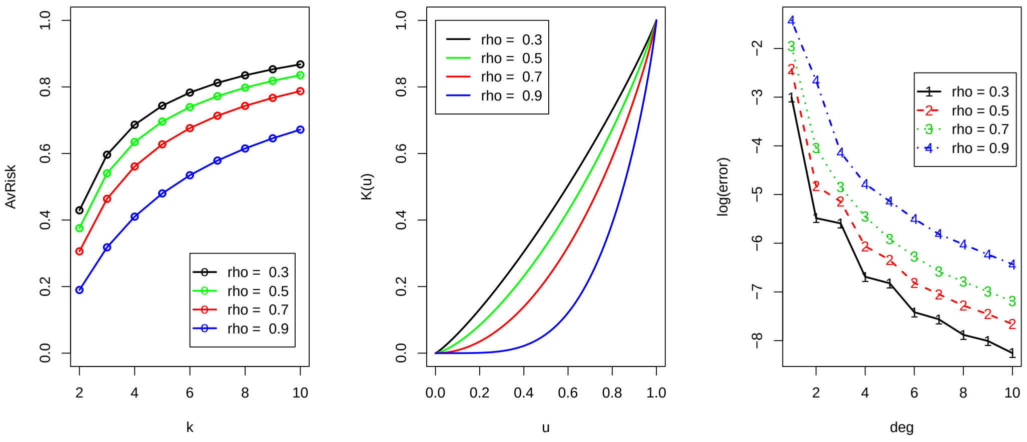
Figure 7: (a) The level curves of the function $U_x(y)$ in the bivariate normal model with $\rho = 0.7$. (b) The function $\bar{D}(u)$, which gives the cumulative distribution function of the random variable $U_Y(X)$.

It is illuminating to consider how the average risk curves and the $\bar{D}(u)$ functions vary as we change the parameter ρ. Higher correlations ρ lead to lower classification risk, as seen in figure 8(a), where the risk curves are

[3] Note however that $\bar{D}(u)$ is only defined as the cumulative distribution function of U in the class of zero-one loss–the definition for general cost functions is somewhat more involved, as we will see.

shifted downward as ρ increases from 0.3 to 0.9. The conditional accuracy $U_y(x)$ tends to be higher on average as well, which leads to lower values of the cumulative distribution function–as we see in figure 8(b), where the function $\bar{D}(u)$ becomes smaller as ρ increases.

In section 3.4, when we consider approximating $\bar{D}(u)$ by polynomials, or some other function basis, it becomes relevant to consider how well $\bar{D}(u)$ can be approximated by such bases in realistic problems. We see in figure 8(c) that, at least in this toy problem, $\bar{D}(u)$ is well-aproximated by low-order polynomials. However, the approximation becomes less adequate as ρ increases. We can see visually why this is the case: as ρ increases, the curvature of $\bar{D}(u)$ near $u = 1$ increases. Hence, higher-degree polynomials become needed to capture the behavior near $u = 1$. More generally, we observe that in cases where classes are relatively well-separated, it becomes necessary to use increasingly precise approximations in order to extrapolate the average risk.



(a) (b) (c)

Figure 8: The (a) average risk, (b) $\bar{D}(u)$ function for $k = 2, \ldots, 7$ for the bivariate normal model with $\rho \in \{0.3, 0.5, 0.7, 0.9\}$. (c) The d-degree ℓ_∞ polynomial approximation error for $\bar{D}(u)$ for the bivariate normal model with $\rho \in \{0.3, 0.5, 0.7, 0.9\}$.

3.2 Easy special cases

Let us first mention two easy special cases, which can be handled using existing machine learning methodology.

3.2.1 Equal numbers of classes

In the special case where $k_1 = k_2 = k$: that is, where the label subsets $\mathcal{S}_1$ and $\mathcal{S}_2$ are the same size, it is clear to see that any unbiased estimate of the risk of the classifier $\mathcal{F}$ for the first classification problem is an unbiased estimate of the average k-class risk. The *test risk* gives one such unbiased estimate of the average k-class risk.

Recall that the data consists of class labels $y^{(i)}$ for $i = 1, \ldots, k_1$, as well as training sample $\hat{F}_{y^{(i)}}$ and test sample $(x_1^{(i)}, \ldots, x_{r_{test}}^{(i)})$ for $i = 1, \ldots, k_1$.

For any given test observation $x_j^{(i)}$, we obtain the predicted label $\hat{y}_j^{(i)}$ by computing the margin for each class,

$$M_{i,j,\ell} = \mathcal{M}(\hat{F}_{y^{(\ell)}})(x_j^{(i)}) = m_{y^{(\ell)}}(x_i^{(j)}),$$

for $\ell = 1, \ldots, k$, and by finding the class with the highest margin $M_{i,j,\ell}$,

$$\hat{y}_j^{(i)} = y_{\text{argmax}_\ell M_{i,j,\ell}}.$$

The test risk is the average cost over test observations,

$$\text{Test Risk} = \frac{1}{r_{test}k} \sum_{i=1}^{k} \sum_{j=1}^{r_{test}} C(\hat{y}_j^{(i)}, y^{(i)}). \tag{2}$$

For each test observation, define the ranks of the margins by

$$R_{i,j,\ell} = \sum_{m \neq \ell} I\{M_{i,j,\ell} \geq M_{i,j,m}\}.$$

Therefore, $\hat{y}_j^{(i)}$ is equal to ℓ if and only if $R_{i,j,\ell} = k$. Thus, an equivalent expression for test risk is

$$\text{Test Risk} = \frac{1}{r_{test}k} \sum_{i=1}^{k} \sum_{\ell=1}^{k} \sum_{j=1}^{r_{test}} C_{ij} I\{R_{ij\ell} = k\}. \tag{3}$$

where

$$C_{ij} = C(y^{(j)}, y^{(i)}).$$

Besides the test risk, other methods, such as cross-validation, can also be used to obtain estimates of the average k-class risk.

