Edibility of Mushroom Species

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1 Introduction to the Problem

1.1 Definition of the Problem

Given a dataset $\mathcal{D}$ with $n = 8124$ samples where each sample represents a mushroom with features being the observations about the characterestics of the mushrooms such as odor, color, etc., we aim to test and compare various supervised learning models for the problem of classifying each sample into either poisonous or edible. Further, we will optimize the Hyperparameters of the model which initially performs the best on the dataset.[1]

1.2 Data Description

We are given $\mathcal{D}$ with $n = 8124$ samples wherein each sample has the following 22 features (excluding the class label).

1. cap-shape
2. cap-surface
3. cap-color
4. bruises
5. odor
6. gill-attachment
7. gill-color
8. stalk-root
9. stalk-surface-above-ring
10. stalk-surface-below-ring
11. stalk-color-above-ring
12. stalk-color-below-ring
13. veil-type
14. veil-color
15. ring-type
16. spore-print-color
17. habitat
18. gill-spacing
19. gill-size
20. stalk-shape
21. ring-number
22. population

These features have been further enumerated in Appendix A.

The labels are binary, namely edible (e) and poisonous(p). Within the original dataset, there are the following number of edible and poisonous mushrooms.

```
>>> df['class'].value_counts()
e    4208
p    3916
```

[1]This dataset can be found at https://www.kaggle.com/uciml/mushroom-classification.

1.3 Encoding the Data

Note that all the features in our dataset are categorical variables. As a result, to proceed with evaluation of model performance, we must first encode these variables into numerical/binary values.

We need to deal with two kinds of categorical variables when encoding the features into numerical data. These are ordinal categorical variables and nominal categorical variables.[2] We will use different techniques to encode both of these kinds of categorical variables as they inherently represent different kinds of categorical data.

1.3.1 Nominal Categorical Variables

To encode nominal categorical variables, we will use one-hot binary features. For instance, if a feature f from a feature set $\mathcal{F}$ has k different categorical values, we can create k different binary features for each feature f of this kind. This is done because the values of each such feature do not hold any ordinal information, in that there should not be different weights for having a specific value of a specific feature.

1.3.2 Ordinal Categorical Variables

The ordinal categorical variables, on the other hand, have been encoded as numerical labels, as these informations contain valueable information about the 'scale' of a certain feature. For instance, if a feature f from a feature set $\mathcal{F}$ has k different features, it would be changed into numeric values $i \in 0, 1, ..., k-1$.

1.3.3 Encoding Process

The following code segment is used to encode the data.[3]

```
def encode(df):
    # Encode Ordinal Variables
    ordinal_columns = ['gill-spacing', 'gill-size',
            'stalk-shape', 'ring-number', 'population', 'class']
    columns = ordinal_columns[:]

    for column in columns:
        df[column] = df[column].astype('category')

        columns = df.select_dtypes(['category']).columns
        df[columns] = df[columns].apply(lambda x: x.cat.codes)

    # Encoding Nominal Variables
    columns = ordinal_columns[:]

    for column in df:
        if column not in columns:
            dummies = pd.get_dummies(df.pop(column))
            column_names = [column + "_" + x for x in dummies.columns]
            dummies.columns = column_names
            df = df.join(dummies)

    return df
```

[2]Information on which features are which kind of categorical variables can be found in Appendix A.
[3]This can be found in the data.py file.

We can now see how our encoded dataset $\mathcal{D}$ is shaped, and then proceed further in our task to classify data.

```
>>> X, y = data.load() # data.load() calls data.encode()
>>> X.shape
(8124, 107)
>>> y.shape
(8124,)
```

2 Machine Learning Pipeline

Before we proceed, let's briefly go through our machine learning pipeline. Consider the encoded dataset $\mathcal{D}$. Given this dataset, we will proceed to solve our classification problem by taking the following steps:

1. Feature selection and test-train split:[4]
   i. Split $\mathcal{D}$ into the training/validation set D and testing set D'.
   ii. Get a set of f best features from D; call this set $\mathcal{F}$.
   iii. Create new training Z and testing sets Z'_1, Z'_2 by choosing only the subset of features $\mathcal{F}$ from D and D' respectively.
2. Model selection and hyperparameter tuning:[5]
   i. Choose a set of models $\mathcal{M}$ and a possible set parameters $\mathcal{P}$ for each model.
   ii. For each model $M \in \mathcal{M}$, choose the best set of parameters $P^* \in \mathcal{P}$ via hyperparameter tuning. Note that the hyperparameter tuning process trains a model on Z with each possible parameter and evaluates performance on Z'_1.
   iii. Use k-fold Cross Validation on testing set Z'_2 to get mean accuracy and standard deviations for each model $M \in \mathcal{M}$ with it's optimal hyperparameters $P^* \in \mathcal{P}$.
   iv. Compare models with hypothesis testing and choose best model.

We will present the metrics and evaluation results for the best selected model.

3 Feature Selection

3.1 The Need for Feature Selection

Feature selection is a useful technique when we want to better understand the input feature set. Having fewer features also leads to a more interpretable model, and is definitely helpful in our case, since we have just created over 100 features from which we want to derive a model to solve the classification problem. As a result, feature selection techniques can help us get a better idea of which features matter more or less while classifying our model.

It is also important to note that feature selection helps us have a control over the complexity of the model. This is a very important aspect, as a less complex model is more useful for generalization.

[4]See get_reduced_data in data.py
[5]See modelSelection.py

3.2 Feature Selection Technique

We are using Greedy Subset Selection for Feature Selection. Greedy Subset Selection is a greedy algorithm for selecting a good subset of feature coordinates. Greedy selection chooses optimum features by minimizing the mean squared error. After selecting a subset of features, it tries to add features based on whichever feature works best with the current subset.

$$S = S \cup \left[\text{argmin}_{j \notin S} \text{min}_{\theta_{S \cup j}} \left(\frac{1}{2} \sum_{t=1}^{n} (y_t - \theta_{S \cup j} \cdot \phi_{S \cup j}(x_t))^2 \right) \right]$$

GSS is computationally faster than Subset Selection. It is also more optimal in comparison to Foward-Fitting and Myopic Forward Fitting algorithms.

3.3 Greedy Subset Selection Results

The following are the 46 best features and their weights obtained from Greedy Subset Selection:

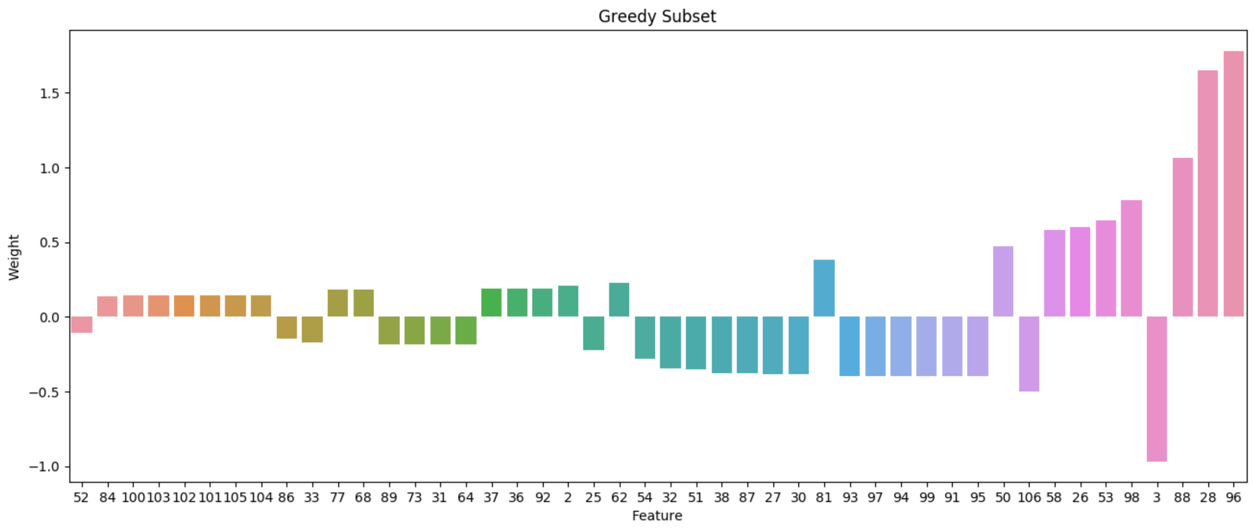


Figure 1: Greedy Subset Selection - 46 features with highest weights. Obtained from featureSelectionPlot.py

