Probabilistic Classification from a K-Nearest-Neighbour Classifier

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Abstract K-nearest-neighbours is a simple classifier, and with increasing size of training set, the accuracy of its class predictions can be made asymptotic to the upper bound. Probabilistic classifications can also be generated: the accuracy of a simple proportional scheme will also be asymptotic to the upper bound, in the case of large training sets. Outside this limit, this and other existing schemes make ineffective use of the available information: this paper proposes a more accurate method, that improves the state-of-the-art performance, evaluated on several public data sets. Criteria such as the degree of unanimity among the neighbours, the observed rank of the correct class, and the intra-class confusion matrix can be used to tabulate the observed classification accuracy within the (cross-validated) training set. These tables can then be used to make probabilistic class predictions for the previously unseen test set, used to evaluate the novel and previous methods in two ways: i) mean *a posteriori* probability and ii) accuracy of the discrete prediction obtained from integrating the probabilistic estimates from independent sources. The proposed method performs particularly well in the limit of small training set sizes.

Keywords Pattern Recognition, Plant Leaves Classification, k-Nearest Neighbours, Density Estimators, Combining Features

1 Introduction

The 'K-nearest neighbour' (K-NN) classifier is a fundamental tool for pattern analysis, providing a straightforward means of estimating to which class a previously unseen sample vector belongs, given a finite training set. It naturally generalises to problems with multiple classes; for a 'test' set of unseen vectors, the resulting precision and recall statistics provide an insight into the separability of the problem. Moreover, its performance can be improved using metric learning approaches [14], and accelerated with enhanced implementations [9]. In this paper, methods are examined for using the training set to estimate the class membership *probabilities* for a test vector. A novel approach is proposed, which has the dual advantages of a fast, non-iterative implementation, and also providing significantly more accurate estimates than the state-of-the-art, over a range of test sets. One challenging set comprises images of leaf specimens from one-hundred species; a sample of which is shown in Figure 1.

The standard K-NN classifier requires a single parameter, K, to select the K nearest elements in the training set: the single most popular class label in this subset is output as the *discrete* estimate. There are some possible variations of a nearest neighbours system in the type of distance measure used and in the tie-break mechanism. With increasing size of training set, the accuracy of the K-NN discrete estimate tends towards the lowest possible – the Bayes error rate – if K can be increased along with the training set size, or twice this rate otherwise [3]. However, the focus of the current work is with small training set sizes: the objective is to use the limited data available as efficiently as possible.

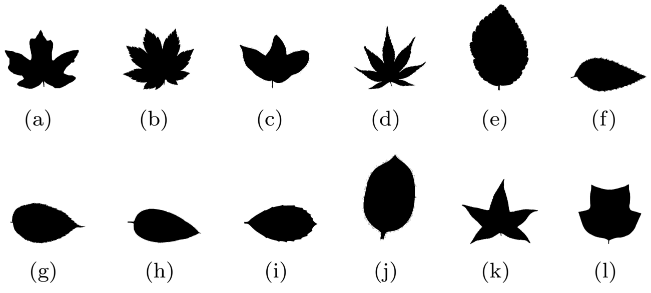


Figure 1. A small variety of plant species that are part of the challenging one-hundred species leaves data set: (a) Acer Campestre. (b) Acer Circinatum. (c) Acer Mono. (d) Acer Palmatum. (e) Alnus Rubra. (f) Alnus Sieboldiana. (g) Betula Austrosinensis. (h) Eucalyptus Urnigera. (i) Ilex Aquifolium. (j) Ilex Cornuta. (k) Liquidambar Styraciflua. (l) Liriodendron Tulipifera.

A probabilistic estimate of class label is not part of the standard output of the K-NN. However, the state-of-the-art standard method [6] is to base the estimate on the proportion of the K neighbours in each class. It can be shown that this will, again in the case of large training set size, provide estimates that converge on the Bayes estimates of the p.d.f.s for each class label. A useful development [1] is to allocate a weight to each member of the training set, and then optimise these weights to maximise the likelihood of this training data. These methods are further described in Section 2. There are also other approaches to density estimation: parametric methods such as Expectation-Maximization of Gaussian Mixture models [12], and non-parametric Kernel-based methods [2, 8] that generalise the histogram-based accumulation of samples. These are not included in this investigation because they are not suitable at the operating range of interest, i.e. problems with scores of classes in hundreds of dimensions, with only a handful of data points per class.

For discrete estimates, the evaluation of a classifier's performance is straightforward: precision and recall can be combined into a single 'mean accuracy' characteristic. The most appropriate evaluation of probabilistic estimates is to report the mean log likelihood of the unseen test data: this is maximised when the Bayes estimate of the p.d.f. is used, and in general its expectation will differ by the Kullback-Leibler distance from the p.d.f. Most importantly, probabilistic estimates from different sources can be combined together much more effectively than discrete estimates. If the sources are conditionally independent then this is a straightforward multiplication: this enables evidence to be combined with prior probabilities, or the separate available channels of evidence to be combined together.

A framework is proposed to tabulate statistical properties of the neighbours from within the training set, and how these characterize the classification performance. These properties can be combined in a robust and straightforward (non-iterative) approach. Within the framework, the K-NN classifier is used to provide statistics about its expected performance within the training set, which are then used to provide estimates for the unseen test set process. The proposed approach is compared against the standard [6] and the recent extension [1].

The paper is organized as following: Section 2 describes the notation and evaluation of the state-of-the-art of probabilistic estimators in a K-NN system. Thereafter, in Section 3, the novel work is described to define a series of estimators based on tabulation of statistics. Section 4 describes the public data sets used to evaluate the estimators, in addition to the experimental results per data set. The paper is concluded in Section 5, which includes comments on further work.

2 Probabilistic Estimators

Let the training set of n vectors, $\mathcal{Y}$, be denoted by $\{\mathbf{y}_1, \ldots, \ \mathbf{y}_n\}$ and the test set $\mathcal{X}$ is formed by m vectors $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$. Both sets are labelled using $\{y_1, \ldots, y_n\}$ and $\{x_1, \ldots, x_m\}$, respectively, where each label one of the C discrete classes (or categories) $1, \ldots, C$. For convenience, an identity operator $I(\cdot)$ is defined to obtain a vector's label, i.e. label, i.e. $I(\mathbf{x}_i) \equiv x_i$, and in particular $p(I(\ \mathbf{x}_i){=}j) \equiv p(x_i{=}j)$.