3.2.2 Fewer classes

Suppose we have data for k_1 classes, and we wish to estimate AvRisk_{k_2} for $k_2 \leq k_1$. Let $\mathcal{S}_1 = \{y_1, \ldots, y_{k_1}\}$. To obtain a classification problem with k_2 classes, we can simply pick a subset S of size k_2 from $\mathcal{S}_1$, and throw away all the training and test data from the other classes $\mathcal{S} \setminus S$. Then, the test risk (3) gives an unbiased estimate of the AvRisk_{k_2}.

Of course, one could obtain a better estimator of the average risk by averaging over all the subsets $S \subset \mathcal{S}_1$ of size k_2. For general classifiers, this may require retraining a classifier over each subset. However, for marginal classifiers, one can compute the average test risk over all $\binom{k_1}{k_2}$ subsets easily.

The reason why the efficient computation is possible is because the test risk for each subproblem can be determined by looking at the margins $M_{i,j,\ell}$, which remain the same as long as both i and ℓ are included in the subsample S.

The computational trick is to look at each combination of test observation $x_j^{(i)}$ and class label $y^{(\ell)}$, and to count the number of subsets $N_{i,j,\ell}$ where (i) both i and ℓ are included in S, and (ii) $\hat{y}_j^{(i)} = y^{(\ell)}$. Then it should be clear that the average test risk over all subsets is equal to

$$\text{AvTestRisk}_{k_2} = \frac{1}{\binom{k_1}{k_2}} \frac{1}{r_{test} k_2} \sum_{i=1}^{k_1} \sum_{\ell \neq i} \sum_{j=1}^{r_{test}} C_{i\ell} N_{i,j,\ell}. \tag{4}$$

Now it is just a matter of simple combinatorics to compute $N_{i,j,\ell}$. We require both $y^{(i)}$ and $y^{(\ell)}$ to be included in S. This implies that if $M_{i,j,i} > M_{i,j,\ell}$, then $y^{(\ell)}$ will never have the highest margin in any of those subsets, so $N_{i,j,\ell} = 0$.

Otherwise, there are $R_{i,j,\ell} - 1$ elements in $\mathcal{S}_1$ with a lower margin than $y^{(\ell)}$. Since $i \neq \ell$, then there are $k_2 - 2$ elements in $S \setminus \{i, \ell\}$, so therefore $N_{i,j,\ell} = \binom{R_{i,j,\ell}-2}{k_2-2}$. Therefore, we can write

$$N_{i,j,\ell} = I\{R_{i,j,\ell} > R_{i,j,i}\} \binom{R_{i,j,\ell} - 2}{k_2 - 2} \tag{5}$$

Therefore, the challenging case is when $k_2 > k_1$: we want to predict the performance of the classification model in a setting with more labels than we currently see in the training set.

3.3 Analysis of the average risk

As we pointed out in the previous section, the challenging case for the analysis is the "undersampled" regime where we wish to predict the loss on a larger label set. Given data with k_1 classes, we already have means to estimate the average risk for all $k \leq k_1$, so the challenge is to understand how the risk will "extrapolate" to $k > k_1$. Hence, the goal of the current analysis is to isolate the effect of k, the size of the label subset, on the average risk.

The result of our analysis is to expose the average risk $\text{AvRisk}_{k,r}$ as the weighted average of a function $\bar{D}(u)$, where $\bar{D}(u)$ is independent of k, and where k only changes the weighting. The result is stated as follows.

Theorem 3.1 *Suppose π, $\{F_y\}_{y\in\mathcal{Y}}$ and marginal classifier $\mathcal{F}$ satisfy the tie-breaking condition. Then, under the definitions* (8)*,* (11)*, and* (13)*, we have*

$$AvRisk_{k,r} = (k-1)\int \bar{D}(u)u^{k-2}du. \tag{6}$$

The tie-breaking condition referred in the theorem is defined as follows.

- *Tie-breaking condition*: for all $x \in \mathcal{X}$, $\mathcal{M}(\hat{F}_Y)(x) = \mathcal{M}(\hat{F}_{Y'})(x)$ with zero probability for Y, Y' independently drawn from π.

The tie-breaking condition is a technical assumption which allows us to neglect the specification of a tie-breaking rule in the case that margins are tied. In practice, one can simply break ties randomly, which is mathematically equivalent to adding a small amount of random noise ϵ to the function $\mathcal{M}$.

Our strategy is to analyze the average risk (1) by means of *conditioning on* the true label and its training sample, $(y^*, \hat{F}_{y^*})$, and the test feature x^* while *averaging* over all the other random variables. Define the *conditional average risk* $\text{CondRisk}_k((y^*, \hat{F}_{y^*}), x^*)$ as

$$\text{CondRisk}_k((y^*, \hat{F}_{y^*}), x^*) = \mathbf{E}[L|Y^* = y^*, X^* = x^*, \hat{F}_{Y^*} = \hat{F}_{y^*}]. \tag{7}$$

Figure 9 illustrates the variables which are fixed under conditioning and the variables which are randomized. Compare to figure 4.

Without loss of generality, we can write the label subset $\mathcal{S} = \{Y^*, Y^{(1)}, \ldots, Y^{(k-1)}\}$. Note that due to independence, $Y^{(1)}, \ldots, Y^{(k-1)}$ are still i.i.d. from π even conditioning on $Y^* = y^*$. Therefore, the conditional risk can be obtained via the following alternative order of randomizations:

C0. Fix $y^*, \hat{F}_y^*$, and x^*. Note that $M_{y^*}(x^*) = \mathcal{M}(\hat{F}_{y^*})(x^*)$ is also fixed.