Our processed data-set contains 8124 samples and 107 features. Hence, the need for reduction of features arises from the size of the dataset, specifically, the large number of features our models need to learn from and the fact that certain features have a high correlations making addition of all features redundant. Further, a lot of the features have little or no correlation with the class label and adding such features just plainly increases our computation time without actually helping our model make 'better' decisions (in some cases, they even increase noise and make the model's decisions worse).

Thus, reduction of features increases the efficiency of training our models, helps us remove redundant features from our data set and learn only from features which have a considerable impact on our class labels. Reduction of features also helps in a control over complexity of some models, as it helps with better generalizability.

The best feature, as can be seen in the graph above is Feature 96, namely, bruises-f. This is a boolean encoded feature, which is 1 if the mushroom does not have any bruises, and 0 if the mushroom has bruises. Now, let's have a look at the following code to understand why this is:

```
>>> import data
>>> X, _, y, _ = data.get_reduced_data(0.6, 1)
>>> n = X.values.size
>>>  np.sum((X.values.resize(n, ) == y))
0
```

This indicates that in the training set $Z = (X, y)$, on which feature selection has been performed, every mushroom with bruises is a poisonous mushroom (since a sum of zero indicates that for each instance of X, the class label $y \in \{0, 1\}$ was not equal to the value of $X \in \{0, 1\}$). As such, this feature seems to be a very good identifier of the edibility of mushrooms.

4 Cross Validation

We use cross-validation to evaluate the chosen predictive model by paritioning it into smaller train and test datasets wherein we train the model on the training set and evaluate it on the testing set. By using better cross-validation techniques, we can get a better understanding of how well our model will generalize, and whether we might be over or underfitting.

In order to conduct cross validation for (i) tuning of hyperparameters [6] and (ii) evaluation of model performance [7], we use a form of nested cross validation as explained previously in our pipeline. We use a combination of k-Fold CV and Train-Validate-Test to make sure that any of the data used in either of the two evaluation sets has not been exposed to the models which are being tuned and evaluated before.

4.1 Basic Methodology

Given the original encoded dataset $\mathcal{D}$, we create a 40:20:40 split, namely D, D'_1, D'_2. We conduct our feature selection process as descibed in the previous section on D to obtain a reduced subset of features $\mathcal{F}$. This reduced subset of features is used to obtain Z, Z'_1, Z'_2, which are used as a train-validate-test sets respectively. Each model is initially trained with different hyperparameters on Z, and evaluated on Z'_1 to get the best set of hyperparameters. Further, we conduct k-Fold CV on Z'_2 by used the optimal set of hyperparameters which we get from the previous step to evaluate the performance of a selected model on unseen data.

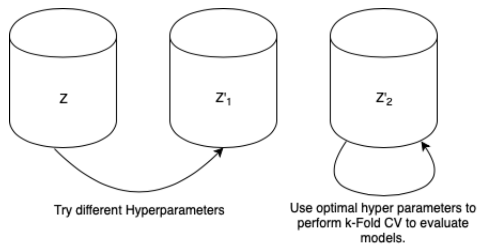

Z
Z'1
Z'2
Try different Hyperparameters
Use optimal hyper parameters to perform k-Fold CV to evaluate models.

Figure 2: Cross Validation Model

[6]See Section 5
[7]See Section 6

4.2 Train-Validate-Test

We obtain the Z, Z' 40:60 split in the data.py file when creating a dataset with a reduced number of features. After doing so, we further split Z' into Z'_1, Z'_2 such that $|Z| \approx 3200, |Z'_1| \approx 1600, |Z'_2| \approx 3200$. Note that all splits are random, and as a result, differing results may be obtain for different splits of the data.[8]

4.3 k-Fold CV

Here, we are using k-Fold Cross Validation on 2, 5, and 10 folds. While we conduct k-Fold Cross Validation in all of these fold sizes, we will only compare models based on their performances in 5-folds.

