CS57800: Project Report

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Contents

Introduction

The aim of the project is to study the performance of various classification algorithms, namely, Support Vector Machines (SVM), K-nearest neighbors (KNN), and neutral networks. We evaluate these algorithms on the task of identifying handwritten digits. The details of the data set and the pre-processing that was done is described next.

Data set Preprocessing

The MNIST data set, which is a subset of a bigger data set from National Institute of Standards and Technology (NIST), is a collection of handwritten digits, each between 0 to 9, and is commonly used as a benchmark data set for evaluating various image processing systems. The data set is preprocessed and has a training set of 60,000 examples, and a test set of 10,000 examples. The pre-processing details are described next.

The original NIST data set which was black and white (i.e. had only two levels) was first processed to fit into a 20×20 pixel image. Each image was then smoothed (anti-aliased) to obtain a grey-scale image which was then centered in a 28×28 pixel box. The centering was performed by computing the center of mass of the pixels, and translating the image so as to position that point at the center of the 28×28 field. The data set was downloaded using the *scikit-learn* python library (`fetch_mldata` method in package `sklearn.datasets`).

Next, we describe the classification algorithms that were used in this project.

Classification Algorithms

In this section, we describe three methods, namely, SVM, KNN and Neural network, for the task of recognizing handwritten digits. The classification task is to learn a function that maps images of handwritten digits $\mathcal{X}$ to digits $\mathcal{Y} = \{0, 1, \ldots 9\}$, from a data set of labeled examples (images of handwritten digits). In our case, $\mathcal{X} = [0, 255]^{784}$ corresponds to the set of flattened 28×28 grey-scale images. Let d (784 in this case) denote the dimension of the feature space and k (10 in this case) denote the number of classes. We have a data set $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$ of n labeled images.

Support Vector Machines

Support Vector Machines (SVM) is one of the most widely used classification algorithm for both binary and multi-task problems. SVM is a maximum margin classifier. To solve the multi-class problem of classifying handwritten digits, we use the one-vs-rest classifier approach where each class gets a classifier bringing the total number of classifiers to 10 in our case. We train each binary classifier using by solving the following optimization problem:

$$\hat{\boldsymbol{\alpha}} = \min_{\boldsymbol{\alpha} \in \mathbb{R}^d} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{subject to} \quad 0 \leq \alpha_i \leq C, i = 1, \ldots, n, \; \sum_{i=1}^{n} \alpha_i y_i = 0,$$

where α_i and α_j are non-negative Lagrange multipliers used to enforce the classification constraints, y_i andy_j are predicted labels for data points $\mathbf{x}_i$ and $\mathbf{x}_j$ and K is the kernel function.

The prediction y for a test data point $\mathbf{x} \in \mathcal{X}$, for each binary classifier, is then obtained as follows:

$$y = \text{sign}\left(\sum_{i=1}^{n} \hat{\alpha}_i y_i K(\mathbf{x}, \mathbf{x}_i)\right)$$

Finally, the class which received the most votes is selected as the predicted label. We have evaluated the performance of the **linear kernel** in our experiments. We used `scikit-learn` python package for an implementation of the above.

K-Nearest Neighbors

K-nearest neighbors (KNN) is a popular non-parameteric classification algorithm which predicts the label of data point by computing the majority label over K nearest neighbors to the data point. In the training phase, a data structure (KD Tree) is constructed over all training data points for efficiently performing nearest neighbor queries during prediction. During prediction, the constructed tree is queried to find the K nearest neighbors, in Euclidean distance, and then the majority label is predicted as the class label of the test data point. We use uniform weighting for computing the votes.

Neural networks

Neural Network / Multi-Layer Perceptron (MLP) is a supervised learning algorithm that uses multiple layers of neurons (perceptrons) to learn a non-linear function $f(\cdot) : \mathbb{R}^d \rightarrow \mathbb{R}^k$. It differs from logistic regression by having multiple non-linear layers between the input layer and the output layer. In our case, the input layer has a dimension of 784(d) and the output layer has a dimension of 10(k - classes). Given training data, we use backpropagation to learn the weights and biases of the perceptrons in the neural network by optimizing a cost function.