Formally, the objective is to calculate the estimator $\hat{p}(\cdot)$ to be as close as possible to the Bayes estimate $p^*(x_i = j)$, i.e. the probability that a given test vector has label j, where $1 \leq j \leq C$.

This can be factored into a likelihood term and a prior probability that sample i is of label j:

$$\underbrace{\hat{p}(x_i{=}j)}_{\text{posterior}} = \underbrace{\hat{L}\big(x_i{=}j \mid \mathbf{x}_i, \mathcal{Y}\big)}_{\text{likelihood}} \underbrace{\pi(x_i{=}j)}_{\text{prior}} \tag{1}$$

Typically, for experimental purposes, the prior terms are often all set to be equal; though naturally, in practical applications they may have specific values determined by the circumstances. The posterior estimator is an estimate of the unknown, optimal, Bayes estimate $p^*(\cdot)$.

Note that, firstly by assuming an exhaustive and exclusive labelling, both $\hat{p}(\cdot)$ and $p^*(\cdot)$ will sum to unity over the C classes. Secondly, the Bayes estimate $p^*(\cdot)$ is optimal in the sense that it minimises the posterior expected loss over the unseen test set $\{\mathbf{x}_i\}$, across all possible estimates $\hat{p}$. Thirdly, the appropriate evaluation measure for any given estimate, is the Kullback-Leibler distance $D(p^*(\cdot), \hat{p}(\cdot))$. However, since in general $p^*(\cdot)$ is unknown, one way to report the accuracy of a particular estimator $\hat{p}_A$ is by evaluating its mean log posterior $\mathbf{LP}_A$, using a sufficiently large unseen test set $\mathcal{X}$:

$$\mathbf{LP}_A = \sum_{i=1}^{m} \log \hat{p}_A\big(I(\mathbf{x}_i){=}x_i\big) \tag{2}$$

This expression quantifies the extent to which this estimator 'picked the right horse to win the race', i.e. the value of $\hat{p}(\mathbf{x})_i$ for the correct label x_i . This quantity is maximised for the Bayes estimator p^*, and it can be used to compare the relative accuracies of any two methods A and B, with estimators $\hat{p}_A$ and $\hat{p}_B$. One aspect of this metric is that it diverges to $-\infty$ if $\exists i : \hat{p}\big(I(\mathbf{x}_i){=}x_i\big) = 0$. As a consequence, the estimator fails to assign a finite probability to an event that did indeed transpire. To address this problem, an estimator should assign finite probabilities to all possible label assignments.

Alternatively, the accuracy of the estimates can be evaluated by combining evidence from S multiple sources, i.e. the set of training sets $\{\mathcal{Y}_1, \ldots, \mathcal{Y}_S\}$, where the vectors in each set have their own associated feature space. If these sources are independent, then the combined estimate $\hat{q}(\cdot)$, using these estimators for these features is:

$$\hat{q}(x_i = j|\mathcal{Y}_1 \ldots \mathcal{Y}_S) = \frac{\displaystyle\prod_{s=1}^{S} \hat{p}(x_i^s = j|\mathcal{Y}_s)}{\displaystyle\sum_{c=1}^{C} \prod_{s=1}^{S} \hat{p}(x_i^s = c|\mathcal{Y}_s)} \tag{3}$$

2.1 The Proportional (Prop) Estimator

The standard approach [6] is to define a proportional estimator, $\hat{p}_{\text{Prop}}(\cdot)$, as follows. For any given input vector $\mathbf{x}_i$, the subset of K nearest training set neighbours is ordered according to their ascending distance to the considered sample $\{\mathbf{y}_1^i, \ldots, \mathbf{y}_\mathbf{k}^\mathbf{i}, \ldots, \mathbf{y}_\mathbf{K}^\mathbf{i}\}$, whereas $K_i(j)$ denotes the number in this set that is of category j. (The superscript i denotes that the order of the indices $1, \ldots, K$ is determined by the test vector $\mathbf{x_i}$). Then, an estimate $\hat{p}'$ of the probability that $\mathbf{x_i}$ belongs to category j, is constructed proportionally to $K_i(j)/K$. It is shown that in the case of large training set size, Equation 4 converges to the definition of probability density. Figure 2 illustrates the Prop estimator and the Bayes Risk.

Furthermore, the estimator is not very efficient at making use of the available information. For instance, it assigns zero probability to those outcomes for $\mathbf{x}_i$ lacking any 'precedent' in the training set, i.e. for which, among the K members of the training set nearest to $\mathbf{x}_i$, none have a matching category, so $K_i(j) = 0$. To overcome this problem, a constant proportion of the probability mass, Δ, is allocated to account for this chance of 'model failure', shared out equally among the C classes:

$$\hat{p}_{\text{Prop}}(x_i = j) = \frac{(1-\Delta)K_i(j)}{K} + \frac{\Delta}{C} \tag{4}$$

A similar approach is integrated into all types of estimator investigated here. While it is possible to optimise the value assigned to Δ, it would take very large, stationary data sets to get any meaningful results, since it is effectively insurance against rare outcomes.

2.2 The Weighted Proportional (wProp) Estimator

Atiya [1] generalises this idea by proposing the assignment of an unconstrained weight w_k to each member of the training set $\mathbf{y}_k$, using a sigmoid function to transform this into g_k, which always lies in the unit interval. As a result, an estimate is given by the following equation:

$$\hat{p}_{\text{wProp}}(x_i = j) = \frac{(1-\Delta)K_i(j)}{K} \sum_{k=1}^{K} g_k \delta(y_k = j) + \frac{\Delta}{C} \tag{5}$$

where the $\delta(\cdot)$ picks out only those neighbours of category j, and Δ is once again the term to guard against model failure.

The key advantage is that, within the training set, the set of unconstrained weights $\{w_k\}$ can be optimised to maximise the likelihood of the training set given this estimator: the cost function can be shown to be convex with the appropriate stationary point. Thanks to this, the efficient search approach by gradient-ascent is applied to find the optimal set of weights.

3 Tabulation of Prior Statistics

To construct an accurate estimate of the posterior probability, it is proposed to investigate various definitions of table that can be used to accumulate statistics from the training set. These tables can be combined and used to record the varying degrees of certainty that have been encountered across the sections of the input space. Hence, for an unseen test vector, its relation to its nearest neighbours in the training set can be used to identify similar sections of the input space, and simply look up the probability that has been measured from the cross-validated statistics. Figure 3 illustrates the proposed framework.