In k-Fold CV, we split the dataset into k different folds. For each i^{th} fold, where $i = 1, 2, ..., k$, we train on the remaining $k-1$ folds and evaluate on the single remaining fold. As a result, we get k different measures of the metrics which we are using for each model we evaluate using the cross-validation technique. These can be aggregated into a single metric as follows:

$$\hat{\mu} = \frac{1}{k} \sum_{1 \le i \le k} M_i, \text{ and } \hat{\sigma}^2 = \frac{1}{k} \sum_{1 \le i \le k} (M_i - \hat{\mu})^2$$

where M_i is the measure for the i^{th} fold (here, it is accuracy). This aggregation may be used in a statistical hypothesis test to compare the performances of two different models.

The following is our implementation of k-fold cross validation:[9]

```
# For each fold
for i in range(k):
    # Find sets S and T
    lower = np.floor(float(n) * i / k).astype('int64')
    upper = np.floor(float(n) * (i + 1) / k - 1).astype('int64')
    T = range(lower, upper + 1)
    S = list(range(0, lower)) + list(range(upper + 1, n))

    # Get training data
    X_train = X[S, :]
    y_train = y[S]

    # Fit model
    m = model(**kwargs)
    m.fit(X_train, y_train)

    # Check prediction accuracy
    y_pred = m.predict(X[T])

    # Update Z values based on accuracy score
    Z[i] = metrics.accuracy_score(y[T], y_pred)

# Return k-Fold results
return Z
```

[8]As we'll see however, even with different splits, we get multiple models which consistently performs with over 98% accuracy on the 5-Fold CV on Z'_2. We will use vc-Dimensions of these models along with results from hypothesis testing (Section 7) to compare these models further.

[9]This can be found in the kfoldcv.py file.

5 Hyperparameter Tuning

Before we conduct any evaluations on a model, we obtain the optimal hyperparameters for the model such that we can compare different models based on each of their tuned hyperparameters. To do this, we utilize Grid Search. For instance, consider the following set of possible hyperparameters for Adaboost:

```
{
    'n_estimators': [3, 5, 10, 20, 50],
    'learning_rate': [0.1, 0.5, 1],
    'algorithm': ['SAMME', 'SAMME.R']
}
```

This python dictionary (which can be found in models.py for each model we use) is used to represent a set of possible values for each of the h different hyperparameters we want to tune.

The key represents the hyperparameters and the value represents the different values of the hyperparameters which we wish to check our models performance on. As such, we create a 'grid' of dimension h all possible combinations of the hyperparameters, and search through the grid to see which combination of hyperparams gives us the best result when the model is trained on Z and evaluated on Z'_1.

The following method returns the best set of parameters given a model, and its possible params (in kwargs) by training the model on Z and evaluating performance on Z'_1. [10]

```
# For all combinations of hyperparams;
# lists contains all possible values of hyperparams
for el in itertools.product(*lists):

    # Create current set of test params
    test = {}
    for i in range(len(el)):
        test[keys[i]] = el[i]

    # Train the model on Z
    m = model(**test)
    m.fit(X_train, y_train)

    # Evaluate the model on Z'_1
    y_pred = m.predict(X_test)
    acc = metrics.accuracy_score(y_test, y_pred)

    # Update max_accuracy and best_params
    if (acc > max_accuracy):
        max_accuracy = acc
        best_params = test

# Return the best set of params
return best_params
```

[10]This method can be found in hyperparameterTuning.py.