When a new test point comes in, we predict the class it belongs based on the output array (k-dimensional) from the output layer by looking at the class which has the highest vote. Various parameters like the learning rate, the activation function for the perceptrons and regularization affect the performance of the neural networks and we use a 10-fold cross-validation approach to tune these parameters.

Experimental Set-up

In this section we describe our experimental setup in detail. We used 10-fold cross validation (CV) with stratified sampling to pick the optimal hyper-parameters for each algorithm, namely, the regularization parameter for SVM, the value of K for KNN, the best activation function, gradient descent learning rate and the regularization parameter for Neural networks. We then plot the mean cross-validation accuracy for each hyper-parameter value used for different algorithms.

After picking the best hyper-parameters for each algorithm from the above step, we ran experiments to find the effect of number of training data samples on accuracy. For different training data set sizes we computed the mean accuracy across 10 randomly sampled (stratified) data sets while keeping test samples fixed at 10,000. We then plot the test set accuracy as the number of samples is varied.

In another set of experiments, we explored the effect of using PCA (Principal Component Analysis) features on the accuracy. We ran experiments to pick the top-K PCA features which explained 90% of the variance in the data. We plot the variance explained versus the number of PCA features. Apart from these, we also performed hypothesis testing and studied a few other parameters, all of which have been explained in the following sections.

We used the implementation provided by the `scikit-learn` python library for the classification algorithms.

Stratified sampling

We used stratified sampling to ensure that the relative proportion of various classes in the full data set is maintained in each of the sampled data set. In stratified sampling the whole dataset is first partitioned into 10 groups (one group for each class 0-9). Then data points are sampled from each group and combined to form samples.

The experimental set-up for 10 fold cross validation, effect of varying number of training data on accuracy and PCA feature generations are explained next.

Implementation details

Receiver Operating Characteristic (ROC) curve

The ROC curve is an useful visual metric to study the classification potential of an algorithm. It is obtained by varying the threshold that is used to classify the data points in the test data set. After running the classification algorithms that we used on the test data, we obtained predicted labels and scores from the corresponding `decision_function()` for the algorithm from the `scikit-learn` python library.

input : *true_labels*, *predicted_scores*, *pos_label*
output: *fpr*, *tpr*

```
1  true_labels ← (true_labels == pos_label)
2  // Sort scores and corresponding truth values
3  desc_score_indices ← Sort(predicted_scores)
4  predicted_scores ← predicted_scores [predicted_scores ]
5  true_labels ← true_labels [predicted_scores ] // Find distinct scores
6  distinct ← DistinctValues(predicted_scores)
7  // Accumulate the true positives with decreasing threshold
8  tps ← CumulativeSum(true_labels)
9  fps ← 1 + distinct- tps
10 // Normalizing the scores to get TPR and FPR
11 fpr ← fps/ fps [-1]
12 tpr ← tps/ tps [-1]
```

Algorithm 1: ROC curve parameters (TPR/FPR)

This information is used to plot the ROC curve. The implementation for plotting the curve which relates the True Positive Rate (TPR) and the False Positive Rate (FPR) is shown in Algorithm 1.

The algorithm shown here returns the FPR and TPR values taking the score and the true labels as the arguments. It should be noted that this implementation is for a binary classification problem (two-labels). Since our problem is a multi-class classification problem, we extended this implementation by performing a "macro-averaging" approach which interpolates all the FPR and TPR scores of all the classes. In this regard, the `roc_curve_params()` method takes in a *pos_label* argument which is the current label (digits 0-9) that is under consideration.

An example of an ROC curve that is generated based on the above implementation is shown in Fig.

