
How many faces can be recognized? Performance extrapolation for multi-class classification

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Abstract

1 The difficulty of multi-class classification generally increases with the number of
2 classes. Using data from a subset of the classes, can we predict how well a classifier
3 will scale with an increased number of classes? Under the assumption that the
4 classes are sampled exchangeably, and under the assumption that the classifier is
5 generative (e.g. QDA or Naive Bayes), we show that the expected accuracy when
6 the classifier is trained on k classes is the $k - 1$ st moment of a *conditional accuracy*
7 *distribution*, which can be estimated from data. This provides the theoretical
8 foundation for performance extrapolation based on pseudolikelihood, unbiased
9 estimation, and high-dimensional asymptotics. We find empirically that some of
10 the methods work well even for non-generative classifiers.

11 1 Introduction

12 In multi-class classification, one observes pairs (z, y) where $y \in \mathcal{Y} \subset \mathbb{R}^p$ are feature vectors, and z
13 are unknown labels, which lie in a countable label set \mathcal{Z} . The goal is to construct a classification rule
14 for predicting the label of a new data point; generally, the classification rule $h : \mathcal{Y} \rightarrow \mathcal{Z}$ is learned
15 from previously observed data points. In many applications of multi-class classification, such as face
16 recognition or image recognition, the space of potential labels is practically infinite. In such a setting,
17 one might consider a sequence of classification problems on finite label subsets $\mathcal{Z}_1 \subset \dots \subset \mathcal{Z}_K$,
18 where in the i -th problem, one constructs the classification rule $h^{(i)} : \mathcal{Y} \rightarrow \mathcal{Z}_i$. Supposing that (Z, Y)
19 have a joint distribution, define the accuracy for the i -th problem as

$$\text{acc}^{(i)} = \Pr[h^{(i)}(Y) = Z | Z \in \mathcal{Z}_i].$$

20 Using data from only \mathcal{Z}_k , can one predict the accuracy achieved on the larger label set \mathcal{Z}_K , with
21 $K > k$? This is the problem of *performance extrapolation*.

22 A practical instance of performance extrapolation occurs in neuroimaging studies, where the number
23 of classes k is limited by experimental considerations. Kay et al. [1] obtained fMRI brain scans which
24 record how a single subject's visual cortex responds to natural images. The label set \mathcal{Z} corresponds
25 to the space of all grayscale photographs of natural images, and the set \mathcal{Z}_1 is a subset of 1750
26 photographs used in the experiment. They construct a classifier which achieves over 0.75 accuracy
27 for classifying the 1750 photographs; based on exponential extrapolation, they estimate that it would
28 take on the order of $10^{9.5}$ photographs before the accuracy of the model drops below 0.10! Directly
29 validating this estimate would take immense resources, so it would be useful to develop the theory
30 needed to understand how to compute such extrapolations in a principled way.

31 However, in the fully general setting, it is impossible to construct non-trivial bounds on the accuracy
32 achieved on the new classes $\mathcal{Z}_K \setminus \mathcal{Z}_k$ based only on knowledge of \mathcal{Z}_k : after all, \mathcal{Z}_k could consist
33 entirely of well-separated classes while the new classes $\mathcal{Z}_K \setminus \mathcal{Z}_k$ consist entirely of highly inseparable

34 classes, or vice-versa. Thus, the most important assumption for our theory is that of *exchangeable*
 35 *sampling*. The labels in \mathcal{Z}_i are assumed to be an exchangeable sample from \mathcal{Z} . The condition of
 36 exchangeability ensures that the separability of random subsets of \mathcal{Z} can be inferred by looking at the
 37 empirical distributions in \mathcal{Z}_k , and therefore that some estimate of the achievable accuracy on \mathcal{Z}_K can
 38 be obtained.

39 The assumption of exchangeability greatly limits the scope of application for our methods. Many
 40 multi-class classification problems have a hierarchical structure [2], or have classes distributed
 41 according to non-uniform discrete distributions, e.g. power laws [3]; in either case, exchangeability
 42 is violated. It would be interesting to extend our theory to the hierarchical setting, or to handle
 43 non-hierarchical settings with non-uniform prior class probabilities, but again we leave the subject
 44 for future work.