To tabulate these statistics from the training set, a 'leave-one-out' cross validation is applied. This means that features are extracted and accumulated, leaving out a single member of the training set. These features are used to predict the label of the left-out sample: the result is stored as a prior statistic. This process is repeated n times, to assemble a table of the prediction performance, conditioned upon the different values that the extracted features can assume. In general, discrete features were chosen, in preference to continuous ones: this allows a tabulation as opposed to a regression. An important design decision is the number of possible feature values, i.e. the number of elements in the conditional tables: a fine-grained model can provide more detail, while a course-grained model allows more statistics to accumulate per element which provides more reliable predictions.

We propose to use four different features of the training set to generate the prior statistics: VoteSplit table, Rank table, Dist feature, and ConfMat (confusion matrix). These are presented in the subsequent sections (3.1 to 3.4). These tables are then combined together in various ways to generate several estimators that can be evaluated on test sets alongside the Prop and wProp methods. The methods for combining the tables are described in section 3.5.

3.1 The VoteSplit Table

It is hypothesised that the *degree of agreement* between the K nearest neighbours to $\mathbf{x}_i$ provides a useful indication about the certainty of the classification result. Intuitively, a unanimous verdict from the K nearest neighbours is a more certain result, than some equivocation between two or more labels. This degree of agreement can be simply modelled by a histogram with K bins: each element k of the histogram is used for those cases in the training set in which k of the nearest neighbours have the same label as the predicted result. The histogram is used to accumulate and then calculate the proportion of these cases in which the predicted result is correct. This is achieved using the 'leave-one-out' methodology to fabricate m test cases from within the training set, in each case omitting it from the list of neighbours used to determine its result.

An example of the accumulation of the VoteSplit table, in addition to the remaining three features, is shown in figure 4.

3.2 The Rank Order of Correct Labels

Another perspective on the performance of the classifier is to rank the distinct labels of the nearest neighbours, by distance, and to assess the relative frequency with which the correct label is present at each of these ranks. Thus, in a specific example, if the labels of the 6 nearest neighbours were, in order, $\{A, C, C, B, A, D\}$, the ordered set of distinct labels would be $\{A, C, B, D\}$, the duplicates having been removed. Following a similar 'leave-one-out' methodology to that presented in Section 3.1, the rank of the correct label is used to increment the respective element of a histogram. After all members of the training set have been tested in this way, this his-

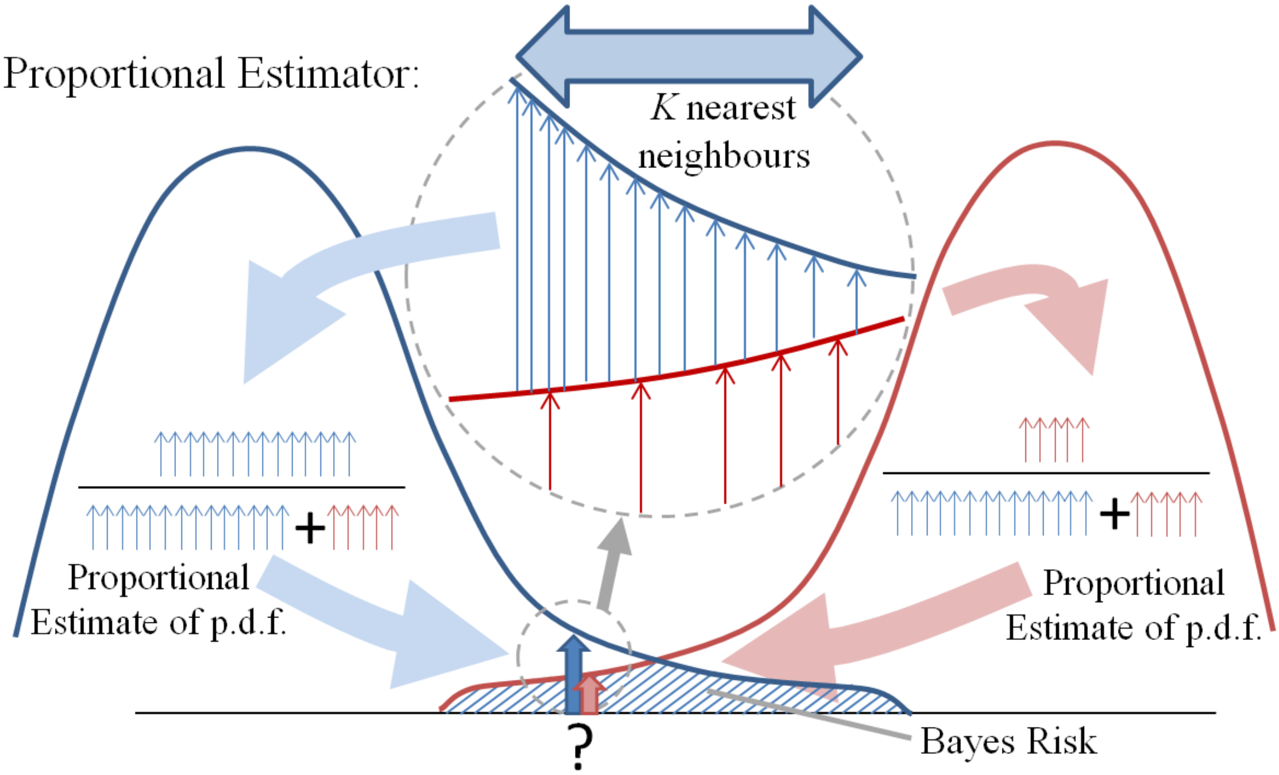

Proportional Estimator:
K nearest neighbours
Proportional Estimate of p.d.f.
+
Proportional Estimate of p.d.f.
+
?
Bayes Risk

Figure 2. Supposing estimates of posterior probability density functions for two classes are required: the Prop estimator uses the proportion of the K neighbours found to have that class label in each case. As the overall density (number) of available neighbours increases, this estimate will converge on the true p.d.f. However, it makes inefficient use of the available information. Also shown is the 'Bayes Risk'; which is the expectation of minimum risk due to some inevitable errors.

togram is normalised to provide an indication of relative frequency.