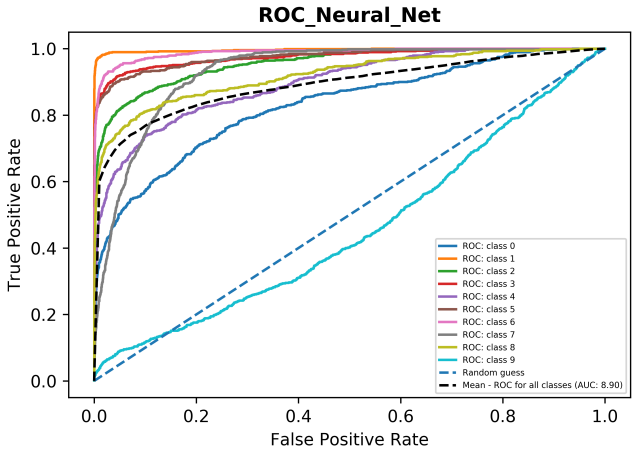


Figure 1: ROC curve example

1. The ROC curve of each of the 10 classes is highlighted along with the *mean_curve* and the Area Under Curve (AUC) metric for the mean curve which is a measure of the accuracy of the classification algorithm. A perfect classification algorithm would have an AUC score of 1. The mean curve is found using the macro-averaging approach shown in the following algorithm.

```
def plot_ROC_curve(y_true,y_score):
    mean_tpr = 0.0
    mean_fpr = np.linspace(0,1,100)
    for i in xrange(10):
        fpr[i], tpr[i] = roc_curve_params(y_true, y_score, pos_label = i)
        mean_tpr += interp(mean_fpr,fpr[i],tpr[i])
        mean_tpr[0] = 0

    mean_tpr /= 10
    mean_tpr[-1] = 1
```

Confusion matrices

Confusion matrices are another way to study the performance of a classification algorithm. While the configuration of a confusion matrix is straightforward for a binary classification, for multi-class classification it can be represented as a matrix of values of size $(n \times n)$, where n is the number of classes.

An example of a confusion matrix for the MNIST dataset is shown in Fig. 2. The confusion matrix is being plotted as a colormap using the in-built capabilities of `matplotlib` Python package and each row represents the proportion of classification of each class being classified as different classes by a classifier. For a perfect classifier, the confusion matrix would be an identity matrix.

Accuracy curve

As part of the experiments, we perform a 10-fold cross validation for parameter tuning, for hypothesis testing, etc. and to study the performance of algorithms in these tests, we study the accuracy score in the test fold. Since this is a multi-class classification, the accuracy of the model is represented as:

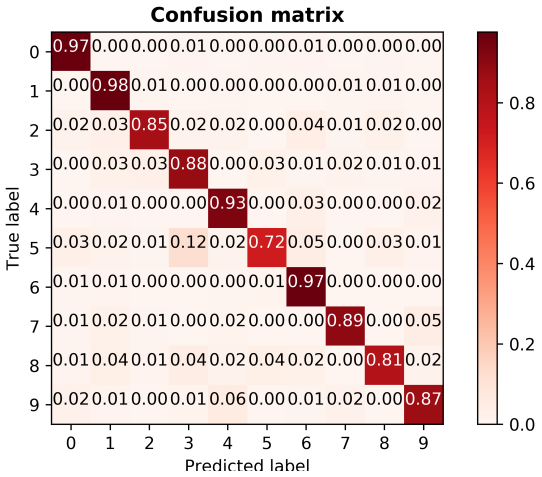


Figure 2: Confusion matrix example

$$Accuracy = \frac{True\_Positives}{Total\_number\_of\_samples}$$

Once we have this information, the plot showing the variation of accuracy with varying parameters were plotted as error bars (containing both mean and variance information) and these have been included in the results section.

Hypothesis testing

Once we had all these performance metrics, we compared the performance of algorithms using hypothesis testing. The data from the 10-fold CV steps were used for comparing the algorithms. Given a pair of means (μ_1, mu_2) and variances (σ_1, σ_2), we determine:

$$x = \frac{(\hat{\mu_1} - \hat{\mu_2})\sqrt{n}}{\sqrt{\hat{\sigma_1}^2 + \hat{\sigma_2}^2}}$$

$$\nu = \left\lceil \frac{\hat{\sigma_1}^2 + \hat{\sigma_2}^{2^2}(n-1)}{\hat{\sigma_1}^4 + \hat{\sigma_2}^4} \right\rceil$$