45 In addition to the assumption of exchangeability, we consider a restricted set of classifiers. We focus on
 46 *generative classifiers*, which are classifiers that work by training a model separately on each class. This
 47 convenient property allows us to characterize the accuracy of the classifier by selectively conditioning
 48 on one class at a time. In section 3, we use this technique to reveal an equivalence between the
 49 expected accuracies of \mathcal{Z}_k to moments of a common distribution. This moment equivalence result
 50 allows standard approaches in statistics, such as U-statistics and nonparametric pseudolikelihood, to be
 51 directly applied to the extrapolation problem, as we discuss in section 4. In non-generative classifiers,
 52 the classification rule has a joint dependence on the entire set of classes, and cannot be analyzed
 53 by conditioning on individual classes. We confirmed that our methods work well for generative
 54 classifiers in simulations, which we have omitted from the paper. Since generative classifiers are
 55 rarely used in large classification problems, we felt that a more interesting demonstration would be to
 56 apply our methods to extrapolate the performance of multinomial logistic regression, support vector
 57 machines, and k -nearest neighbors—three commonly used non-generative classifiers. In Section 5,
 58 we see that our methods achieve accurate extrapolation for these three non-generative classifiers. A
 59 possible reason for this fact is that since the Bayes classifier (the optimal classifier as implemented by
 60 an oracle) is generative, our theory must also apply to any classifier which adequately approximates
 61 the Bayes classifier. We discuss this idea further in Section 6.

62 To our knowledge, we are the first to formalize the problem of prediction extrapolation. We introduce
 63 three methods for prediction extrapolation: the method of extended unbiased estimation and the
 64 constrained pseudolikelihood method are novel. The third method, based on asymptotics, is a new
 65 application of a recently proposed method for estimating mutual information [4].

66 2 Setting

67 Having motivated the problem of performance extrapolation, we now reformulate the problem for
 68 notational and theoretical convenience. Instead of requiring \mathcal{Z}_k to be a random subset of \mathcal{Z} as we
 69 did in section 1, take $\mathcal{Z} = \mathbb{N}$ and $\mathcal{Z}_k = \{1, \dots, k\}$. We fix the size of \mathcal{Z}_k without losing generality,
 70 since any monotonic sequence of finite subsets can be embedded in a sequence with $|\mathcal{Z}_k| = k$. In
 71 addition, rather than randomizing the labels, we will randomize the marginal distribution of each
 72 label; Towards that end, let $\mathcal{Y} \subset \mathbb{R}^p$ be a space of feature vectors, and let $\mathcal{P}(\mathcal{Y})$ be a measurable
 73 space of probability distributions on \mathcal{Y} . Let \mathcal{F} be a probability measure on \mathcal{P} , and let F_1, F_2, \dots
 74 be an infinite sequence of i.i.d. draws from \mathbb{F} . We refer to \mathbb{F} , a probability measure on probability
 75 measures, as a *meta-distribution*. The distributions F_1, \dots, F_k are the marginal distributions of the
 76 first k classes. We therefore rewrite the accuracy as

$$\text{acc}^{(t)} = \frac{1}{t} \sum_{i=1}^t \Pr_{F_i}[h^{(t)}(Y) = i].$$

77 where the probabilities are taken over $Y \sim F_i$.

78 In order to construct the classification rule $h^{(t)}$, we need data from the classes F_1, \dots, F_t . In most
 79 instances of multi-class classification, one observes independent observations from each F_i which
 80 are used to construct the classifier. Since the order of the observations does not generally matter, a
 81 sufficient statistic for the training data for the t -th classification problem is the collection of empirical
 82 distributions $\hat{F}_1^{(t)}, \dots, \hat{F}_t^{(t)}$ for each class. Henceforth, we make the simplifying assumption that
 83 the training data for the i -th class remains fixed from $t = i, i + 1, \dots$, so we drop the superscript on

84 $\hat{F}_i^{(t)}$. Write $\hat{\mathbb{F}}(F)$ for the conditional distribution of \hat{F}_i given $F_i = F$; also write $\hat{\mathbb{F}}$ for the marginal
 85 distribution of \hat{F} when $F \sim \mathbb{F}$. As an example, suppose every class has the number of training
 86 examples $r \in \mathbb{N}$; then \hat{F} is the empirical distribution of r i.i.d. observations from F , and $\hat{\mathbb{F}}(F)$ is the
 87 empirical meta-distribution of \hat{F} . Meanwhile, $\hat{\mathbb{F}}$ is the meta-distribution of the empirical distribution
 88 of r i.i.d. draws from a random $F \sim \mathbb{F}$.