6 Model Evaluations

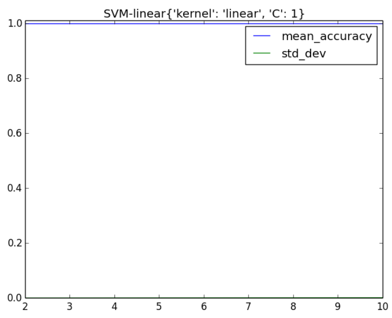
In order to solve the classification problem, with a reduced number of features, we will test the following machine learning algorithms with $\{2, 5, 10\}$-Fold Cross Validation and different metrics, including Hypothesis Testing, ROC Curves, etc. to compare the results:

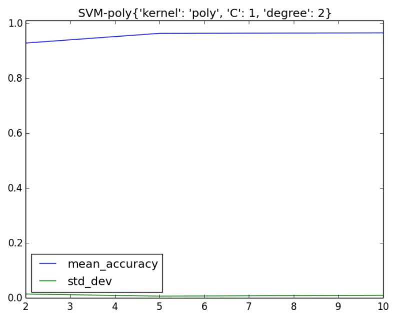
1. Support Vector Machine
   (a) Linear Kernel
   (b) Polynomial Kernel
   (c) RBF Kernel
2. Logistic Regression
3. Adaboost

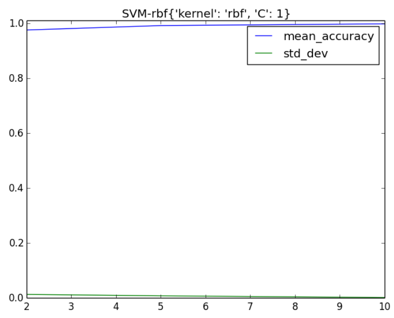
We conduct hyperparameter tuning and run 2,5,10-fold CV for each of these models as in modelSelection.py.

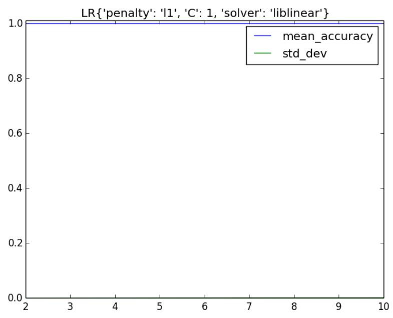
6.1 Model k-Fold CV Results

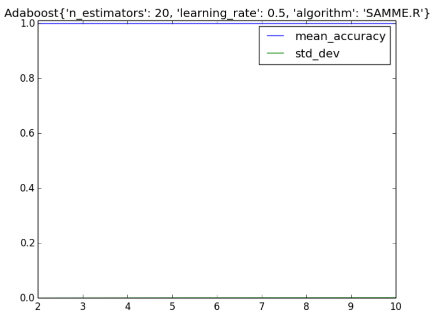
The following graphs are the graphs for number of folds (2, 5, 10) vs accuracy for the tuned hyperparameters of each of the models as generated by modelSelection.py. Note that the title contains the dictionary which represents the optimal hyperparameters.











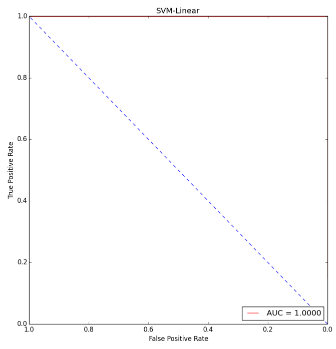
The following table contains the mean and standard deviations of 5-fold CV for each of the models on this instance of running modelSelection.py.

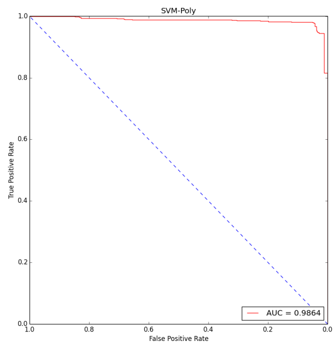
Models	Adaboost	Logistic Regression	SVM-Linear	SVM-RBF	SVM-Polynomial
μ	0.99937	0.99937	0.99906	0.99222	0.00840
σ	0.00076	0.00076	0.00076	0.96395	0.00711

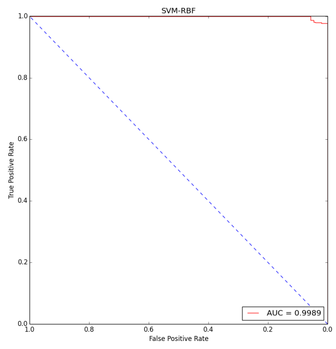
6.2 ROC Curves

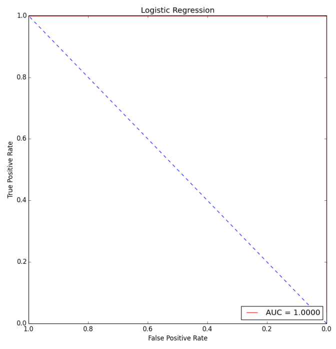
ROC is metric to evaluate classifier output quality. ROC is a plot of signal (True Positive Rate) against noise (False Positive Rate). The model performance is determined by looking at the area under the ROC curve (or AUC).