From these values, we reject the null hypothesis $\mu_1 = \mu_2$, in favor of $\mu_1 > \mu_2$, if $x > x_{1-\alpha,\nu}$. We fixed the confidence level $\alpha = 0.95$. In our case, we performed hypothesis testing for comparing the following pairs of algorithms:

- SVM vs. Neural Net (using PCA data)
- SVM vs. KNN (using PCA data)
- Neural Net vs. KNN (using PCA data)
- SVM vs. Neural Net (using actual data)
- SVM vs. KNN (using actual data)

- Neural Net vs. KNN (using actual data)
- SVM (with PCA) vs. SVM (without PCA)
- Neural Net (with PCA) vs. Neural Net (without PCA)
- KNN (with PCA) vs. KNN (without PCA)

All of these hypothesis tests were done with the results from the 10-fold cross validation (which use the tuned parameters that were found earlier using the parameter tuning experiments explained earlier). So, in a sense each algorithm is performing at it's best for the MNIST dataset. Of course, considering more parameters and tuning within a finer range of these parameters might result in better performance of the respective algorithms.

Principal Component Analysis (PCA)

TODO

Other Miscellaneous Metrics

Apart from these parameters, we also report Precision and Recall scores for the final test runs (10-fold CV using the tuned parameters). While precision and recall are not as efficient as accuracy in gauging the performance of an algorithm, they have been included to provide a sense of completion and in understanding the performance from different perspectives.

Since we use a multi-class dataset, the precision and recall scores have been calculated using a "*weighted-averaging*" technique. Here, the metrics are calculated for each label and a weighted average of them is taken based on the support (the number of samples for each label in the dataset).

Experiments/Results

10-Fold Cross Validation For Parameter Tuning

Support Vector Machines

Neural Networks

K-Nearest Neighbors

For 10-fold cross validation we used stratified sampling using all 70,000 MNIST data. We first divided the whole data into 10 groups (data belonging to each digit from 0-9). Then for each fold in 10-fold CV, we picked one fold from each group and combined them to form our test data set (approximately 7,000 data points) and rest of the data i.e. the other 9-folds were our training data set (approximately 63,000 data points). The results are shown in Figure 3 and 4.

From the plots we see that, the hyper-parameter C for SVM was selected to be **70**, value of K for KNN was selected to be **3** since the accuracy is highest at K=3, and in case of the neural networks, the following configuration was chosen:

- Regularization parameter (α): 100
- Activation function: Logistic
- Learning rate (η): 0.0003

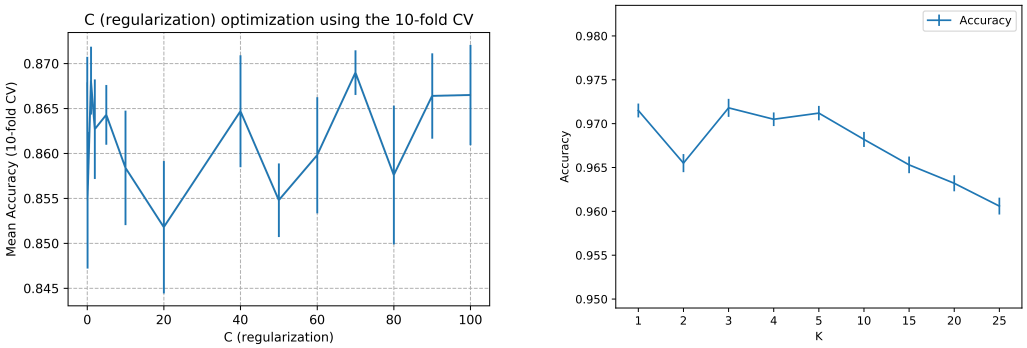


Figure 3: (Left) CV for SVM. (Right) CV for KNN.