89 2.1 Multiclass classification

90 Extending the formalism of Tewari and Bartlett [5]¹, we define a classifier as a collection of mappings
 91 $\mathcal{M}_i : \mathcal{P}(\mathcal{Y})^k \times \mathcal{Y} \rightarrow \mathbb{R}$ called *margin functions*. Intuitively speaking, each margin function *learns*
 92 a model from the first k arguments, which are the empirical marginals of the k classes, $\hat{F}_1, \dots, \hat{F}_k$;
 93 for each class, the classifier assigns a *margin* or *score* to the *query point* $y \in \mathcal{Y}$. A higher score
 94 $\mathcal{M}_i(\hat{F}_1, \dots, \hat{F}_k, y)$ indicates a higher estimated probability that y belongs to the k -th class. Therefore,
 95 the classification rule corresponding to a classifier \mathcal{M}_i assigns a class with maximum margin to y :

$$h(y) = \operatorname{argmax}_{i \in \{1, \dots, k\}} \mathcal{M}_i(y).$$

96 For some classifiers, the margin function \mathcal{M}_i is especially simple in that \mathcal{M}_i is only a function of \hat{F}_i
 97 and y . Furthermore, due to symmetry, in such cases one can write

$$\mathcal{M}_i(\hat{F}_1, \dots, \hat{F}_k, y) = \mathcal{Q}(\hat{F}_i, y),$$

98 where \mathcal{Q} is called a *single-class margin* (or simply *margin*), and we say that \mathcal{M} is a *generative*
 99 *classifier*. Quadratic discriminant analysis and Naive Bayes [6] are two examples of generative
 100 classifiers².

101 For notational convenience, we assume that ties occur with probability zero: that is, Note that the
 102 tie-breaking property implies that \mathbb{F} contains no atoms. The *generative* property allows us to prove
 103 strong results about the accuracy of the classifier under the exchangeable sampling assumption, as we
 104 see in Section 3.

105 3 Performance extrapolation for generative classifiers

106 Let us specialize to the case of a generative classifier, with margin \mathcal{Q} . Consider estimating the
 107 expected accuracy for the t -th classification problem,

$$p_t \stackrel{\text{def}}{=} \mathbf{E}[\operatorname{acc}^{(t)}]. \quad (1)$$

108 In the case of a generative classifier, we have

$$p_k = \mathbf{E}[\operatorname{acc}^{(k)}] = \mathbf{E} \left[\frac{1}{k} \sum_{i=1}^k \Pr_{Y \sim F_i} [\mathcal{Q}(\hat{F}_i, Y) > \max_{j \neq i} \mathcal{Q}(\hat{F}_j, Y)] \right].$$

109 Define the *conditional accuracy* function $u(\hat{F}, y)$ which maps a distribution \hat{F} on \mathcal{Y} and a *test*
 110 observation y to a real number in $[0, 1]$. The conditional accuracy gives the probability that for
 111 independently drawn \hat{F}' from $\hat{\mathbb{F}}$, that $\mathcal{Q}(\hat{F}, y)$ will be greater than $\mathcal{Q}(\hat{F}', y)$:

$$u(\hat{F}, y) = \Pr_{\hat{F}' \sim \hat{\mathbb{F}}} [\mathcal{Q}(\hat{F}, y) > \mathcal{Q}(\hat{F}', y)].$$

¹We borrow their terminology of *margin functions*, but introduce the notion of a classifier as a multiple-argument functional on empirical distributions. The functional formulation of a classifier echoes the functional formulation of estimators common in the statistical literature.

²For QDA, the margin is given by

$$\mathcal{Q}_{QDA}(\hat{F}, y) = -(y - \mu(\hat{F}))^T \Sigma(\hat{F})^{-1} (y - \mu(\hat{F})) - \log \det(\Sigma(\hat{F})),$$

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 is

$$\mathcal{Q}_{NB}(\hat{F}, y) = \sum_{i=1}^n \log \hat{f}_i(y_i),$$

where \hat{f}_i is a density estimate for the i -th component of \hat{F} .