C1. Draw the *incorrect labels* $Y^{(1)}, \dots, Y^{(k)}$ i.i.d. from π. (Note that $Y^{(i)} \neq y^*$ with probability 1 due to the continuity assumptions on $\mathcal{Y}$ and π.)

C2. Draw the training samples for the incorrect labels $\hat{F}_{Y^{(1)}}, \dots, \hat{F}_{Y^{(k-1)}}$. This determines
$$\hat{Y} = \text{argmax}_{y \in \mathcal{S}} M_y(x^*)$$
and hence
$$L = C(\hat{Y}, y^*).$$

Compared to four randomization steps listed in section 2.3, we have essentially conditioned on steps A3 and A4 and randomized over steps A1 and A2.

Now, in order to analyze the k-class behavior of the conditional average risk, we begin by considering the *two-class* situation.

In the two-class situation, we have a true label y^* and one incorrect label, Y. Define the *U-function* $U_{x^*}(y^*, \hat{F}_{y^*})$ as the *probability of correct classification* in the two-class case. The classification is correct if the margin $M_{y^*}(x^*)$ is greater than the margin $M_Y(x^*)$, and incorrect otherwise. Since we are fixing x^* and $(y^*, \hat{F}_{y^*})$, the probability of correct classification is obtained by taking an expectation:

$$\begin{aligned} U_{x^*}(y^*, \hat{F}_{y^*}) &= \Pr[M_{y^*}(x^*) > \mathcal{M}(\hat{F}_Y)(x^*)] && (8) \\ &= \int I\{M_{y^*}(x^*) > \mathcal{M}(\hat{F}_y)(x)\} d\Pi_{y,r}(\hat{F}_y) d\pi(y). && (9) \end{aligned}$$

See also figure 10 for an graphical illustration of the definition.

An important property of the U-function, and the basis for its name, is that the random variable $U_x(Y, \hat{F}_Y)$ for $Y \sim \pi$ and $\hat{F}_Y \sim \Pi_{Y,r}$ is uniformly distributed for all $x \in \mathcal{X}$. This is proved in Lemma A.1 in the appendix.

Now, we will see how the U-function allows us to understand the k-class case. Suppose we have true label y^* and incorrect labels $Y^{(1)}, \dots, Y^{(k-1)}$. Note that the U-function $U_{x^*}(y, \hat{F}_y)$ is monotonic in $M_y(x^*)$. Therefore,

$$\hat{Y} = \text{argmax}_{y \in \mathcal{S}} M_y(x^*) = \text{argmax}_{y \in \mathcal{S}} U_{x^*}(y, \hat{F}_y).$$

Therefore, we have a correct classification if and only if the U-function value for the correct label is greater than the maximum U-function values for the

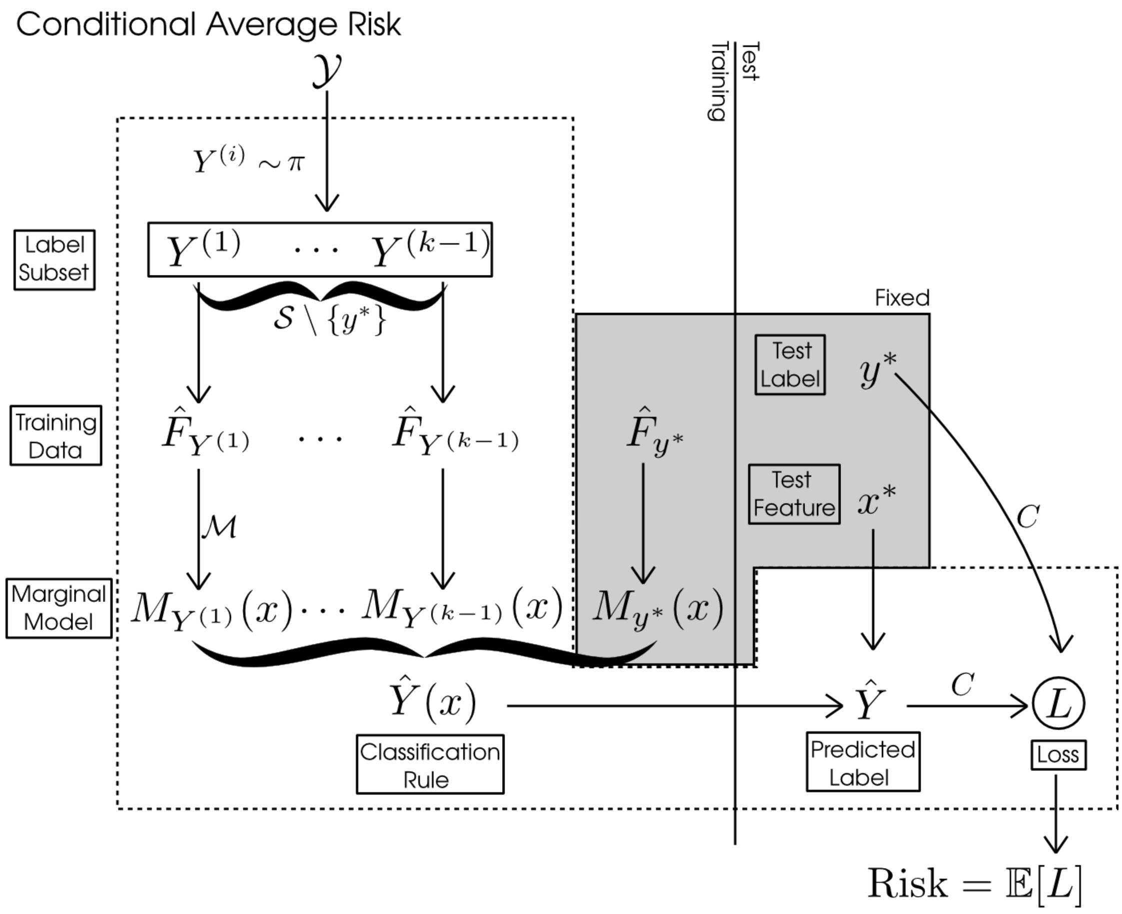


Figure 9: Conditional average risk

incorrect labels:

$$\Pr[\hat{Y} = y^*] = \Pr[U_{x^*}(y^*, \hat{F}_{y^*}) > \max_{i=1}^{k-1} U_{x^*}(Y^{(i)}, \hat{F}_{Y^{(i)}})] = \Pr[u^* > U_{max}].$$

where $u^* = U_{x^*}(y^*, \hat{F}_{y^*})$ and $U_{max,k-1} = \max_{i=1}^{k-1} U_{x^*}(Y^{(i)}, \hat{F}_{Y^{(i)}})$. But now, observe that we know the distribution of $U_{max,k-1}$! Since $U_{x^*}(Y^{(i)}, \hat{F}_{Y^{(i)}})$ are i.i.d. uniform, we know that

$$U_{max,k-1} \sim \text{Beta}(k-1, 1). \tag{10}$$

We now have the insights needed to analyze the simplest special case: zero-one loss.

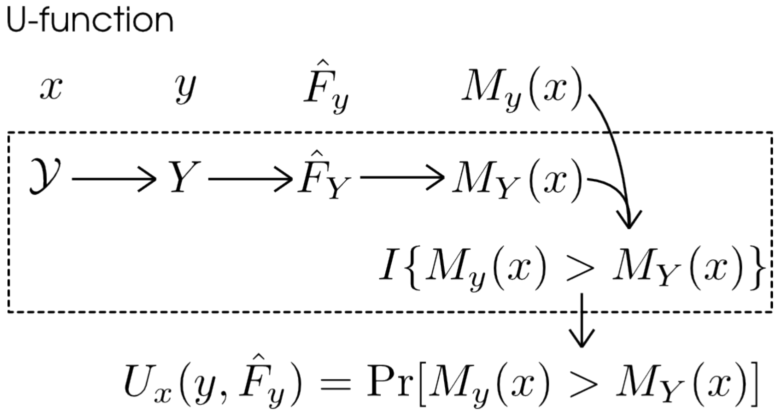


Figure 10: U-functions

Special case: 0-1 loss. For zero-one loss, which is $C(y, y') = I\{y = y'\}$, we have $L = 1$ if and only if $U_{max} > u^*$ and $L = 0$ otherwise. Therefore, the conditional average risk is

$$\text{CondRisk}_k((y^*, \hat{F}_{y^*}), x^*) = \Pr[U_{max} > u^*] = \int_{u^*}^1 (k-1)u^{k-2}du.$$

Now the average risk can be obtained by integrating over the distribution of $U^* = U_{x^*}(y^*, \hat{F}_{y^*})$. We have

$$\begin{aligned}\text{AvRisk}_k &= \mathbf{E}[\int_{U^*}^1 (k-1)u^{k-2}du] \\ &= \mathbf{E}[\int_0^1 I\{u \geq U^*\}(k-1)u^{k-2}du] \\ &= (k-1)\int_0^1 \Pr[U^* \leq u]u^{k-2}du.\end{aligned}$$

Or equivalently,

$$\text{AvRisk}_{k,r,\nu}((y^*, \hat{F}_{y^*}), x^*) = (k-1)\int \bar{D}(u)u^{k-2}du.$$

where $\bar{D}(u)$ denote the cumulative distribution function of U^* on $[0, 1]$:

$$\bar{D}(u) = \Pr[U_{x^*}(y^*, \hat{F}_{y^*}) \leq u].$$

We have expressed the average risk expressed as a weighted integral of a certain function $\bar{D}(u)$ defined on $u \in [0,1]$. We have clearly isolated the part of the average risk which is independent of k–the univariate function $\bar{D}(u)$, and the part which is dependent on k–which is the density of U_{max}.

In section 3.4, we will develop estimators of $\bar{D}(u)$ in order to estimate the k-class average risk. But now let us return to the general case.

General loss functions. The case for general cost functions is somewhat more complicated, since knowledge of U_{max} is not sufficient to determine L. In short, this is because U_{max} by itself is insufficient to determine $\hat{Y}$, and therefore $L = C(\hat{Y}, y^*)$. However, we can resolve this issue by noting that for the purposes of computing the expected loss, it suffices to have the *conditional distribution* of $\hat{Y}$ given U_{max}. Even though U_{max} does not deterministically map onto a unique $\hat{Y}$, it determines a conditional distribution of $\hat{Y}$ which allows us to compute $\mathbf{E}[L|U_{max}, x^*, y^*, \hat{F}_{y^*}]$.