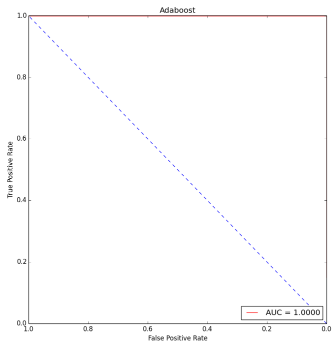
ROC curves typically have the and false positive rate on the X axis and true positive rate on the Y axis. The top left corner of the plot is the “ideal” point - a false positive rate of zero, and a true positive rate of one. The “steepness” of ROC curves is also important, since it is ideal to maximize the true positive rate while minimizing the false positive rate. An ideal model would have AUC = 1.0, since it would mean that the false positive rate is zero for all observations. Here are the ROC Curves generated from the tuned hyperparameters for each model:











6.3 A Note Variability of Results

Recall that, as we mentioned in Section 4.2 and in Footnote 8, we are splitting the data into the three dataset we use for training and evaluation randomly. As such, the results obtained on different instances may be different. Furthermore, the tuned hyperparameters might be different as well.

However, we obtain very good results when performing 2,5,10-fold cross-validation using the tuned SVM-linear, Logistic Regression, and Adaboost models consistently (more than 98% accuracy each time). As a result, we must employ other techniques such as statistical hypothesis testing and comparison of VC-Dimensions of these models to determine which model best fits our problem. We have done so in section 7. Regardless, we have presented the results for one such split of Z, Z_1', Z_2'.

7 Model Comparison

To compare the performance of different models based on the 5-fold cross validation on Z_2', we can conduct hypothesis testing on their results. The purpose of hypothesis testing is to make a decision in the face of uncertainty. We used hypothesis testing to understand which model would be better to predict the edibility of the Mushrooms based on the data. Since none of our models are "perfect" we used hypothesis testing to understand which algorithm is more likely to perform better.

7.1 Hypothesis Testing

We used t-distribution because we don't know the population standard deviation; we did not use all the mushroom data to train our algorithm. We ran k-fold cross validation for the different algorithms and compared them pairwise with t-distribution. We calculated the mean and standard deviation of the errors obtained from each of the k-folds. Let's call these mean errors μ_1, σ_1 be the mean error and standard deviation of the first model and μ_2, σ_2 be the mean error and standard deviation of the second model. We can conduct hypothesis testing as follows:

1. Null hypothesis: $\mu_1 = \mu_2$
2. Calculating test parameters:
$$x = \frac{(\mu_1 - \mu_2)\sqrt{n}}{\sqrt{\sigma_1^2 + \sigma_2^2}}$$
3. Calculating degrees of freedom:
$$\nu = \left\lceil \frac{(\sigma_1^2 + \sigma_2^2)^2 (n-1)}{\sigma_1^4 + \sigma_2^4} \right\rceil$$
4. Reject null hypothesis in favor of first algorithm if
$$x > x_{1-\alpha,\nu}$$
where α is the level of significance (Note that we chose $\alpha = 0.01$).