112 Define the *conditional accuracy* distribution ν as the law of $u(\hat{F}, Y)$ where \hat{F} and Y are generated
 113 as follows: (i) a true distribution F is drawn from \mathbb{F} ; (ii) the query Y is drawn from F , and (iii) the
 114 empirical distribution \hat{F} is drawn from $\hat{\mathbb{F}}(F)$ (e.g., the distribution of the empirical distribution of
 115 r i.i.d. observations drawn from F), with Y independent of \hat{F} . The significance of the conditional
 116 accuracy distribution is that the expected generalization error p_t can be written in terms of its
 117 moments.

118 **Theorem 3.1.** *Let \mathcal{Q} be a single-distribution margin, and let $\mathbb{F}, \hat{\mathbb{F}}(F)$ be a distribution on $\mathcal{P}(\mathcal{Y})$.
 119 Further assume that $\hat{\mathbb{F}}$ and \mathcal{Q} jointly satisfy the tie-breaking property:*

$$\Pr[\mathcal{Q}(\hat{F}, y) = \mathcal{Q}(\hat{F}', y)] = 0 \quad (2)$$

120 *for all $y \in \mathcal{Y}$, where $\mathbb{F}, \mathbb{F}' \stackrel{iid}{\sim} \hat{\mathbb{F}}$. Let U be defined as the random variable*

$$U = u(\hat{F}, Y)$$

121 *for $F \sim \mathbb{F}$, $Y \sim F$, and $\hat{F} \sim \hat{\mathbb{F}}(F)$ with $Y \perp \hat{F}$. Then*

$$p_k = \mathbf{E}[U^{k-1}],$$

122 *where p_k is the expected accuracy as defined by (1).*

123 **Proof.** Write $q^{(i)}(y) = \mathcal{Q}(\hat{F}_i, y)$. By using conditioning and conditional independence, p_k can be
 124 written

$$\begin{aligned} p_k &= \mathbf{E} \left[\frac{1}{k} \sum_{i=1}^k \Pr[q^{(i)}(Y) > \max_{j \neq i} q^{(j)}(Y)] \right] \\ &= \mathbf{E} \left[\Pr[q^{(1)}(Y) > \max_{j \neq 1} q^{(j)}(Y)] \right] \\ &= \mathbf{E}_{F_1} [\Pr[q^{(1)}(Y) > \max_{j \neq 1} q^{(j)}(Y) | \hat{F}_1, Y]] \\ &= \mathbf{E}_{F_1} [\Pr[\cap_{j>1} q^{(1)}(Y) > q^{(j)}(Y) | \hat{F}_1, Y]] \\ &= \mathbf{E}_{F_1} [\prod_{j>1} \Pr[q^{(1)}(Y) > q^{(j)}(Y) | \hat{F}_1, Y]] \\ &= \mathbf{E}_{F_1} [\Pr[q^{(1)}(Y) > q^{(2)}(Y) | \hat{F}_1, Y]^{k-1}] \\ &= \mathbf{E}_{F_1} [u(\hat{F}_1, Y)^{k-1}] = \mathbf{E}[U^{k-1}]. \end{aligned}$$

125 \square

126 Theorem 3.1 tells us that the problem of extrapolation can be approached by attempting to estimate
 127 the conditional accuracy distribution. The $(t-1)$ -th moment of U gives us p_t , which will in turn be
 128 a good estimate of $\text{acc}^{(t)}$.

129 While $U = u(\hat{F}, Y)$ is not directly observed, we can obtain unbiased estimates of $u(\hat{F}_i, y)$ by using
 130 test data. For any $\hat{F}_1, \dots, \hat{F}_k$, and independent test point $Y \sim F_i$, define

$$\hat{u}(\hat{F}_i, Y) = \frac{1}{k-1} \sum_{j \neq i} I(\mathcal{Q}(\hat{F}_i, Y) > \mathcal{Q}(\hat{F}_j, Y)). \quad (3)$$