3.3 Conditional Dependence on Dist

The accumulation of statistics to measure the recorded (Euclidean) distance between samples that are either the same label or different labels, is well established in the literature [15]. In this context, the set $\{|\mathbf{y}' - \mathbf{y_k}|\}$ denote the distances between the cross-validation probe $\mathbf{y}'$ and its K nearest neighbours $\{\mathbf{y_k}\}$. The distances are quantised into the histogram bins; for those distances for which the neighbour and the probe have the same label, i.e. $y' = y_k$, histogram H_1 is incremented. Otherwise, histogram H_2 is incremented.

To obtain a probability that is conditioned upon a given quantised distance (and histogram bin) b, the histograms are normalised to their respective priors and then the conditional probability is $H_1(b)/(H_1(b) + H_2(b))$.

3.4 The ConfMat Confusion Matrix

The confusion matrix [13], ConfMat, is a standard methodology for cross-validation; whereby a matrix of relative performance of a classifier per class is visualised in a specific table layout. Each column of the matrix represents the instances in a predicted class, while each row represents the instances in an actual class; for each associated correct or incorrect prediction, a 1 value is tallied to the respective row and column of the table. This represents the frequency over the training set that category j_1 is classified as category j_2. An example confusion matrix is shown in table 1. The ConfMat table uses the classifier precision from each class in the confusion matrix as the direct probabilistic estimate for any future prediction of that specific class.

Table 1. Example confusion matrix with three class labels: A, B, and C, and three samples of each class. The relative tallies can be evaluated in various ways to provide estimates of the classification accuracy. In the case of class A there are three true positives, where A was correctly predicted; three false positives, where one B sample and two C samples were confused to be as class A; no false negatives; and lastly three true negatives. The respective classification accuracy (precision) for class A would therefore be equal to: $\frac{3}{3+3} = 0.50$ (where the true positives for class A are shown in bold, and the false positives shown in italics).

		Predicted		
		A	B	C
Actual	A	**1+1+1**	0+0+0	0+0+0
	B	*1+0+0*	0+1+0	0+0+1
	C	*1+0+1*	0+0+0	0+1+0

3.5 Combination of Tables

Combinations of the various feature tables can be implemented to create additional novel estimators. In the simplest combination, an additional column is added to the table, which provides more discrimination between various values in the table. Some of the combinations are documented as the following:

1. The Dist$_\&$VoteSplit estimator: This combined table uses the Dist feature from the K-NN frame-

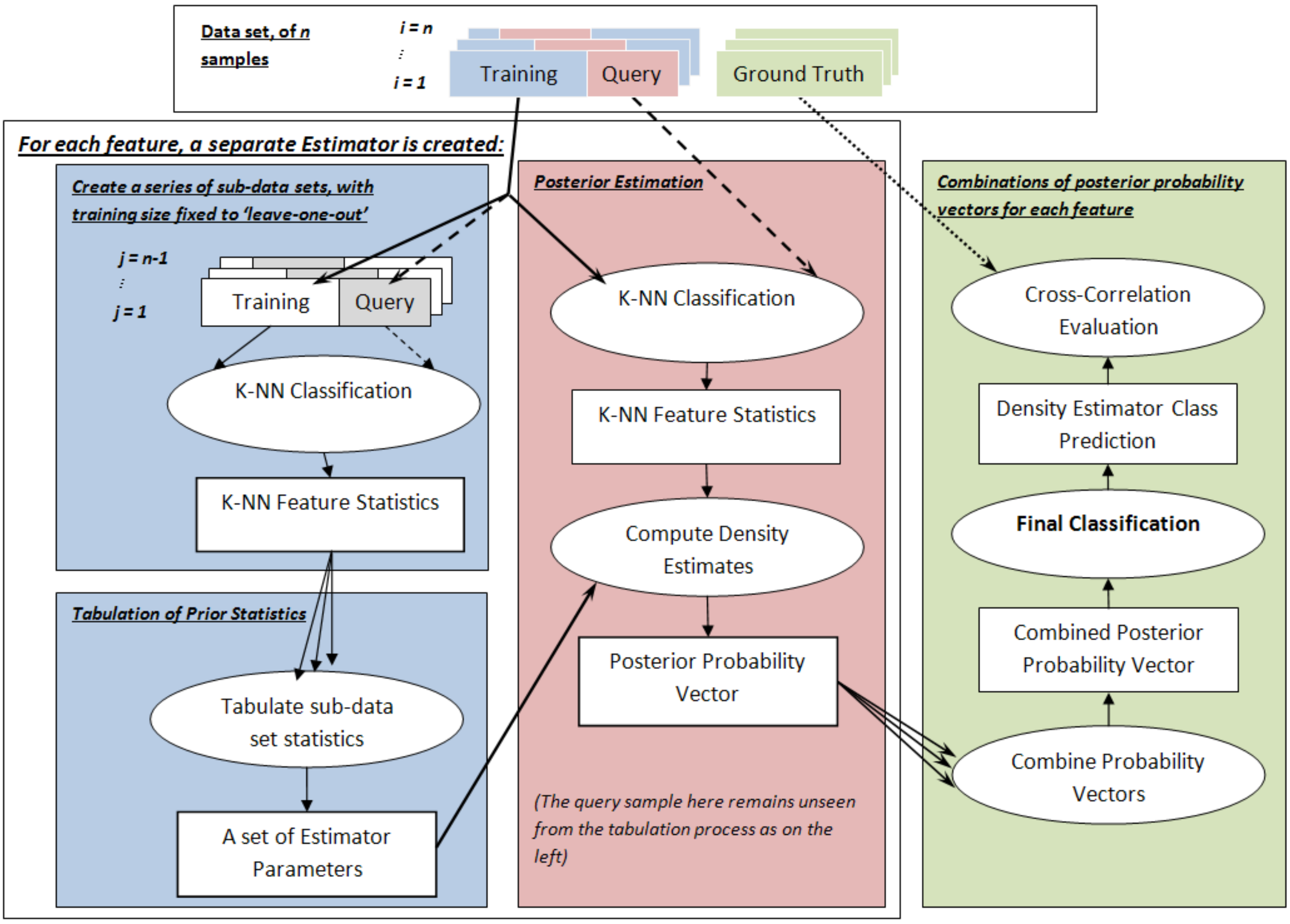

Data set, of n samples
i = n
i = 1
Training
Query
Ground Truth
For each feature, a separate Estimator is created:
Create a series of sub-data sets, with training size fixed to 'leave-one-out'
j = n-1
j = 1
Training
Query
K-NN Classification
K-NN Feature Statistics
Tabulation of Prior Statistics
Tabulate sub-data set statistics
A set of Estimator Parameters
Posterior Estimation
K-NN Classification
K-NN Feature Statistics
Compute Density Estimates
Posterior Probability Vector
(The query sample here remains unseen from the tabulation process as on the left)
Combinations of posterior probability vectors for each feature
Cross-Correlation Evaluation
Density Estimator Class Prediction
Final Classification
Combined Posterior Probability Vector
Combine Probability Vectors