Now, a key fact is that the conditional distribution of $\hat{Y}$ given U_{max} *does not depend* on k. To see this fact, suppose without loss of generality that $\hat{Y} = Y^{(k-1)}$. Then the joint density of $Y^{(1)}, \dots, Y^{(k-1)}$ given $U_{max} = u$ can be written

$$p(y^{(1)}, \dots, y^{(k-1)}) \propto \pi(y^{(k-1)}) \frac{d}{dt} \Pr[U_{x^*}(y^{(k-1)}, \hat{F}_{y^{(k-1)}}) \leq t]|_{t=u} \prod_{i=1}^{k-2} \pi(y^{(i)}) \Pr[U_{x^*}(y^{(k-1)}, \hat{F}_{y^{(k-1)}}) < u]$$

up to a normalizing constant. Note that the term $\frac{d}{dt}\Pr[U_{x^*}(y^{(k-1)}, \hat{F}_{y^{(k-1)}}) \leq t]$ is the density of the random variable $U_{x^*}(Y^{(k-1)}, \hat{F}_{Y^{(k-1)}})$. From the density, we can see that $Y^{(1)}, \dots, Y^{(k-1)}$ are conditionally independent given $U_{max} = u$, hence the marginal density of $\hat{Y} = Y^{(k-1)}$ can be written

$$p(\hat{y}) \propto \pi(\hat{y}) \frac{d}{dt} \Pr[U_{x^*}(y^{(k-1)}, \hat{F}_{y^{(k-1)}}) \leq t]|_{t=u}.$$

The only property of the conditional distribution of $\hat{Y}|U_{max} = u$ that is needed is the expectation of $L = C(\hat{Y}, y^*)$. Therefore, define the *conditional expected loss* $D((y^*, \hat{F}_{y^*}), x^*, u)$ by

$$D((y^*, \hat{F}_{y^*}), x^*, u) = \begin{cases} 0 \text{ if } u < u^* \\ \mathbf{E}[C(\hat{Y}, y^*)|U_{max} = u, x^*, y^*, \hat{F}_{y^*}] \text{ otherwise.} \end{cases} \tag{11}$$

We have the two cases $u < u^*$ and $u > u^*$ since when $U_{max} < u^*$, the correct label is chosen and the loss is zero. Otherwise, an incorrect label is chosen, and the expected loss must be calculated using the conditional distribution of $\hat{Y}$.

Again, since the conditional distribution of $\hat{Y}|U_{max}, x^*, (y^*, \hat{F}_{y^*})$ is independent of k, the conditional cost function is also independent of k.

With the conditional cost function and the distribution of U_{max} both in hand, we can compute the average conditional risk

$$\text{CondRisk}_k((y^*, \hat{F}_{y^*}), x^*) = (k-1) \int D((y^*, \hat{F}_{y^*}), x^*, u) u^{k-2} du. \tag{12}$$

Now the average risk can be obtained by integrating over $(Y^*, \hat{F}_{Y^*})$, and X^*.

$$\text{AvRisk}_{k,r} = (k-1) \int \bar{D}(u) u^{k-2} du.$$

where

$$\bar{D}(u) = \int D((y^*, \hat{F}_{y^*}), x^*, u) \pi(y^*) dy dF_{y^*}(x^*) d\Pi_{y^*,r}(\hat{F}_{y^*}). \tag{13}$$

This is the key result behind our estimation method, which was stated in theorem 3.1. The proof is given in the appendix.

Having this theoretical result allows us to understand how the expected k-class risk scales with k in problems where all the relevant densities are known. However, applying this result in practice to estimate Average Risk$_k$ requires some means of estimating the unknown function $\bar{D}$–which we discuss in the following.

3.4 Estimation in the general case

Now we address the problem of estimating AvRisk$_{k_2, r_{train}}$ from data. As we have seen from Theorem 3.1, the k-class average risk of a marginal classifier $\mathcal{M}$ is a functional of a object called $\bar{D}(u)$, which depends marginal model $\mathcal{M}$ of the classifier, the joint distribution of labels Y and features X when Y is drawn from the sampling density ν.

Therefore, the strategy we take is to attempt to estimate $\bar{D}$ for then given classification model, and then plug in our estimate of $\bar{D}$ into the integral (6) to obtain an estimate of AvRisk$_{k_2, r_{train}}$.

Having decided to estimate $\bar{D}$, there is then the question of what kind of model we should assume for $\bar{D}$. While a nonparametric approach may be ideal, for the case of general loss functions we will adopt a parametric model: that is the subject of this section.

Let us assume the linear model

$$\bar{D}(u) = \sum_{\ell=1}^{m} \beta_\ell h_\ell(u), \tag{14}$$

where $h_\ell(u)$ are known basis functions, and β are the model parameters to be estimated. We can obtain *unbiased* estimation of $\text{AvRisk}_{k_2,r_{train}}$ via the unbiased estimates of k-class average risk obtained from (4).

If we plug in the assumed linear model (14) into the identity (6), then we get

$$\begin{aligned}
\text{AvRisk}_{k,r_{train}} &= (k-2)\int \bar{D}(u)u^{k-2}du && (15)\\
&= (k-2)\int_0^1 \sum_{\ell=1}^{m} \beta_\ell h_\ell(u)u^{k-2}du && (16)\\
&= \sum_{\ell=1}^{m} \beta_\ell H_{\ell,k} && (17)
\end{aligned}$$

where

$$H_{\ell,k} = (k-2)\int_0^1 h_\ell(u)u^{k-2}du. \tag{18}$$

The constants $H_{\ell,k}$ are moments of the basis function h_ℓ: hence we call this method the *moment method.* Note that $H_{\ell,k}$ can be precomputed numerically for any $k \geq 2$.