131 Then $\hat{u}(\hat{F}_i, Y)$ is an unbiased estimate of $u(\hat{F}_i, Y)$, as stated in the following theorem.

132 **Theorem 3.2.** *Assume the conditions of theorem 3.1. Then defining*

$$V = (k-1)\hat{u}(\hat{F}_i, y), \quad (4)$$

133 *we have*

$$V \sim \text{Binomial}(k-1, u(\hat{F}_i, y)).$$

134 *Hence,*

$$\mathbf{E}[\hat{u}(\hat{F}_i, y)] = u(\hat{F}_i, y).$$

135

136 In section 4, we will use this result to estimate the moments of U . Meanwhile, since U is a random
 137 variable on $[0, 1]$, we also conclude that p_t follows a *mixed exponential decay*. Let α be the law of
 138 $-\log(U)$. Then from change-of-variables $\kappa = -\log(u)$, we get

$$\mathbf{E}[\text{acc}^{(t)}] = \mathbf{E}[U^{t-1}] = \int_0^1 u^{t-1} d\nu(u) = \int_0^1 e^{t \log(u)} \frac{1}{u} d\nu(u) = \int_{\mathbb{R}^+} e^{-\kappa t} d\alpha(\kappa).$$

139 This fact immediately suggests the technique of fitting an mixture of exponentials to the test error at
 140 $t = 2, 3, \dots, k$: we explore this idea further in Section 4.1.

141 3.1 Properties of the conditional accuracy distribution

142 The conditional error distribution ν is determined by \mathbb{F} and \mathcal{Q} . What can we say about the the
 143 conditional accuracy distribution without making any assumptions on either \mathbb{F} or \mathcal{Q} ? The answer
 144 is: not much—for an arbitrary probability measure ν' on $[0, 1]$, one can construct \mathbb{F} and \mathcal{Q} such that
 145 $\nu = \nu'$, even if one makes the *perfect sampling assumption* that $\hat{F} = F$.

146 **Theorem 3.3.** *Let U be defined as in Theorem 3.1, and let ν denote the law of U . Then, for any*
 147 *probability distribution ν' on $[0, 1]$, one can construct a meta-distribution \mathbb{F} and a margin \mathcal{Q} such*
 148 *that $\nu = \nu'$ under perfect sampling (that is, $\hat{F} = F$).*

149 **Proof.** Let G be the cdf of ν , $G(x) = \int_0^x d\nu(x)$, and let $H(u) = \sup_x \{G(x) \leq u\}$. Define \mathcal{Q} by

$$\mathcal{Q}(\hat{F}, y) = \begin{cases} 0 & \text{if } \mu(\hat{F}) > y + H(y) \\ 0 & \text{if } y + H(y) > 1 \text{ and } \mu(\hat{F}) \in [H(y) - y, y] \\ 1 + \mu(\hat{F}) - y & \text{if } \mu(\hat{F}) \in [y, y + H(y)] \\ 1 + y + \mu(\hat{F}) & \text{if } \mu(\hat{F}) + H(y) > 1 \text{ and } \mu(\hat{F}) \in [0, H(y) - y]. \end{cases}$$

150 Let $\theta \sim \text{Uniform}[0, 1]$, and define $F \sim \mathbb{F}$ by $F = \delta_\theta$, and also $\hat{F} = F$. A straightforward calculation
 151 yields that $\nu = \nu'$. \square

152 On the other hand, we can obtain a positive result if we assume that the classifier approximates
 153 a *Bayes classifier*. Assuming that F is absolutely continuous with respect to Lebesgue measure
 154 Λ with probability one, a Bayes classifier results from assuming perfect sampling ($\hat{F} = F$) and
 155 taking $\mathcal{Q}(\hat{F}, y) = \frac{dF}{d\Lambda}(y)$. Theorem 3.4. states that for a Bayes classifier, ν has a density $\eta(u)$
 156 which is monotonically increasing. Since a ‘good’ classifier approximates the Bayes classifier, we
 157 intuitively expect that a monotonically increasing density η is a good model for the conditional
 158 accuracy distribution of a ‘good’ classifier.