We conduct hypothesis test for the model with the best average performance against all the other models at the end of modelSelection.py using the t-test in hypothesisTest.py. The following are the results for one instance of running modelSelection.py (the same as the one for which results have been provided in section 6.1):

```
Adaboost > LR: False
Adaboost > SVM-linear: False
Adaboost > SVM-rbf: False
Adaboost > SVM-poly: True
```

As we can see on various instances, it is not clear even from hypothesis testing whether SVM-linear, Adaboost, or LogisticRegression are better suited to our problem. As a result, we must use some other way to compare how these models will

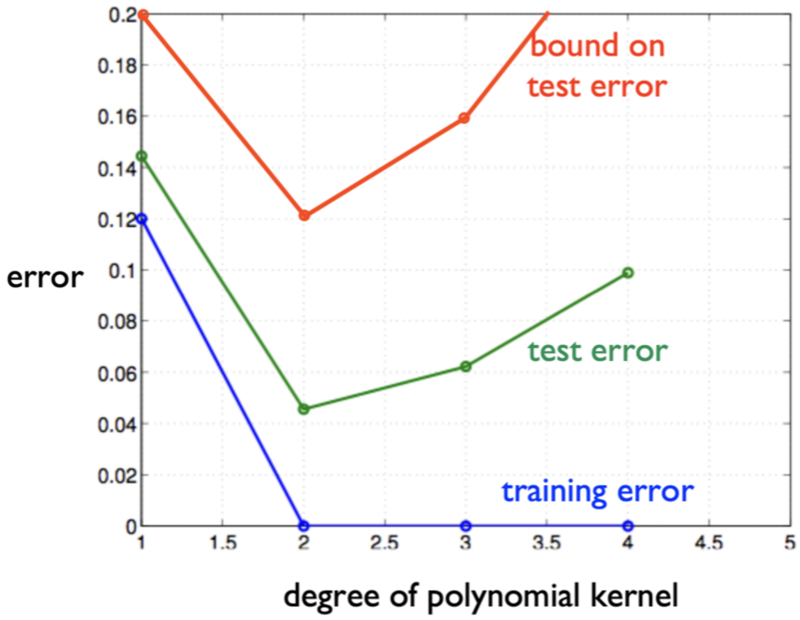
7.2 VC Dimensions and Generalizability

The Vapnik - Chervonenkis dimension of each model is given by:

$$d_{vc} = \max_n \{n : N_F(n) = 2^n\}$$

where N_F is the growth function.

For our mushroom classification problem, we have tried multiple models and each of models display different characteristics for different train-test data splits and have differing accuracies and standard deviations. However, since each of them consistently have a performance of more than 98% accuracy, and since hypothesis testing is inconclusive, we can use VC-dimensions for each of these models to get a theoretical upper bound on the test errors for each of the models. As such, the model with the best theoretical lower bound would be most suited to out problem.



The relation between the test error $R(f)$, training error $R_n(f)$ and VC-dimension is given by the following equation:

$$R(f) \leq R_n(f) + \sqrt{\frac{\log N_F(2n) + \log(4/\delta)}{n}}$$

where it is true for N_F given that the number of samples $n \geq d_{vc}$ (which, in our case it is) that:

$$\log N_F(2n) \leq d_{vc}\left(1 + \log\frac{2n}{d_{vc}}\right)$$

As a result, a model with lower vc-dimension would have an increased generalizability as it would result in a smaller upper bound for R_f. The following are the VC-dimensions for all the models we use (where $d =$ number of features, $m =$ number of decision stumps):

1. SVM Linear: $d_{vc} = d + 1$
2. SVM RBF: $d_{vc} = \infty$
3. Logistic Regression: $d_{vc} = d + 1$
4. Adaboost: $d_{vc} \geq m/2$

Since we are using $d = 50$ features, we are using at most 20 decision stumps for Adaboost, we know that Adaboost has a lower vc-Dimension than any of the other models we are using and would, as a result, have the lowest upper bound for the test error.

8 Conclusion

After doing hypothesis testing we concluded that Adaboost, SVM linear and logistic regression perform equally well; when we compared each of them, we did not reject the null hypothesis (mean accuracy are equal). So, to choose the best out of these three we calculated the VC Dimension of each of these algorithms. As mentioned before, Adaboost has the lowest VC-Dimension out of these three models and thus has the lowest relative test-error bound. A lower test-error bound means that, theoretically, there is lesser gap between training error and testing error. Hence, with Adaboost we can be more certain about the testing error. Using feature selection in our algorithm discarded all the “noise” features and improved generalization. Exploring the data, helped us understand the correlations between the features and between a feature and the class label.

