Report for Project 3

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December 16, 2018

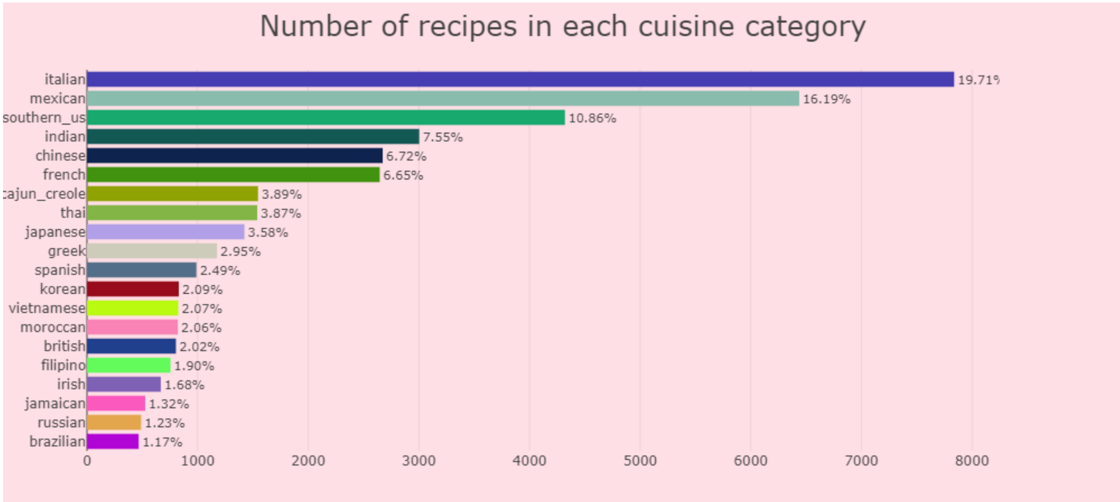
In this project we analysed some cooking data and did fairly well.

1 Introduction

In this project we explore a delicious classification problem: Given a list of ingredients, can you predict what cuisine the final dish will be? There are certainly cases where this is easy. If you meet you friend at the store and they have burritos, guacamole, salad, and beef in their basket, you can feel confident they are having Mexican food. But what if they have flour, yeast, and milk? They are probably baking, but are they making a French baguette our Indian naan bread?

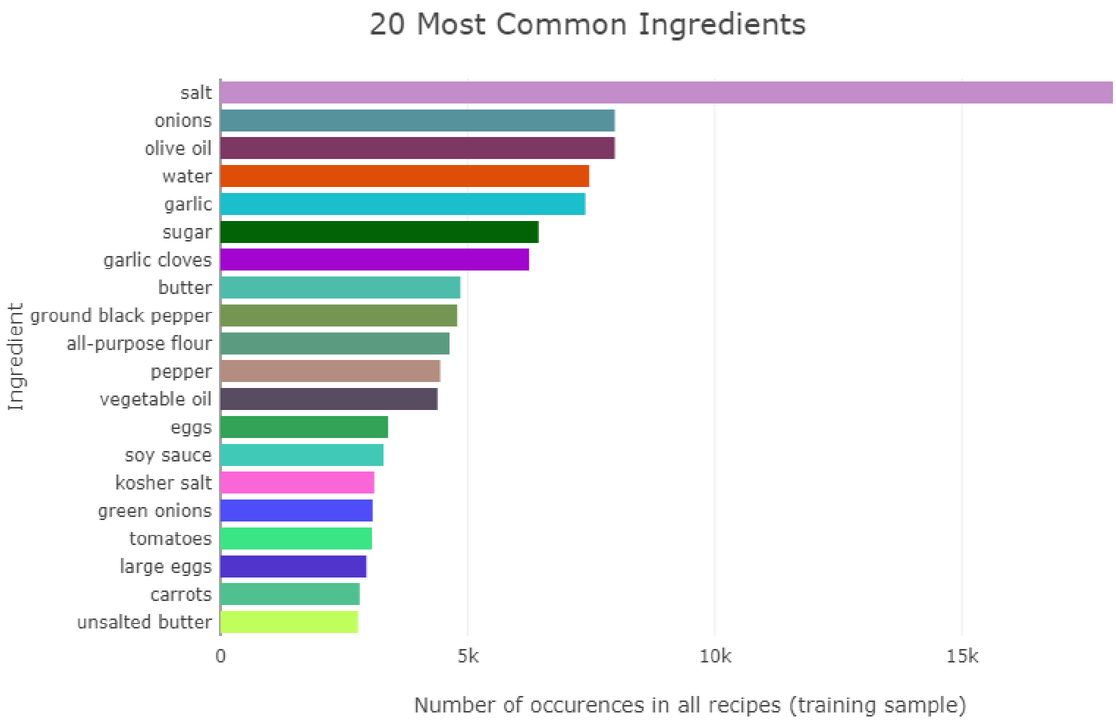
In this project we will use various machine learning techniques to solve this classification problem. Our data comes from an old kaggle competition.