159 **Theorem 3.4.** *Assume the conditions of theorem 3.1, and further suppose that $\hat{F} = F$, F is*
 160 *absolutely continuous with respect to Λ with probability one, that $\mathcal{Q}(\hat{F}, y) = \frac{dF}{d\Lambda}(y)$, and that $F|Y$*
 161 *has a regular conditional probability distribution. Let ν denote the law of U . Then ν has a density*
 162 *$\eta(u)$ on $[0, 1]$ which is monotonic in u .*

163 **Proof.** It suffices to prove that

$$\nu([u, u + \delta]) < \nu([v, v + \delta])$$

164 for all $0 < u < v < 1$ and $0 < \delta < 1 - v$. Let $\mathcal{P}_{ac}(\mathcal{Y})$ denote the space of distributions supported
 165 on \mathcal{Y} which are absolutely continuous with respect to p -dimensional Lebesgue measure Λ . Let \mathbb{Y}
 166 denote the marginal distribution of Y for $Y \sim F$ with $F \sim \mathbb{F}$. Define the set

$$J_y(A) = \{F \in \mathcal{P}_{ac}(\mathcal{Y}) : u(F, y) \in A\}.$$

167 for all $A \subset [0, 1]$. One can verify that for all $y \in \mathcal{Y}$,

$$\Pr_{\mathbb{F}}[J_y([u, u + \delta]) | Y = y] \leq \Pr_{\mathbb{F}}[J_y([v, v + \delta]) | Y = y],$$

168 using the fact that \mathbb{F} has no atoms. Hence, we obtain

$$\Pr[U \in [u - \delta, u + \delta]] = \mathbf{E}_{\mathbb{Y}}[\Pr_{\mathbb{F}}[J_Y([u, u + \delta]) | Y]] \leq \mathbf{E}_{\mathbb{Y}}[\Pr_{\mathbb{F}}[J_Y([v, v + \delta]) | Y]] = \Pr[U \in [v - \delta, v + \delta]].$$

169 Taking $\delta \rightarrow 0$, we conclude the theorem. \square

170

4 Estimation

Suppose we have m independent test repeats per class, $y^{(i),1}, \dots, y^{(i),m}$. Let us define

$$V_{i,j} = \sum_{\ell \neq i} I(\mathcal{M}_i(\hat{F}_1, \dots, \hat{F}_k, y^{(i,j)}) > \mathcal{M}_\ell(\hat{F}_1, \dots, \hat{F}_k, y^{(i,j)})),$$

which coincides with the definition (4) in the special case that \mathcal{M} is generative.

At a high level, we have a hierarchical model where U is drawn from a distribution ν on $[0, 1]$ and then $V_{i,j} \sim \text{Binomial}(k, U)$. Let us assume that U has a density $\eta(u)$: then the marginal distribution of $V_{i,j}$ can be written

$$\Pr[V_{i,j} = \ell] = \binom{k}{\ell} \int_0^1 u^\ell (1-u)^{k-\ell} \eta(u) du.$$

However, the observed $\{V_{i,j}\}$ do *not* comprise an i.i.d. sample.

We discuss the following three approaches for estimating $p_t = \mathbf{E}[U^{t-1}]$ based on $V_{i,j}$. The first is an extension of *unbiased estimation* based on binomial U-statistics, which is discussed in Section 4.1. The second is the *pseudolikelihood* approach. In problems where the marginal distributions are known, but the dependence structure between variables is unknown, the *pseudolikelihood* is defined as the product of the marginal distributions. For certain problems in time series analysis and spatial statistics, the maximum pseudolikelihood estimator (MPLE) is proved to be consistent [7]. We discuss pseudolikelihood-based approaches in Section 4.2. Thirdly, we note that the high-dimensional theory of Anon 2006 can be applied for prediction accuracy, which we discuss in Section 4.3.

4.1 Extensions of unbiased estimation

If $V \sim \text{Binomial}(k, U)$, then an unbiased estimator of U^t exists if and only if $0 \leq t \leq k$.

The theory of U-statistics [8] provides the minimal variance unbiased estimator for U^t :

$$U^t = \mathbf{E} \left[\binom{V}{t} \binom{k}{t}^{-1} \right].$$

This result can be immediately applied to yield an unbiased estimator of p_t , when $t \leq k$:

$$\hat{p}_t^{UN} = \frac{1}{km} \sum_{i=1}^k \sum_{j=1}^m \binom{V_{i,j}}{t-1} \binom{k}{t-1}^{-1}. \quad (5)$$