Now, since the AvTestRisk_k are unbiased estimates of $\text{AvRisk}_{k,r_{train}}$, this implies that the regression estimate

$$\hat{\beta} = \text{argmin}_\beta \sum_{k=2}^{k_1} w_k \left(\text{AvTestRisk}_k - \sum_{\ell=1}^{m} \beta_\ell H_{\ell,k} \right)^2$$

is unbiased for β, under any choice of positive weights w_k. The estimate of $\text{AvRisk}_{k_2,r_{train}}$ is similarly obtained from (17), via

$$\widehat{\text{AvRisk}_{k_2,r_{train}}} = \sum_{\ell=1}^{m} \hat{\beta}_\ell H_{\ell,k_2}. \tag{19}$$

3.5 Large-Sample Theory

How good are the estimated average risks (19)? Let us investigate the accuracy of the estimates in the limit where $k_1 \to \infty$, first in the case where the model (14) is correctly specified, and then considering possible model misspecification.

If we fix the number of classes k_2 which defines the estimation target, then we need not use the estimator (19), since once $k_1 > k_2$, we can use the AvTestRisk_{k_2} as an estimator instead, which can easily be shown to a have a convergence rate of $O(1/\sqrt{k_1})$ to the true average risk. Therefore, if we want to quantify the performance of the regression-based estimator (19), it does not make sense to look at asymptotic settings where k_2 is fixed. One approach is to specify a setting where k_2 changes as a function of k_1. However, the approach we will take is to look at the minimax error: that is, to look at the maximum discrepancy between the estimate and the true average risk over all k_2 simultaneously. The performance criterion is the minimax error, defined

$$\text{MinimaxError} = \sup_{k_2 > 2} |\widehat{\text{AvRisk}_{k_2, r_{train}}} - \text{AvRisk}_{k_2, r_{train}}|. \tag{20}$$

Well-specified case.

Let us first assume that the parametric model (14) is correct. Then

$$\text{AvRisk}_{k_2, r_{train}} = \sum_{\ell=1}^{m} \beta_\ell H_{\ell, k_2} = \langle \vec{H}_{k_2}, \beta \rangle$$

where $\vec{H}_{k_2} = (H_{\ell, k_2})_{\ell=1}^m$. Then, we get

$$\text{MinimaxError} = \sup_{k_2 > 2} |\langle \vec{H}_{k_2}, \beta - \hat{\beta} \rangle|.$$

If we assume that all the basis functions $h_\ell(u)$ are bounded by a common constant M, then it follows that H_ℓ, k are also bounded by the same constant M, and we have

$$\text{MinimaxError} \leq M||\beta - \hat{\beta}||_1 \leq M\sqrt{m}||\beta - \hat{\beta}||_2$$

Therefore, any convergence rate we can establish for $\hat{\beta}$ is inherited by the minimax error. Meanwhile, we can show that choosing k_0 sufficiently large that $(\vec{H}_2, \ldots, \vec{H}_{k_0})$ is full-rank, and setting weights $w_k = I\{k \leq k_0\}$, then the resulting $\hat{\beta}$ converges to the true β at the usual $O(1/\sqrt{n})$ rate. We state the result in the following theorem.

Theorem 3.2 *Consider a sequence of problems where the model $\mathcal{M}$, r_{train}, r_{test}, joint distribution $\{F_y\}_{y \in \mathcal{Y}}$, and class sampling distribution η are fixed as $k_1 \to \infty$. Further assume that the function $\bar{D}(u)$ defined by $\{F_y\}_{y\in\mathcal{Y}}$, η, and $\mathcal{M}$ satisfies*

$$\bar{D}(u) = \sum_{\ell=1}^{m} \beta_\ell h_\ell(u)$$

for some basis functions $h_\ell(u)$. Let k_0 be an integer sufficiently large so that

$$Rank(\vec{H}_2, \ldots, \vec{H}_{k_0}) = m.$$

Then, defining

$$\hat{\beta} = argmin_\beta \sum_{k=2}^{k_0} \left(AvTestRisk_k - \sum_{\ell=1}^{m} \beta_\ell H_{\ell,k} \right)^2$$

there exists some constant $C < \infty$ such that

$$\lim_{k_1 \to \infty} \sqrt{k_1} ||\hat{\beta} - \beta||_2 = C.$$

Proof. Note that the statistics AvTestRisk_k are U-statistics of the k_1 pairs of test and training samples. Therefore, by Hoeffding 1948, it follows that $(\text{AvTestRisk}_2, \ldots, \text{AvTestRisk}_{k_0})$ is asymptotically normal with covariance satisfying

$$\lim_{k_1 \to \infty} k_1 \text{Cov}(\text{AvTestRisk}_2, \ldots, \text{AvTestRisk}_{k_0}) = \Sigma,$$

for some positive semidefinite matrix Σ. Defining $\boldsymbol{H}$ to be the matrix with rows $\vec{H}_2, \ldots, \vec{H}_{k_0}$, this then implies that

$$\lim_{k_1 \to \infty} k_1 \text{Cov}(\hat{\beta}) = (\boldsymbol{H}^T \boldsymbol{H})^{-1} \boldsymbol{H}^T \Sigma \boldsymbol{H} (\boldsymbol{H}^T \boldsymbol{H})^{-1}.$$

It follows that defining

$$C = \sqrt{\text{tr}(\boldsymbol{H}^T \boldsymbol{H})^{-1} \boldsymbol{H}^T \Sigma \boldsymbol{H} (\boldsymbol{H}^T \boldsymbol{H})^{-1}}$$

we have

$$\lim_{k_1 \to \infty} \sqrt{k_1} ||\hat{\beta} - \beta||_2 = C.$$

□.

Misspecified case.