Our data consists of 39,774 recipes which spans over 20 different cuisines. They are distributed between the 20 cuisines like this:



We can tell from the plot that around 36% of the data is labeled as either italian or mexican cuisine. So we should be prepared on that this uneven distribution of the recipes will affect how our predictors will do.

It is also interesting to look at what the most common ingredients are:



Salt is the most common ingredient by far. It is so common, that we can expect it to not be as good of a classifier as it probably won't be particular for a certain cuisine. The other ingredients are more evenly spread out, which is expected.

The paper is organized as follows: A section on methods, a section on selection and so on.

Machine learning has gained a huge popularity boost over the last couple of years. And this is no wonder: the techniques have a wide range of applications and can be a major asset if you know when to use what.

When to use what is exactly what we're going to have a brief peek into in this project. We will evaluate the performance of three different methods for classification on a data set consisting of recipies labeled with the cuisines they belongs to. That is we are looking at a classification problem with multiple classes. The methods we will look at are logistic regression, support vector machines and random forests.

All the code we have implemented can be found at `https://github.com/???`. A print of the jupyter notebook is also attached at the end of this report.

2 Methods

First we need to establish some notation. In the following we assume that we are given $N \in \mathbb{N}$ samples consisting of $p \in \mathbb{N}$ features and one target. Further we let $K \in \mathbb{N}$ be the number of classes in our classification problem. We then denote by $x_{i,j}$ the j-th feature of the i-th sample and by $t_i \in \{1, 2, \ldots, K\}$ the target of the i-th sample.

2.1 Reading in the data

The raw data lives in a .json file, which we load using Pandas. Each recipe has a cuisine and a list of ingredients. The first thing we do is to join all the ingredients into one string, and then we use scikit learns `CountVectorizer` on the corpus of all recipes to get a matrix representation of the data. The `CountVectorizer` works by making each individual word in the whole corpus a feature. Each recipe is then a vector in $\mathbb{R}^p$, with the k'th entry equal to the number of times the k'th feature (ingredient) appears in the recipe, usually this will be 0 or 1. This means that a recipe that calls for tomato sauce will have the features tomato and sauce set to 1, even if it does not use a tomato.

Before using the `CountVectorizer` we clean up the data a little bit, namely we replace hyphens with spaces, to make sure e.g. *low-fat* and *low fat* are treated the same, and we drop all numbers and special characters. The latter because the recipes are not all formatted in the same way, with some including amounts. When using `CountVectorizer` we set the parameter `min_df` to 3. This means we only include features that appear at least 3 times in all lists of ingredients. A feature that only appears once is useless for prediction, because it will either be contained only in the training data or only in the test data. We also excluded features that only appeared twice because the likelihood for them to appear in just the training data or just the test data are relatively high, approximately 68%.

2.2 Logistic Regression

Since we now are dealing with a classification problem with multiple categories, there are at least two different ways to approach this. The first one is maybe the easiest one technically, we simply make one binary model (as explained in[**?**]) for each category. We thus have K models P_k, where $P_k(\boldsymbol{x})$ is the likelihood of the sample with features $\boldsymbol{x}$ being in category k, and $1 - P_k(\boldsymbol{x})$ is the likelihood that the sample is not in category k. One drawback with this approach is that we don't necessarily have $\sum_{k=1}^{K} P_k(x) = 1$, that is, our model doesn't act very much like a probability distribution. In many cases this is not a problem, but if this property is desirable there's a slightly different way of doing it.