Figure 3. The proposed novel density estimator framework using tabulated statistics calculated from an internal data-set. A posterior estimate for the unseen query sample can then be calculated using the prior estimates. The evaluation method is also illustrated, whereby each probabilistic estimate per feature can be combined to produce various class predictions. The selected classifier features used to build the estimator, in addition to the test sample feature combinations, can thus be evaluated like-for-like, (allowing a selection of the preferred classification solution).

work. For additional granularity, the table contains two columns: the first remains as distance with the second adding the range of categories from the VoteSplit table.

2. The Rank&VoteSplit matrix estimator: Similar to the above method, however instead of using the distance feature uses the Rank feature as the first column of the table, and the VoteSplit table as the second.

3. The ConfMat&Rank estimator: Whereby probability mass is accumulated into the confusion matrix instead of the discrete 1 assigned if the prediction matches the ground truth. In this case, the probability mass from the Rank lookup table is calculated and accumulated in the relevant row and column of the confusion matrix (see section 3.4). This new confusion matrix requires normalisations so that the total probability mass across each row of the matrix sums to one; this also means that there are no zero-value elements in this table (to avoid model failure), therefore all elements have a constant value added to them (such as +1). The ConfMat&Rank matrix is then used in the same way as the standard ConfMat table. An example is shown in table 2.

4. The ConfMat&Rank&VoteSplit estimator: Similar to the above method, however instead uses the additional information from the combined Rank&VoteSplit table to estimate the probability mass which, again, in turn is accumulated into the ConfMat matrix instead of discrete 1 values.

Table 2. Example confusion matrix, aggregating probability mass instead of discrete values. In this example, the results are roughly equivalent to table 2 The respective classification accuracy (precision) for each class is readily available after adding a constant value to each element (such as 1), then normalise each row by the total of that row (so the sum becomes equal to 1).

		Predicted		
		A	B	C
Actual	A	0.9 + 0.85 + .78	0 + 0 + 0	0 + 0 + 0
	B	0.4 + 0 + 0	0 + 0.75 + 0	0 + 0 + 0.43
	C	0.85 + 0 + 0.7	0 + 0 + 0	0 + 0.8 + 0

4 Experimental Evaluation

The following estimators are tested in this paper: Prop (Section 2.1), wProp (Section 2.2), Dist&VoteSplit, ConfMat, Rank, Rank&VoteSplit, ConfMat&Rank and ConfMat&Rank&VoteSplit combinations of tabulated