Now consider the more realistic setting where the model (14) is misspecified. We quantify the degree of misspecification by the ℓ_∞ error on [0,1]. Define

$$\delta = \inf_\beta \|\bar{D}(u) - \sum_{\ell=1}^m \beta_\ell h_\ell(u)\|_\infty,$$

and let $\tilde{\beta}$ be the coefficients β which attain the infimum, with $\tilde{D}(u) = \sum_{\ell=1}^m \tilde{\beta}_\ell h_\ell(u)$. To deal with this case, refer to the theory in section A.3. For each $u = [0,1]$, find a matrix $A(u)$ such that (i) the first column equals

$$A_1(u) = (h_1(u), \ldots, h_m(u))$$

and that (ii) the rest of the columns are orthogonal to the first, and (iii) $A(u)$ is full-rank. Then define $Z(u) = XA(u)$, and consider the column vector

$$Z_{1|-1}(u) = (I - P_{Z_{-1}})Z_1(u).$$

It can be shown that $Z_{1|-1}(u)$ is well-defined, regardless of how $A(u)$ is chosen. Then, by the theory in section A.3, the extra bias due to approximation error for predicting $\hat{D}(u)$ is given by

$$\text{Bias}^2(u) = \frac{||Z_{1|-1}(u)||_1^2}{||Z_{1|-1}(u)||_2^4}.$$

Define the maximum bias as

$$\text{Bias}^2_{max} = \sup_{u \in [0,1]} \text{Bias}^2(u).$$

From the analysis of the well-specified case, we know that the variance component of the prediction risk decreases at order $O(1/k)$. Therefore, the misspecified minimax error is of order

$$\text{MinimaxError} = O(1/\sqrt{k}) + \text{Bias}^2_{max}.$$

4 Results

5 Discussion

- In non-marginal classifiers, the classification rule has a joint dependence on the entire set of classes, and cannot be analyzed by conditioning on

Classifier	Test err$^{(20)}$	Test err$^{(400)}$	$\hat{p}_{400}^{EXP}$	$\hat{p}_{400}^{POS}$	$\hat{p}_{400}^{(5)}$
Naive Bayes	0.049	0.399	0.108	**0.142**	0.079
Logistic	0.078	0.289	0.166	**0.188**	0.130
SVM	0.140	0.455	0.299	**0.313**	0.227
ϵ-NN	0.049	0.409	0.084	**0.590**	0.102
Deep neural net	0.005	0.014	**0.011**	0.093	0.010

Table 1: Performance extrapolation: predicting the accuracy on 400 classes using data from 20 classes on a Telugu character dataset. $\epsilon = 0.002$ for ϵ-nearest neighbors.

individual classes.

- Now recall that the prior probabilities π_i for each classification task are free for the user to define, unlike the population distribution π_0 of class labels which is assumed to have an objective existence. Since the subsampled or 'small-scale' classification tasks (with label subsets $\mathcal{S}_i$) are presumably intended to approximate the 'full' classification problem (with the label set $\mathcal{Y}$), and since the prior in the full problem is π_0, a sensible choice would be to choose

$$\pi_i(y) = \frac{\pi_0(y)}{\sum_{y' \in \mathcal{S}_i} \pi_0(y')}.$$

  as the prior for the ith classification task. As it turns out, such a prior assignment also simplifies the theory, so we will assume that π_i is defined according to the above.

- $\mathcal{S}_{k_1} \subset \mathcal{S}_{k_2}$ with $\mathcal{S}_{k_1}$ being a subsample of $\mathcal{S}_{k_2}$.

A Appendix

A.1 Proofs

Lemma A.1 *Suppose π, $\{F_y\}_{y \in \mathcal{Y}}$ and marginal classifier $\mathcal{F}$ satisfy the tie-breaking condition. Take $x \in \mathcal{X}$. Defining $U_{y,\hat{F}_y}(x)$ as in* (8)*, and defining the random variable U by*

$$U = U_{Y,\hat{F}_Y}(x)$$

for $Y \sim \pi$, $\hat{F}_Y \sim \Pi_{Y,r}$, the distribution of U is uniform on $[0,1]$*, i.e.*

$$\Pr[U \leq u] = max\{u, 1\}.$$

Proof of Lemma A.1.

Define the variable $Z = \mathcal{M}(\hat{F}_Y)(x)$ for $Y \sim \pi$. By the tie-breaking condition, Z has a continuous density on $[0,1]$. Consider the survivor function of Z, $g(z) = \Pr[Z \geq z]$. From the definition (8), we see that

$$U = g(\mathcal{M}(\hat{F}_Y)(x)) = g(Z).$$

Now note that the survivor function of any continuous random variable, when applied to itself, is uniformly distributed. □

Proof of Theorem 3.1.

By the property of conditional expectations, and by definitions (7) and (1) and identity (12) , for $Y \sim \pi$, $\hat{F}_Y \sim \Pi_{Y,r}$ and $X \sim F_Y$ we have

$$\begin{aligned}\text{AvRisk}_{k,r} &= \mathbf{E}[\text{CondRisk}_k((Y, \hat{F}_Y), X)] \\ &= \int \text{CondRisk}_k((y, \hat{F}_y), x) d\pi(y) dF_y(x) d\Pi_{y,r}(\hat{F}_y) \\ &= (k-1) \int \int D((y^*, \hat{F}_{y^*}), x^*, u) u^{k-2} du d\pi(y) dF_y(x) d\Pi_{y,r}(\hat{F}_y) \\ &= (k-1) \int \bar{D}(u) u^{k-2} du,\end{aligned}$$

where

$$\bar{D}(u) = \int D((y^*, \hat{F}_{y^*}), x^*, u) \pi(y^*) dy dF_{y^*}(x^*) d\Pi_{y^*,r}(\hat{F}_{y^*}).$$

□

A.2 Background: Multiclass terminology

In this section we review the key terminology for multi-class classification and discuss examples of problems and algorithms which we will use throughout the paper to serve as concrete examples. We assume some degree of familiarity with statistical learning: however, this section can probably be skipped by the expert. Meanwhile, those new to the field might be aided by having a good introduction to the subject at hand, such as (Hastie et al, ESL) or (?? other book.)