Let $\boldsymbol{x}_i := (1, x_{i,1}, x_{i,2}, \ldots, x_{i,p})$ be the row-vector in $\mathbb{R}^{p+1}$ consisting of a one followed by the features of sample i. Also let $\boldsymbol{\beta_k}$ be a column-vector in $\mathbb{R}^{p+1}$ for $k \in \{1, 2, \ldots, K-1\}$

and let $\boldsymbol{\theta} := [\boldsymbol{\beta}_1 \; \boldsymbol{\beta}_2 \; \dots \; \boldsymbol{\beta}_{K-1}]$ be the matrix with the $\boldsymbol{\beta}_k$'s as it's columns. Our model is then given by

$$\begin{aligned} P_k(\boldsymbol{x};\boldsymbol{\theta}) &= \frac{\exp(\boldsymbol{x}\boldsymbol{\beta}_k)}{1+\sum_{l=1}^{K-1}\exp(\boldsymbol{x}\boldsymbol{\beta}_l)} \qquad k \in \{1,2,\dots,,K-1\} \\ P_K(\boldsymbol{x};\boldsymbol{\theta}) &= \frac{1}{1+\sum_{l=1}^{K-1}\exp(\boldsymbol{x}\boldsymbol{\beta}_l)} \end{aligned} \tag{1}$$

where the $\boldsymbol{\beta_k}$'s are the coefficients we wish to estimate. $P_k(\boldsymbol{x};\boldsymbol{\theta})$ is then the likelihood that a sample with features $\boldsymbol{x}$ belongs to category k. In this case we have the neat property that $\sum_{k=1}^{K} P_k(x) = 1$ [Hastie et al., 2009]. Hence our model act's more like a probability distribution. In this project we use a scikit-learn method that emphazises this last approach.

The way we fit our model in the case of logistic regression deviates slightly from the usual proceedure with the introduction of a loss function. We now instead define a function we wish to maximize, namely the log-likelihood function given by

$$L(\boldsymbol{\theta}) = \sum_{i=1}^{N}\sum_{k=1}^{K} \chi_{\{k\}}(t_i)\log(P_k(\boldsymbol{x}_i;\boldsymbol{\theta})) \tag{2}$$

However the difference doesn't go further than the fact that this function shouldn't be interpreted exactly as a loss function. Other than that we proceed as usual by minimizing the negative of this function in order to maximize the original function. To do this we first need to compute the derivative of this function with respect to $\boldsymbol{\theta}$. Some computations gives us

$$\frac{\partial L(\boldsymbol{\theta})}{\partial \beta_{k,j}} = \sum_{i=1}^{N} \chi_{\{k\}}(t_i) x_{i,j}(1 - P_k(x_i;\theta)) \tag{3}$$

We are now all set to use the gradient method of your choice to minimize $-L$ as a function of $\boldsymbol{\theta}$. This way we fit our model to the given set of training data. For an explanation of some gradient-methods consult [**?**].

2.3 Support Vector Machines

This section is based on [James et al., 2013, Chapter 9] and [Hastie et al., 2009, Chapter 12].

2.3.1 Linearly separable data

Support vector machines where originally introduced to be used for a two class classification, so we will discuss that case first. For ease of notation let the classes be $\{-1, 1\}$. Recall that if $\beta_0, \beta_1, \dots, \beta_p \in \mathbb{R}$, then we can define a hyperplane H in $\mathbb{R}^p$ by

$$H = \left\{ \begin{pmatrix} z_1 & z_2 & \cdots & z_p \end{pmatrix} \;\middle|\; \beta_0 + z_1\beta_1 + z_2\beta_2 + \cdots + z_p\beta_p = 0 \right\}.$$

We can always assume that

$$\sum_k \beta_k^2 = 1,$$

and from here on out we will do just that.