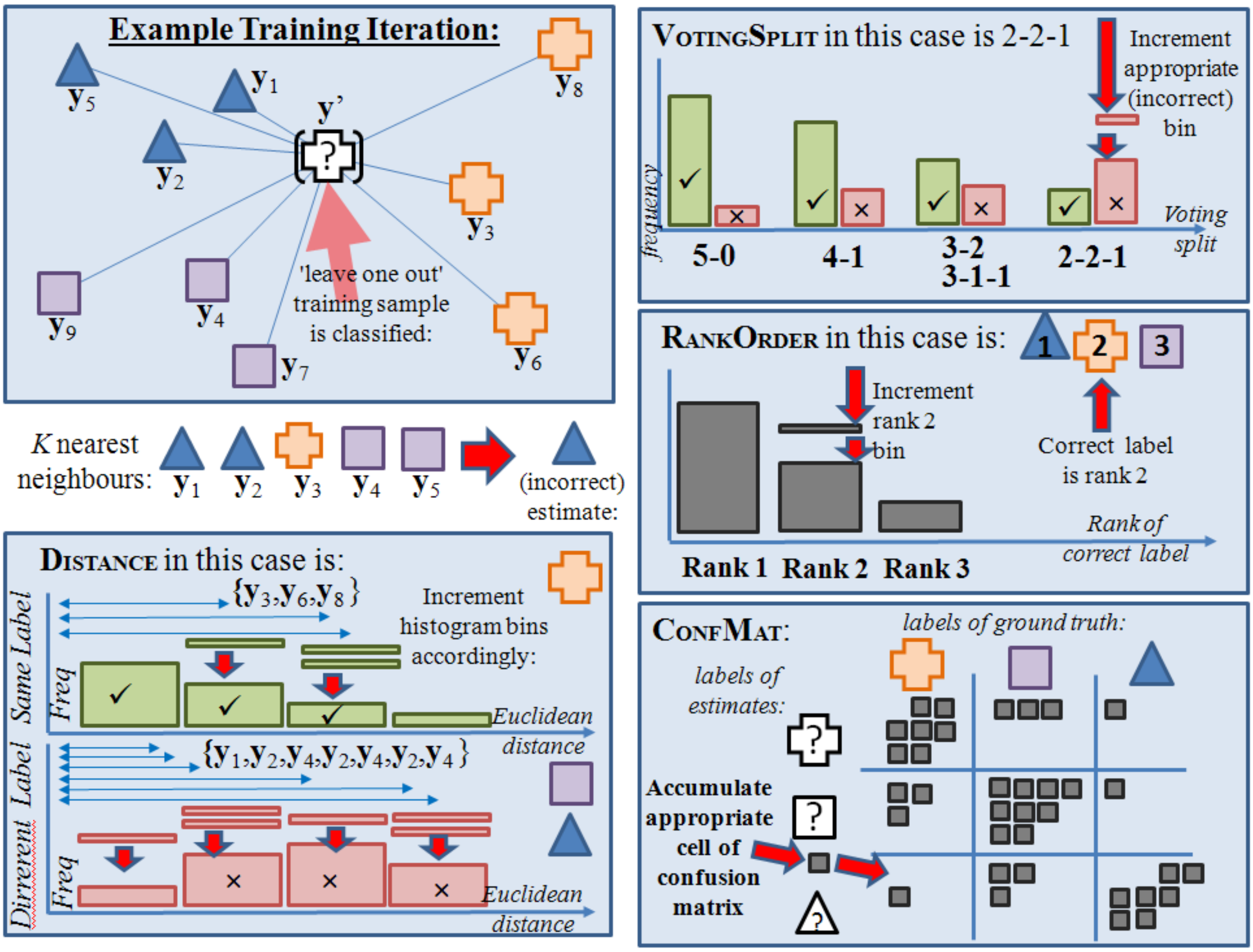

Example Training Iteration:
y1 y2 y3 y4 y5 y6 y7 y8 y9
y'
'leave one out' training sample is classified:
K nearest neighbours: y1 y2 y3 y4 y5
(incorrect) estimate:
VotingSplit in this case is 2-2-1
Increment appropriate (incorrect) bin
frequency
Voting split
5-0
4-1
3-2 3-1-1
2-2-1
RankOrder in this case is: 1 2 3
Increment rank 2 bin
Correct label is rank 2
Rank of correct label
Rank 1 Rank 2 Rank 3
Distance in this case is:
{y3,y6,y8}
Increment histogram bins accordingly:
Same Label
Freq
Euclidean distance
{y1,y2,y4,y2,y4,y2,y4}
Dirrerent Label
Freq
Euclidean distance
ConfMat:
labels of ground truth:
labels of estimates:
Accumulate appropriate cell of confusion matrix
?

Figure 4. An example iteration of the accumulation of the tabulated statistics: VoteSplit, Rank, Dist, and ConfMat features. These features would eventually be tabulated over all of the training iterations, using each training sample as a new leave-one-out test sample.

statistics (Section 3). The eight estimators are evaluated using unseen test sets. Results are accumulated using ten-fold evaluation (for Iris and Wheat data sets) and sixteen-fold evaluation of the leaves data set. In each of these iterations, the estimator is rebuilt completely, thus ensuring that a sample used as a test vector in one iteration, can be used as a training vector in another iteration, without compromising the integrity of the experiments. In all cases there are an equal number of samples used from each class, effectively setting the priors to be equal. The performance results reported consist of the mean log posterior (**LP**), i.e. expected log likelihood, of the density estimates and the mean classification accuracy (Acc) of the estimators. For the results concerning the Leave data set, we additionally report the mean precision and mean recall accuracies (due to the number of classes and complexity of the data set).

For each estimator, the number of separate features to be included in the classification can be varied. Each feature has its own separate K-NN system that is trained on the respective training data. There are two, three and four separate K-NN systems created, for the Iris, Leaves and Wheat data sets; the Leaves features are multivariate (64-dimensions each); the Iris and Wheat features are univariate. In the current investigation, the K-NN system is configured with a Euclidean distance measure and the first-nearest neighbour is used as the tie-break mechanism. Additionally, the 'model failure' value of $\Delta = 0.01$ is used for all experiments, i.e. 1% of the probability mass is reassigned to all classes thus removing zero valued elements (Section 2.1).

In each case, the evaluation reports two measures of performance: the log posterior of the probabilistic estimate, and the accuracy of the final discrete estimate. The main objective of the experiments is to understand which of the available estimators provides the most accurate classification results. Subsequently, the performance as a function of training size is investigated, using the high-dimensional (Leaves) data set.

4.1 Test Data sets

Two public benchmark data sets are employed to validate the performance of considered methods: Iris Flower and Wheat Seed Kernel (Section 4.1.1). The experimental design restricts the processing of these data sets to a single variable per K-NN classifier, to examine the efficacy with which the probabilistic estimates from each classifier can be combined. Additionally, a one-hundred species leaves data set is included, which is a challenging classification problem due to major/minor species of plant leaves (Section 4.1.2).

4.1.1 Iris Flowers & Wheat Seed Kernels

A well-known data set in the pattern recognition literature is Fisher's iris data [5, 4]. It consists of 50 samples from 3 varieties of Iris plant. The features of the iris data consist of four scalar values; these refer to the Length and Width of the Petal (PL and PW), and the Length and Width of the Sepal (SL and SW). Guvenir et al, [7], use the iris data set (amongst others) to validate the performance of their own weighted K-NN classifier. In the case of $K = 3$, using a ten-fold cross-validation evaluation, the mean classification accuracy was reported to be 90.7% for the standard classifier definition. The authors report an accuracy of 94% using their weighted K-NN metric (with the same $K = 3$ parameter). We create four separate feature vectors per iris sample, which relate to each of the petal and sepal dimensions (rather than use all values in one feature vector).

Another publicly available data set consists of seven attributes of wheat seed kernels [10]. The data set consists of 70 samples from 3 different varieties of wheat. The attributes refer to the Area (AR), Perimeter (PE), Compactness (CO), Length of Kernel (LK), Width of Kernel (WK), Asymmetry Coefficient (AS) and Length of Kernel Groove (LKG). The authors report a mean classification accuracy of 92% using a clustering algorithm technique. Similarly to the Iris data set, we create separate feature vectors using each of these attributes within the test framework.

4.1.2 Plant Leaves

The 'leaves' data set comprises one-hundred species of leaves [11]. For each species, there are sixteen distinct specimens, photographed as a colour image on a white background. Figure 1 contains a sample set of silhouette images. From these samples, three distinct features were extracted: a Centroid Contour Distance Curve shape signature (Sha), an interior texture feature histogram (Tex), and a fine-scale margin feature histogram (Mar). Each feature is represented by a 64 element vector.

The data set inherently consists of having a wide set of classes with a low number of samples. Additionally, many sub species resemble the appearance of other major species, as well as many sub species with a major species can resemble a radically different appearance. As such, this data set provides the main classification challenge from the three data sets described in this paper.

4.2 Iris Flower & Wheat Seed Results

The experimental results using the Iris Flower data set is shown in Table 3. All described density estimation methods were tested in this case with $K = 3$. Note, no significant differences were observed when experiments were conducted with $K = 5$ and $K = 7$. The results using the Wheat Seeds data set is shown in Table 4. Some minor differences were noted when experimenting with $K = 5$ and $K = 7$, however we include results using $K = 3$. For both cases, results of three different feature combinations are shown for comparative purposes.

Table 3. Experimental results using the Iris Flower data set.