However, since \hat{p}_t^{UN} is undefined for $k \geq t$, we can use exponential extrapolation to define an extended estimator \hat{p}_t^{EXP} for $k > t$. Let $\hat{\alpha}$ be a measure defined by solving the optimization problem

$$\text{minimize} \sum_{t=2}^k \left(\hat{p}_t^{UN} - \int_0^\infty \exp[-t\kappa] d\hat{\alpha}(\kappa) \right)^2.$$

After discretizing the measure $\hat{\alpha}$, we obtain a convex optimization problem which can be solved using non-negative least squares [9]. Then define

$$\hat{p}_t^{EXP} = \begin{cases} \hat{p}_t^{UN} & \text{for } t \leq k, \\ \int_0^\infty \exp[-t\kappa] d\hat{\alpha}(\kappa) & \text{for } t > k. \end{cases}$$

4.2 Maximum pseudolikelihood

The pseudolikelihood is defined as

$$\ell(\eta) = \sum_{i=1}^k \sum_{j=1}^m \log \left(\int u^{V_{i,j}} (1-u)^{k-V_{i,j}} \eta(u) du \right), \quad (6)$$

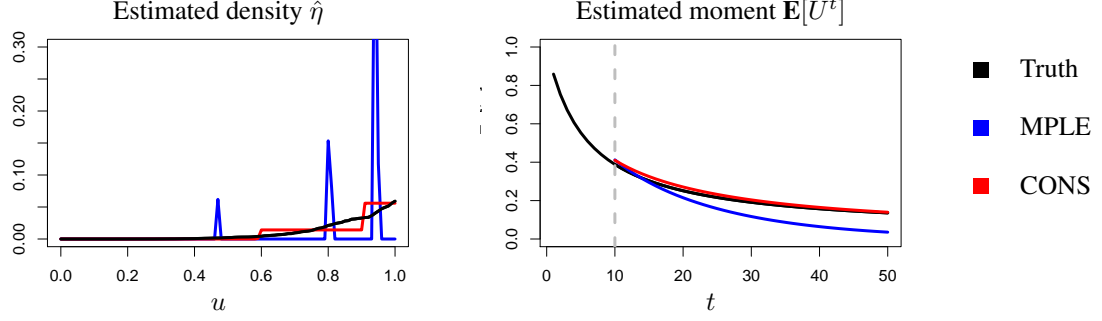


Figure 1: Maximum pseudolikelihood (MPLE) versus constrained pseudolikelihood (CONS). Adding constraints improves the estimation of the density $\eta(u)$, as well as moment estimation.

and a maximum pseudolikelihood estimator (MPLE) is defined as any density $\hat{\eta}$ such that

$$\ell(\hat{\eta}_{MPLE}) = \sup_{\eta} \ell(\eta).$$

The motivation for $\hat{\eta}_{MPLE}$ is that it consistently estimates η in the limit where $k \rightarrow \infty$. However, in finite samples, $\hat{\eta}_{MPLE}$ is not uniquely defined, and if we define the plug-in estimator

$$\hat{p}_t^{MPLE} = \int u^{t-1} \hat{\eta}_{MPLE}(u) du,$$

\hat{p}_t^{MPLE} can vary over a large range, depending on which $\hat{\eta} \in \text{argmax}_{\eta} \ell_t(\eta)$ is selected. These shortcomings motivate the adoption of additional constraints on the estimator $\hat{\eta}$.

Theorem 3.4. motivates the *monotonicity constraint* that $\frac{d\hat{\eta}}{du} > 0$. A second constraint is to restrict the k -th moment of $\hat{\eta}$ to match the unbiased estimate. The addition of these constraints yields the constrained PMLE $\hat{\eta}_{CON}$, which is obtained by solving

$$\text{maximize } \ell(\eta) \text{ subject to } \int u^{k-1} \eta(u) du = \hat{p}_k^{UN} \text{ and } \frac{d\hat{\eta}}{du} > 0.$$

By discretizing η , all of the above maximization problems can be solved using a general-purpose convex solver³. As seen in Figure 1, the added constraints can improve estimation of η and thus improve moment estimation.