We say that a given data set is linearly separable, if there exists a hyperplane H in $\mathbb{R}^p$ such that all data points $x_i = \begin{pmatrix} x_{i1} & x_{i2} & \cdots & x_{ip} \end{pmatrix}$ with $t_i = 1$ satisfy

$$\beta_0 + x_{i1}\beta_1 + x_{i2}\beta_2 + \cdots + x_{ip}\beta_p > 0, \tag{4}$$

and all data points $x_j = \begin{pmatrix} x_{j1} & x_{j2} & \cdots & x_{jp} \end{pmatrix}$ with $t_j = -1$ satisfy

$$\beta_0 + x_{j1}\beta_1 + x_{j2}\beta_2 + \cdots + x_{jp}\beta_p < 0. \tag{5}$$

Intuitively all points with $t_i = 1$ lie on one side of H and all points with $t_i = -1$ lie on the other side. This intuition is entirely correct if $p = 2$, if $p > 2$ then it is still correct, provided one has the right mental image of the sides of hyperplane. Note that equations (4) and (5) can be combined to the single equation

$$t_i(\beta_0 + x_{i1}\beta_1 + x_{i2}\beta_2 + \cdots + x_{ip}\beta_p) > 0. \tag{6}$$

Given some new data point $z = \begin{pmatrix} z_1 & z_2 & \cdots & z_p \end{pmatrix}$, we then predict $t \in \{-1, 1\}$ such that

$$t(\beta_0 + z_1\beta_1 + z_2\beta_2 + \cdots + z_p\beta_p) > 0.$$

2.3.2 Data that is not linearly separable

If a given data set is linearly separable, then there will be infinitely many separating hyperplanes. From one point of view, any one of these will do to make predictions. However, it seems intuitively correct to pick a hyperplane that is in the middle of the two classes. This is achieved by choosing the so called maximal margin hyperplane. That is, we want to choose $\beta_0, \beta_1, \cdots, \beta_p$ such that we maximize $M > 0$ under the condition that

$$t_i(\beta_0 + x_{i1}\beta_1 + x_{i2}\beta_2 + \cdots + x_{ip}\beta_p) \geq M,$$

for all data points x_i.

Of course, or data will not usually be linearly separable. To still get useful classification, we will accept hyperplanes that do not cleanly separate the points. This is achieved by introducing for each data point x_i a slack variable $\varepsilon_i \geq 0$. Then aim to find $\beta_0, \beta_1, \dots, \beta_p$ that maximize $M > 0$ under the conditions

$$t_i(\beta_0 + x_{i1}\beta_1 + x_{i2}\beta_2 + \cdots + x_{ip}\beta_p) \geq M(1 - \varepsilon_i),$$
$$\sum \varepsilon_i \leq C,$$

where $C \geq 0$ is a tuning parameter. We note that if $\varepsilon_i = 0$, then the point x_i is outside the margin of the hyperplane, if $0 < \varepsilon_i < 1$, then x_i is inside the margin but on the right side of the hyperplane, and if $1 < \varepsilon_i$, then x_i is on the wrong side of the hyperplane, i.e. it is misclassified. Hence C is an upper bound on the number of point we are allowed to misclassify when we choose H. However, a choice of $C < 1$ is still very valid, it just corresponds to choosing a very narrow margin, is we do not allow many points to be inside the margin.

2.3.3 Kernels

Actually solving the maximization problem of finding a hyperplane H and a margin M is done using Lagrange multipliers. We will not discuss how this is done in detail, but will just focus on two aspect of this approach (see equation (12.17) in [Hastie et al., 2009])

(a) To find H and M one does not actually need the data points x_i but rather all inner products $\langle x_i, x_j \rangle$.

(b) H and M will not depend on all the datapoints x_i, the points they do depend on are called the support vectors.