Estimator	Features	**LP**	Acc
Prop	PW	-0.165	96.00
	PL$_\&$PW	-0.064	94.67
	PL$_\&$PW$_\&$SL$_\&$SW	-0.113	90.00
wProp	PW	-0.103	96.00
	PL$_\&$PW	-0.061	95.33
	PL$_\&$PW$_\&$SL$_\&$SW	-0.115	90.67
Dist$_\&$ VoteSplit	PW	-0.967	28.67
	PL$_\&$PW	-0.345	24.67
	PL$_\&$PW$_\&$SL$_\&$SW	-0.387	25.33
ConfMat	PW	-0.093	96.00
	PL$_\&$PW	-0.302	92.67
	PL$_\&$PW$_\&$SL$_\&$SW	-0.349	92.67
Rank	PW	-0.077	96.00
	PL$_\&$PW	-0.267	96.00
	PL$_\&$PW$_\&$SL$_\&$SW	-0.313	90.67
Rank$_\&$ VoteSplit	PW	-0.088	94.00
	PL$_\&$PW	-0.221	95.33
	PL$_\&$PW$_\&$SL$_\&$SW	-0.263	93.33
ConfMat$_\&$ Rank	PW	-0.072	96.00
	PL$_\&$PW	-0.071	96.00
	PL$_\&$PW$_\&$SL$_\&$SW	-0.211	92.67
ConfMat$_\&$ Rank$_\&$ VoteSplit	PW	-0.074	96.00
	PL$_\&$PW	-0.204	96.00
	PL$_\&$PW$_\&$SL$_\&$SW	-0.245	92.00

Table 4. Experimental results using the Wheat Seed data set.

Estimator	Features	**LP**	Acc
Prop	AR$_\&$AS$_\&$LKG	-0.182	88.10
	PE$_\&$WK$_\&$AS$_\&$LKG	-0.133	88.57
	AR$_\&$PE$_\&$CO$_\&$LK$_\&$AS$_\&$LKG	-0.137	88.57
wProp	AR$_\&$AS$_\&$LKG	-0.171	87.62
	PE$_\&$WK$_\&$AS$_\&$LKG	-0.134	88.57
	AR$_\&$PE$_\&$CO$_\&$LK$_\&$AS$_\&$LKG	-0.169	87.62
Dist$_\&$ VoteSplit	AR$_\&$AS$_\&$LKG	-0.177	78.57
	PE$_\&$WK$_\&$AS$_\&$LKG	-0.192	81.43
	AR$_\&$PE$_\&$CO$_\&$LK$_\&$AS$_\&$LKG	-0.162	86.19
ConfMat	AR$_\&$AS$_\&$LKG	-0.172	86.67
	PE$_\&$WK$_\&$AS$_\&$LKG	-0.163	88.57
	AR$_\&$PE$_\&$CO$_\&$LK$_\&$AS$_\&$LKG	-0.183	89.05
Rank	AR$_\&$AS$_\&$LKG	-0.163	90.48
	PE$_\&$WK$_\&$AS$_\&$LKG	-0.154	88.57
	AR$_\&$PE$_\&$CO$_\&$LK$_\&$AS$_\&$LKG	-0.184	88.10
Rank$_\&$ VoteSplit	AR$_\&$AS$_\&$LKG	-0.159	90.48
	PE$_\&$WK$_\&$AS$_\&$LKG	-0.148	87.14
	AR$_\&$PE$_\&$CO$_\&$LK$_\&$AS$_\&$LKG	-0.181	87.14
ConfMat$_\&$ Rank	AR$_\&$AS$_\&$LKG	-0.152	92.38
	PE$_\&$WK$_\&$AS$_\&$LKG	-0.143	90.00
	AR$_\&$PE$_\&$CO$_\&$LK$_\&$AS$_\&$LKG	-0.183	89.52
ConfMat$_\&$ Rank$_\&$ VoteSplit	AR$_\&$AS$_\&$LKG	-0.151	90.00
	PE$_\&$WK$_\&$AS$_\&$LKG	-0.143	87.14
	AR$_\&$PE$_\&$CO$_\&$LK$_\&$AS$_\&$LKG	-0.185	87.62

4.3 Plant Leaves Results

The experimental results using the plant leaves data set is shown in Table 5. All described density estimation methods were tested in this case with $K = 3$ and $K = 5$. The results shown consist of the combined Sha$_\&$Tex$_\&$Mar classified features (unanimously, the best feature combination across all estimators for the leaves data set). In addition to the mean classification accuracy, we report the mean precision and mean recall metrics in order to provide more detail on the performance of the estimators using this more complex data set.

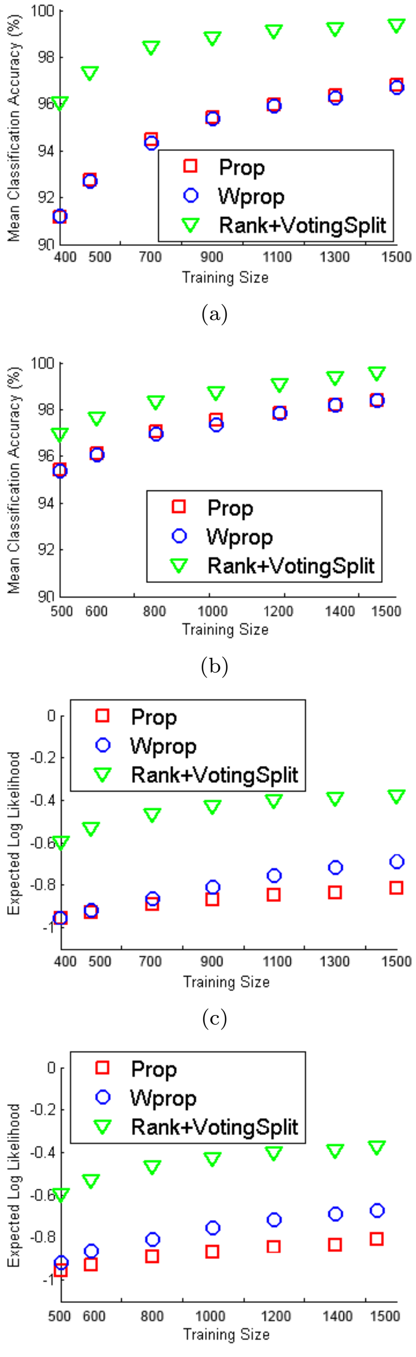
The classification accuracy is then reported as a function of training size, in addition to the mean log posterior metric. The respective plots are shown in Figure 5.

Table 5. Results of the sixteen-fold evaluation of the leaves data set using only the Sha$_{\&}$Tex$_{\&}$Mar features combination.