While a *binary classification* problem generally refers to a class with two labels, $\mathcal{Y} = \{0, 1\}$, problems with three or more classes are called *multi-class classification* problems. The most famous dataset for illustrating a multi-class classification problem is Fisher's iris data (Fisher 1936), where the classification task is to assign a flower to one of three iris species based on four features: the lengths and widths of the sepals and the lengths and widths of the petals.

In classification problems, it is assumed that each observation belongs exclusively to a single class. In contrast, in *multi-label* classification, each observation can belong to multiple classes at the same time, or none at all. We do not address multi-label classification in this paper: however, we remark that any multi-label classification problem can be recoded as a single-label classification problem [find a reference so we don't have to explain this.]

The performance of a classification rule on a problem is evaluated by specifying a *cost function.* If the true class is y, but the classifier outputs y', the severity of this misclassification is quantified by $C(y', y)$. The most common cost function is *zero-one loss*: the cost is zero for correct classifications, and the cost is one for all incorrect classifications, i.e. $C(y', y) = \delta_y(y')$.

One setting where alternative cost functions are used is when there exists *hierarchical structure* of the label sets. For example, in image recognition, the label "golden retriever" may be a member of the class "dog," which is in itself another label. If we work under the single-label framework, then a picture of a golden retriever might be considered to have the true class of "golden retriever." While labelling the picture as "dog" would be semantically correct, we might prefer the more specific label. But while on a technical level we may consider "dog" to be the incorrect label for the picture, we would not want to overly penalize the assignment of "dog" to the picture. Therefore, in hierarchichal problems it is often appropriate to use a cost function which is reflective of the *semantic distance* between two labels, rather than the strict zero-one loss.

In our terminology, a *classification model* is an algorithm which learns a *classification rule* from *training data.* Examples of multi-class classification models include k-nearest neighbors, multinomial logistic regression, linear discriminant analysis (LDA), quadratic discriminant analysis (QDA), decision trees, and random forests, as well as the two 'divide and conquer' approaches, one-vs-one (OVO) and one-vs-all (OVA) (Friedman et al, 2008.)

The *generalization risk* is the expected cost over the population of label-feature pairs. Given *test data* sampled from the population, it is possible to obtain an unbiased estimate of the risk fof a classification rule.

A.3 Prediction risk in the misspecified linear model

Consider a misspecified linear model, such that

$$\mathbf{E}[Y|X=x] = f(x) = x^T\beta + a(x),$$

and

$$\text{Var}[Y|X=x] = \sigma^2.$$

Define $\delta = ||a||_\infty$.

Suppose now that we obtain observations (x_i, y_i) for $i = 1, ..., n$. The estimated coefficients $\hat{\beta}$ are given by $(X^TX)^{-1}X^Ty$. Let x_0 be a new point. The prediction $\hat{y}_0$ is given by

$$\hat{y}_0 = h^Ty = x_0^T(X^TX)^{-1}X^Ty.$$

What can we say about the prediction risk $R = E[(\hat{y}_0 - y_0)^2]$?

The prediction error can be computed via the bias-variance decomposition

$$R = \text{Bias}^2 + \text{Var},$$

where the variance term is

$$\text{Var} = \sigma^2(1 + ||h||^2)$$

Meanwhile, the bias term is

$$\begin{aligned}\text{Bias} = E[h_0^Ty - f(x)] &= h_0^T(X^T\beta + a(X)) - (x_0^T\beta + a(x_0)) \\ &= h^Ta(X) - a(x_0)\end{aligned}$$

where $a(X) = (a(x_1), ..., a(x_n))$. By assumption, $||a(X)||_\infty \leq \delta$ and $a(x_0) \leq \delta$.

Let us find a bound on the bias. The bias term is the same no matter what the true value of β, so we can take $\beta = 0$ without loss of generality. Also note that the prediction risk is invariant to change-of-basis, so without loss of generality we can take $x_0 = (1, 0, ...)$. This means that $\hat{y}_0 = \hat{\beta}_1$. But since the true signal is zero, we also have $E[\hat{y}_0] = E[\hat{\beta}_1] = h^T a(X)$–which is the estimated $\hat{\beta}_1$ for an OLS regression of response $a(X)$ on X.

Let us change the problem accordingly to the problem of the maximum size of $\hat{\beta}1$ for an OLS regression of y on X where it is known that $||y||\infty \leq \delta$. The maximum size of $\hat{\beta}_1$ in this problem gives us the bound on the bias which we originally sought.

Now note that by Holder's inequality,

$$|\hat{\beta}1| = |h^T y| \leq ||y||\infty ||h||_1 = \delta ||h||_1$$

so the key problem is to bound the L1-norm of h.

We know that $\hat{\beta}1$ for the regression $y \sim X$ is the same as the $\hat{\beta}$ obtained in the univariate regression of y on $X_{1|-1} = (I - P_{X_{-1}})X_1$. Here, P_A denotes the projection matrix onto the column space of matrix A, $P_A = A(A^TA)^{-1}A^T$. This means that the h vector can be written

$$h = \frac{1}{||X_{1|-1}||^2} X_{1|-1}.$$

Therefore, we have

$$||h||_1 = \frac{||X_{1|-1}||_1}{||X_{1|-1}||^2}.$$

It therefore follows that

$$\text{Bias} \leq \frac{||X_{1|-1}||_1}{||X_{1|-1}||^2}$$

and hence

$$R \leq \sigma^2(1 + ||h||^2) + \left(\frac{||X_{1|-1}||_1}{||X_{1|-1}||^2}\right)^2.$$

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