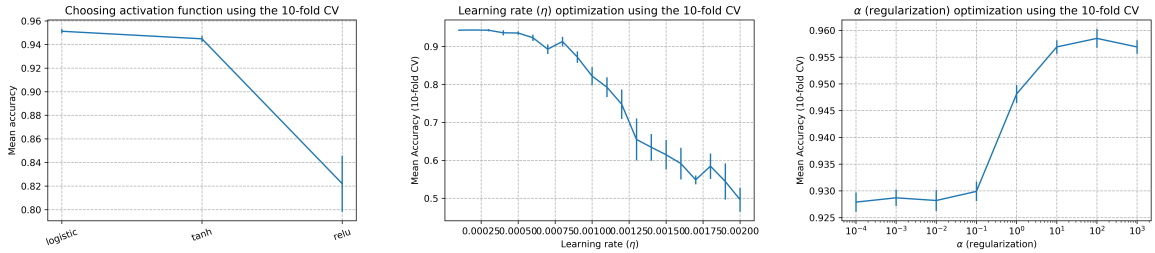
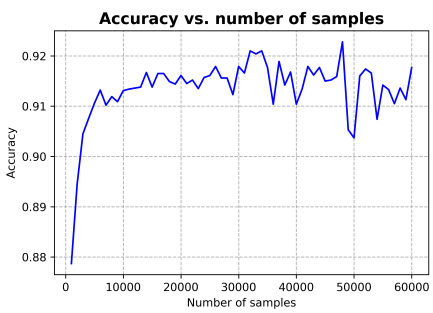


Figure 4: CV for Neural networks.

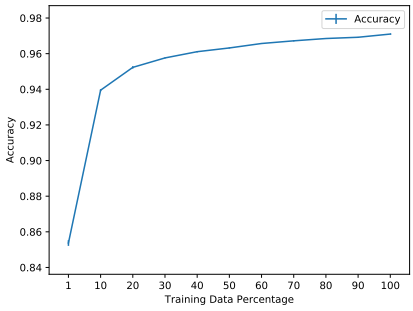
Effect of number of samples on accuracy

For this experiment, we progressively varied the fraction of samples used for training from 1% to 100% out of the entire 60,000 samples using randomized stratified sampling, taking the fraction of data from each class (digits 0-9) and combining them to form the training data and computed the accuracy on the test data (fixed size 10,000) for each case. Here we fixed the hyper-parameters for respective algorithm found using CV. The results are shown in Figure 5.

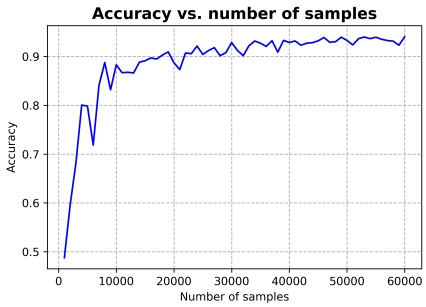
From the plots we see that, approximately 20% (12,000) of the training data points (60,000) is required for high accuracy. After 20% data points, the accuracy almost remains in the same range even if we increase the number of training data points.



(a) SVM



(b) KNN



(c) Neural Network

Figure 5: Training set size vs. accuracy

PCA features

For this experiment, we computed the top-K principal component features such that the top-K principal components explained 90% of the variance in the data. The results is shown in Figure 6.

From the plot we can see that the number PCA features are 87 out of 784 features which explains 90% variance in the data.

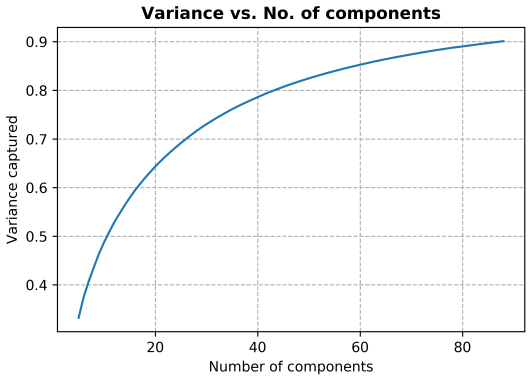


Figure 6: PCA features.

Hypothesis testing

Comparison using PCA data

Comparison using actual data

Within algorithm comparison

Miscellaneous results