Estimator	K	**LP**	Acc	Pre	Rec
Prop	3	-0.814	96.81	96.98	96.81
	5	-0.569	98.19	98.33	98.19
wProp	3	-0.554	96.69	96.87	96.69
	5	-0.368	98.19	98.31	98.19
Dist$_{\&}$ VoteSplit	3	-0.394	97.75	97.88	97.75
	5	-0.282	97.81	97.97	97.81
ConfMat	3	-0.327	92.25	92.96	92.25
	5	-0.251	90.13	91.22	90.13
Rank	3	-0.263	99.25	99.31	99.25
	5	-0.202	99.31	99.36	99.31
Rank$_{\&}$ VoteSplit	3	-0.221	**99.38**	99.42	99.38
	5	-0.170	**99.38**	99.42	99.38
ConfMat$_{\&}$ Rank	3	-0.197	97.69	97.88	97.69
	5	-0.155	97.19	97.31	97.19
ConfMat$_{\&}$Rank$_{\&}$ VoteSplit	3	-0.189	94.63	94.75	94.56
	5	-0.158	91.81	92.29	91.81

4.4 Algorithm Computation Speed

The experiments introduced in this paper were conducted on a workstation using the Microsoft Windows XP operating system with a 3.2 GHz processor and 3 GB of RAM; the algorithm was implemented in the MATLAB programming environment. We report the mean experiment time taken to classify one trial of the one-hundred species leaves data set, i.e. the average time to compute one-fold of 100 test samples using 1500 training samples. Note that one trial comprises of building a separate K-NN density estimator for *each* feature vector i.e. the classification timings noted here indicate timing of the entire experiment using all features. Our implementation of the Prop estimator had completed this task in 21.8 seconds, whereas the wProp estimator was completed in 31.7 seconds. The Dist$_{\&}$VoteSplit estimator performs slowest with 41 seconds processing time, and the remaining estimators all completed within 33 seconds.



(a)

(b)

(c)

(d)

Figure 5. Estimator performance as a function of training size using the leaves data set: Using $K = 3$, (a) and (c) show the mean classification accuracy and expected log likelihood, respectively. Similarly, (b) and (d) show the results using $K = 5$.

4.5 Discussion

The Prop and wProp estimators perform similarly with respect to mean classification accuracy over the ten-fold cross-validation evaluation. Using the Iris Flower data set, a 96% mean accuracy with the PW feature alone and 90% with all four of the PL$_{\&}$PW$_{\&}$SL$_{\&}$SW features. With regards to the expected log likelihood using the PW feature alone: -0.165 to -0.103 for Prop and wProp, respectively. For all estimators the single PW feature worked better than any combination of the PL, PW, SL, and SW features. Comparatively, Guvenir et al [7] reported an accuracy of 94% using their proposed weighted K-NN metric using all four values. All of the tested estimators performed less than this, however the Rank$_{\&}$VoteSplit method was closest with 93.33% mean accuracy using the four features.

Similarly to the Iris Flower data set, results using Wheat Seeds show that many of the features combined together from the seven available did not give the optimal solution. Generally, the framework worked optimally with the AR, AS, and LKG features. We observe that of all estimators, the ConfMat$_{\&}$VoteSplit method performs the strongest with a mean classification accuracy of 92.38% and expected log likelihood of -0.152, using the combination of AR$_{\&}$AS$_{\&}$LKG features. Comparatively, Charytanowicz et al [10] reported a mean classification accuracy of 92% using a proposed clustering algorithm on the same data set using all seven features. The Rank$_{\&}$VoteSplit estimator performed next best with 90.48% mean accuracy and mean log posterior of -1.159 (also using the AR$_{\&}$AS$_{\&}$LKG features).

The most complex data set consisting of the Plant

Leaves have further supported the performance of the Rank&VoteSplit estimator. The mean classification accuracy for the sixteen-fold evaluation was 99.38%, with an expected log likelihood of -0.17 (using $K = 5$). Comparatively, the Prop and wProp methods performed well with a mean classification accuracy of 98.19%, respectively. The expected log likelihood for these methods were -0.569 and -0.368, respectively.

The K parameter selection from $K = 3$ to $K = 5$ had shown a 1.38% and 1.5% boost in classification accuracy for the Prop and wProp methods. However the Rank&VoteSplit method worked consistently across the two tested K values. The remaining estimator methods performed with varying success, most notably the ConfMat based methods worked worse for the plant leaves data set.

5 Conclusion and Further Work

This paper has introduced a novel framework for estimating the posterior probability density, using information available to a K-nearest neighbour classifier. Four different types of statistics were tabulated from within the training set, and various ways of combining these tables were investigated. Experiments on several data sets indicated that the best performing estimator is the joint table that conditions the estimate on the VoteSplit and the Rank of the hypothesis provided by K-NN.

For the one-hundred species leaf data set, integrating all three Sha, Tex and Mar features, the novel Rank&VoteSplit method was the best performing estimator. This was inferred from the standard discrete metric (99.38% mean classification accuracy). For the standard probabilistic metric (mean log likelihood of the test set), the values obtained from the combinations of Rank, VoteSplit and ConfMat were in the range of -0.155 to -0.21, compared to the values obtained from the conventional estimators of -0.814 and -0.368. Thus these represent very sizeable improvements in the accuracy with which an unseen test set's classification probabilities are estimated.

As a function of the training set size, the discrete classification performance is readily interpreted: at low values of available samples, and especially for low values of K (number of nearest neighbours), the Rank&VoteSplit estimator provides significantly better performance. Thus, the effectiveness of the framework is shown when combining the probabilistic estimates from individually processed features. For the leaves data set, the optimal configuration used all available features; however, this may not always be the case as shown with the iris flower and wheat seeds data sets. It has been shown to be effective in the particular task of classification with low training samples and a relatively large variety of categories.

There are several avenues of future work. For leaf recognition, it will be useful to validate the framework with noisy and missing data, e.g. missing parts of the sample leaf or focus errors. More generally, there are other areas of probabilistic estimation for which the proposed framework may be useful, e.g. correct estimation of face or vehicle registration plate details apparently permit a similar analysis. The evaluation of probability density will extend to check that kernel-based methods and Parzen windows do not offer any advantage under these conditions. Finally, it will be useful to investigate the extent to which properties of the training set statistics can predict the out-of-sample performance on the test set, to enable the most appropriate combination of tabulated data to be automatically selected and used.

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