4.3 High-dimensional asymptotics

Under a number of conditions on the distribution \mathbb{F} , including (but not limited to) having a large dimension p , Anon et al. [4] relate the accuracy p_t of the Bayes classifier to the mutual information between the label z and the response y :

$$p_t = \bar{\pi}_t(\sqrt{2I(Z; Y)}).$$

where

$$\bar{\pi}_k(c) = \int_{\mathbb{R}} \phi(z - c) \Phi(z)^{k-1} dz.$$

While our goal is not to estimate the mutual information, we note that the results of Anon 2016 imply a relationship between p_k and p_K for the Bayes error under the high-dimensional regime:

$$p_K = \bar{\pi}_K(\bar{\pi}_k^{-1}(p_k)).$$

Therefore, under the high-dimensional conditions of [4] and assuming that the classifier approximates the Bayes classifier, we naturally obtain the following estimator

$$\hat{p}_t^{HD} = \bar{\pi}_K(\bar{\pi}_k^{-1}(\hat{p}_k^{UN})).$$

³ We found that the CVX discipline convex programming language, using the ECOS second-order cone programming solver, succeeds in optimizing the problems where the dimension of the discretized η is as large as 10,000 [10, 11].

| Classifier | Test acc ⁽²⁰⁾ | Test acc ⁽⁴⁰⁰⁾ | \hat{p}_{400}^{EXP} | \hat{p}_{400}^{CON} | \hat{p}_{400}^{HD} |
|----------------|--------------------------|---------------------------|-----------------------|-----------------------|----------------------|
| Logistic | 0.922 | 0.711 | 0.844 | 0.721 | 0.686 |
| SVM | 0.860 | 0.545 | 0.737 | 0.575 | 0.546 |
| ϵ -NN | 0.880 | 0.591 | 0.903 | 0.608 | 0.839 |

Figure 2: Performance extrapolation: predicting the error on 400 classes using data from 20 classes on a Telugu character dataset. $\epsilon = 0.002$ for ϵ -nearest neighbors.

5 Results

We applied the methods described in Section 4 to predict the 400-class accuracy of multinomial logistic regression, SVM [6], and ϵ -nearest neighbors⁴ on a Telegu character classification task [12], using 20-class data with 100 examples per class. The results are displayed in Figure 2.

Taking the test accuracy on 400 classes (using 50 test examples per class) as a proxy for $\text{acc}^{(400)}$, we compare the performance of the three extrapolation methods. The exponential extrapolation method makes use of the fewest theoretical assumptions, but performs badly on all three problems. Meanwhile, constrained PMLE makes an extra assumption in the monotonicity of $\eta(u)$, which is true if the classifier is sufficiently close to the Bayes classifier, and achieves the best and most consistent results. The high-dimensional estimator \hat{p}^{HD} is the most assumption-heavy; in addition to assuming approximation to the Bayes classifier, it also requires Y to be high-dimensional, and to satisfy a number of other technical conditions (Anon 2016). Nevertheless, it performs well on the multinomial logistic and SVM classifiers. That said, all three classifiers studied are non-generative, hence violating an assumption common to both the \hat{p}^{EXP} and \hat{p}^{CON} estimators: therefore, it is doubtful if the theory developed so far can do much to explain the relative performance of these methods.

6 Discussion

We have developed a theory of prediction extrapolation for generative classifiers, under the assumption of exchangeable classes. The equivalence between the expected t -class accuracy and the $t - 1$ -th moment of the conditional accuracy distribution allows a variety of methods to be applied to the problem. We develop two novel extrapolation methods, and also propose a new application of the mutual information estimator [4] as a third method for prediction extrapolation.

Empirical results indicate that our methods generalize beyond generative classifiers. A possible explanation is that since the Bayes classifier is generative, any classifier which approximates the Bayes classifier is also ‘approximately generative.’ However, an important caveat is that the classifier must already attain close to the Bayes accuracy on the smaller subset of classes. If the classifier is initially far from the Bayes classifier, and then becomes more accurate as more classes are added, our theory could underestimate the accuracy on the larger subset. This is a non-issue for generative classifiers when the training data per class is fixed, since a generative classifier approximates the Bayes rule if and only if the single-class margin approximates the Bayes optimal single-class margin. On the other hand, for classifiers with built-in *model selection* or *representation learning*, it is expected that the individual class margins become more accurate, in the sense that they better approximate a monotonic function of the class margins of the Bayes classifier, as data from more classes is added.

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⁴ k -nearest neighbors with $k = \epsilon n$ for fixed $\epsilon > 0$

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