The first of these points leads to the kernel techniques for support vector machines. In a variety of classification problems it can be helpful to change the feature space. This is done by finding some mapping $\phi\colon \mathbb{R}^p \to \mathbb{R}^q$ and then classifying $\phi(x_i)$ instead of x_i. A typical example is to add polynomial features, if $p = 2$ say, we might want to consider not only $\begin{pmatrix} z_1 & z_2 \end{pmatrix}$ but instead $\begin{pmatrix} z_1 & z_2 & z_1^2 & z_1 z_2 & z_2^2 \end{pmatrix}$. Computing all these extra features can be a time and memory consuming task, but for support vector machines one does not need to do it. Since we only need inner products of datapoints, it suffices to find a kernel function K such that

$$K(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle.$$

For instance using the kernel function

$$K(x_i, x_j) = \sum \left(1 + \sum_{k=1}^{p} x_{ik} x_{jk} \right)^d,$$

corresponds, upto some constants, to adding polynomial features of degree d.

2.3.4 More than two classes

To use support vector machines in a situation where there are $K > 2$ classes, scikit learn by default uses a so called one-vs-rest approach. For each class c we use a support vector machine classifier with classes $\{-1, 1\}$ chosen so that class c is coded 1 and all other classes are coded -1. This gives K hyperplanes with parameters $\beta_0^c, \beta_1^c, \ldots, \beta_p^c$, $c = 1, 2, \ldots, K$. Given an unseen datapoint z we classify it as belonging to the class c for which $\beta_0^c + \beta_1^c z_1 + \cdots \beta_p^c z_p$ is the largest.

2.3.5 Getting probabilities

While support vector machines do not provide a probability estimate as described above, there is some research into how to get that. Scikit learn implements a methods developed in [Wu et al., 2004]. However, computing these are expensive and they are not guaranteed to give the same prediction as the usual support vector machine, so we will not use this approach in this project.

2.4 Decision trees

Building a classification decision tree works in roughly two steps:

1. We divide the predictor space - that is, the set of possible values for X_1, X_2, ..., X_p into J distinct and non-overlapping regions, R_1, R_2, ..., R_J.

2. For every observation that falls into the region R_j, we make the same prediction, which is simply the *most commonly occurring class* of training observations in the region to which it belongs.

Each X_i uses all data points as data to split into the regions, R_j. The result of this is then that you get a classifier which predicts well on the training data, but falls short on testing data. This is because it fits its classifier perfectly to the data which it has seen. If it just splits up into enough R_i's, it would be able to place every sample perfectly. So a lone decision tree with all features will almost always be overfitted.

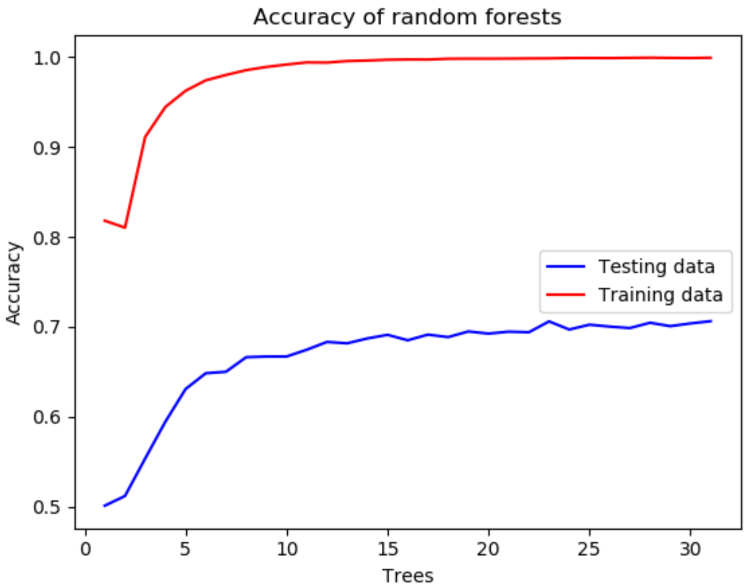
2.4.1 Rather a forest, then just a tree

This is why random forests are more popular. A random forest can usually generalise much better then what a lone tree can.
A random forest is constructed by choosing how many decision trees you want in the forest and then train every tree on your data. But the construction of these trees is done differently then a lone decision tree.

Each tree just use a subset of the features, typically $features = \sqrt{all - features}$. This makes it so each tree functions a bit differently and will then predict different things. The final prediction then becomes which of the classes which gets voted most for when every tree predicts their own.