Appendix A: Data Description

Classes: edible=e, poisonous=p (y-values)

Size of dataset (before encoding): $(n = 8124, d = 22)$
Size of dataset (after encoding): $(n = 8124, d = 107)$
Attribute Information and Encoding:

1. Nominal Categorical Variables:
   These variables will be encoded as binary one-hot features. As a result, each feature in this category would be replace by the k features in the encoded dataset if the feature has k possible values. These featues include:

   i. **cap-shape**: bell=b, conical=c, convex=x, flat=f, knobbed=k, sunken=s
   ii. **cap-surface**: fibrous=f, grooves=g, scaly=y, smooth=s
   iii. **cap-color**: brown=n, buff=b, cinnamon=c, gray=g, green=r, pink=p, purple=u, red=e, white=w, yellow=y
   iv. **bruises**: bruises=t, no=f
   v. **odor**: almond=a, anise=l, creosote=c, fishy=y, foul=f, musty=m, none=n, pungent=p, spicy=s
   vi. **gill-attachment**: attached=a, descending=d, free=f, notched=n
   vii. **gill-color**: black=k, brown=n, buff=b, chocolate=h, gray=g, green=r, orange=o, pink=p, purple=u, red=e, white=w, yellow=y
   viii. **stalk-root**: bulbous=b, club=c, cup=u, equal=e, rhizomorphs=z, rooted=r, missing=?
   ix. **stalk-surface-above-ring**: fibrous=f, scaly=y, silky=k, smooth=s
   x. **stalk-surface-below-ring**: fibrous=f, scaly=y, silky=k, smooth=s
   xi. **stalk-color-above-ring**: brown=n, buff=b, cinnamon=c, gray=g, orange=o, pink=p, red=e, white=w, yellow=y
   xii. **stalk-color-below-ring**: brown=n, buff=b, cinnamon=c, gray=g, orange=o, pink=p, red=e, white=w, yellow=y
   xiii. **veil-type**: partial=p, universal=u
   xiv. **veil-color**: brown=n, orange=o, white=w, yellow=y
   xv. **ring-type**: cobwebby=c, evanescent=e, flaring=f, large=l, none=n, pendant=p, sheathing=s, zone=z
   xvi. **spore-print-color**: black=k, brown=n, buff=b, chocolate=h, green=r, orange=o, purple=u, white=w, yellow=y
   xvii. **habitat**: grasses=g, leaves=l, meadows=m, paths=p, urban=u, waste=w, woods=d

2. Ordinal Categorical Variables:
   These variables will be encoded in place by encoding labels, as the data here has ordinal meaning to it. These variables include:

   i. **gill-spacing**: close=c$\rightarrow$0, crowded=w$\rightarrow$1, distant=d$\rightarrow$2
   ii. **gill-size**: broad=b$\rightarrow$0, narrow=n$\rightarrow$1
   iii. **stalk-shape**: enlarging=e$\rightarrow$0, tapering=t$\rightarrow$1
   iv. **ring-number**: none=n$\rightarrow$0, one=o$\rightarrow$1, two=t$\rightarrow$2
   v. **population**: abundant=a$\rightarrow$0, clustered=c$\rightarrow$1, numerous=n$\rightarrow$2, scattered=s$\rightarrow$3, several=v$\rightarrow$4, solitary=y$\rightarrow$5

Appendix B: List of Scripts

The following scripts have been included with the preliminary report in the zip file:

1. data.py - Interface to load encoded data.
2. project.py - Contains project config.
3. kfoldcv.py - Conduct kfoldcv.
4. greedySubset.py - Conduct Greedy Subset Selection.
5. featureSelection.py - Graph the results for Greedy Subset Selection.
6. hyperparameterTuning.py - Tunes hyperparams for a model.
7. hypothesisTest.py - Conducts hypothesis testing.
8. rocCurve.py - Plots the ROC Curve for a model.
9. models.py - Contains all models used and their hyperparameters.
10. modelSelection.py - Main driver file. Makes calls to data, kfoldcv, hyperparameterTuning, hypothesisTest, models to conduct all discussed steps regarding model selection.