2.4.2 Difference in number of trees

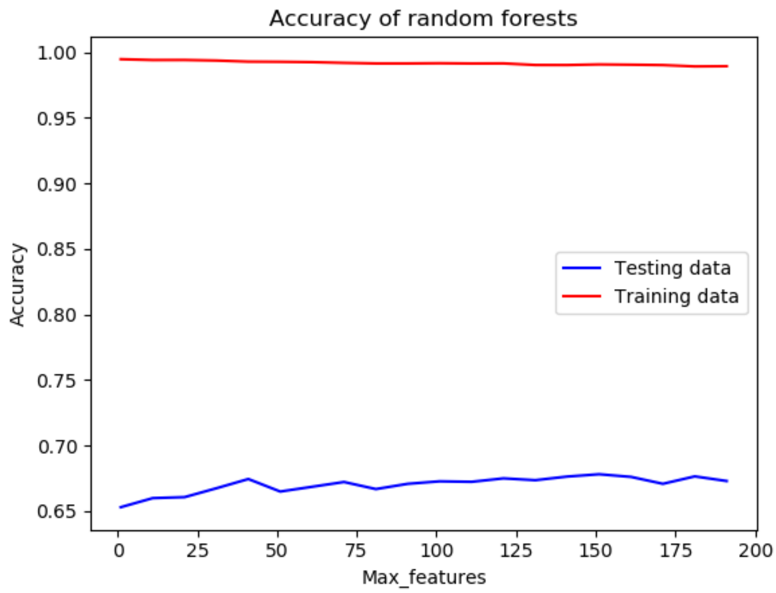
The number of trees in the forest is the main hyper parameter we have used to tweak this classifier. But it seems like the rule of thumb was the more, the merrier. Here is a plot of how well the random forest did:



So more trees provides a better accuracy. But the classifier starts to have a decent accuracy after 10 trees.

2.4.3 Difference in number of max_features

Here is a plot on how well the accuracy is using different numbers as max_features:



The number of trees used is 10.

The default in the scikitlearn classifier is using the root of the number of all the features as max_features. Since we have approximately 2000 features, the root becomes 44.72. That's why I computed different accuracies around this number.

The plot tells us that it doesn't seem to matter much what we use as max_features. The optimum in the plot is around 40 which gives us just more reason to stick with the default of using the root of all the features as max_features.

2.5 Voting Classifiers

Voting classifiers provide a way to combine a collection of classifiers `clf_k`, $k = 1, 2, \ldots, n$ to form a single classifier, `voting_clf`. There are two ways to form voting classifiers, using hard or soft voting. In hard voting, to predict the class of a data point z, we ask each classifier to predict what class a z belongs to, and then the voting classifier returns the class with the most votes. In case of a tie, the scikit learn implementation simply picks the label that comes first when the the labels are sorted. For soft voting, we can only use classifiers that assign a probability to each label. The voting classifier asks each of `clf_k` for their probability distribution of the labels, sums them up and picks the label with the highest sum.

As an example, suppose we have three classifiers A, B, C and 2-labels. Suppose further that on a datapoint z they give the following predictions.

	P(-1)	P(1)
A	0.55	0.45
B	0.51	0.49
C	0.10	0.90
SUM	1.16	1.74

Since both A and B predict the label -1, a hard voting scheme will lead to the voting classifier predicting the label -1. On the other hand, if we use a soft voting scheme the voting classifier will predict 1. So when using soft voting we take into account how "sureÂ´Â´ each classifier is in its prediction, but we are restricted to using classifiers that return probabilities.

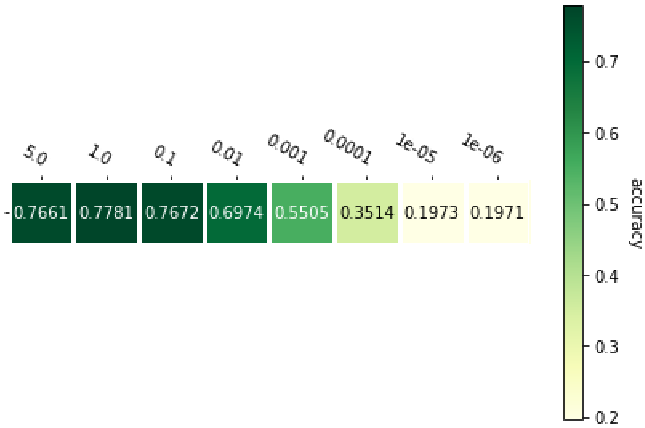
3 Model Selection and Verification

We used cross validation to decide how to tune our models. Because of the size of our data set we felt that three folds would suffice. To preform the cross validation we used the scikit learn method `cross_val_score`, which returns a list of accuracies, one for each fold. We simply took the average of this to the expected accuracy of a method on unseen data, similar to how cross validation for MSE is treated in [Hastie et al., 2009, Chapter 7.10].

3.1 Single model

For Logistic Regression, we tune the C parameter. The following figure shows the results of our cross validation computations.

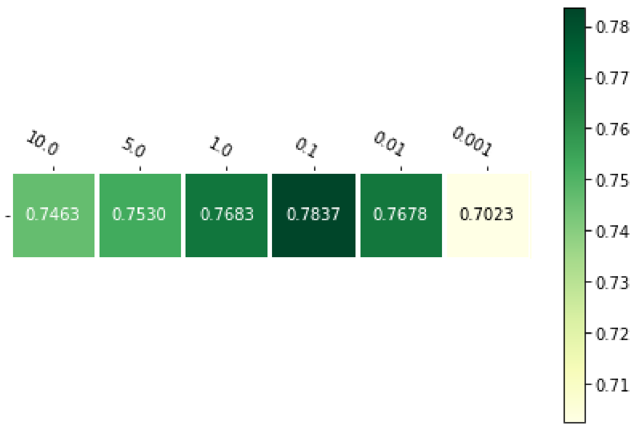
Figure 1: Choosing C for logistic regression.



We get the best results when using $C = 1$.

For the linear support vector machine the tuning parameter is also called C. Below are the most important outputs of our cross validation computations.

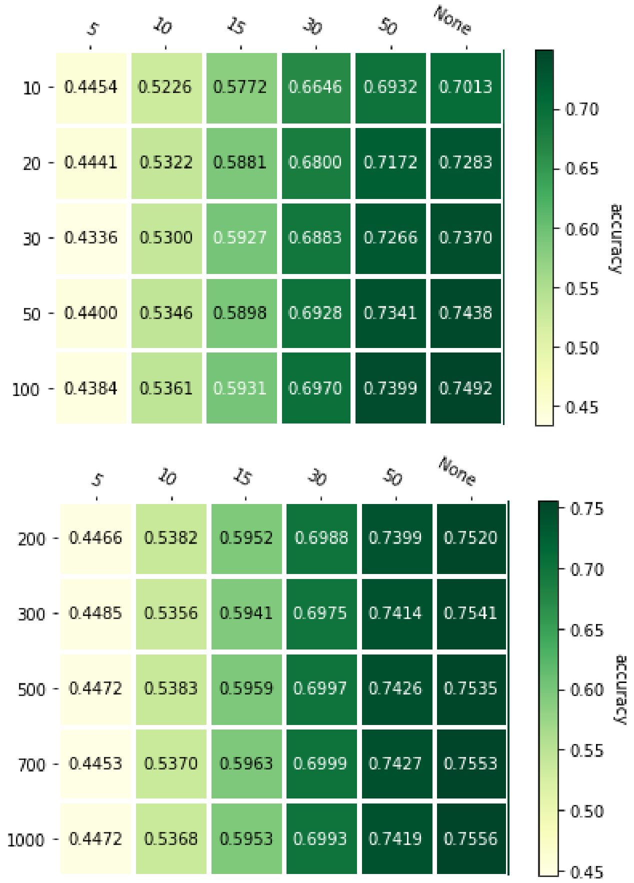
Figure 2: Choosing C for support vector machines.



Here the best constant is $C = 0.1$.

Random forrest are a voting classifier, so we would expect that more trees yield better results. We might be concerned that having too many leafs could lead to over fitting, but as the figure below shows, that is not the case. The horizontal axis is the maximal depth of the trees, and the vertical indicates the number of trees.

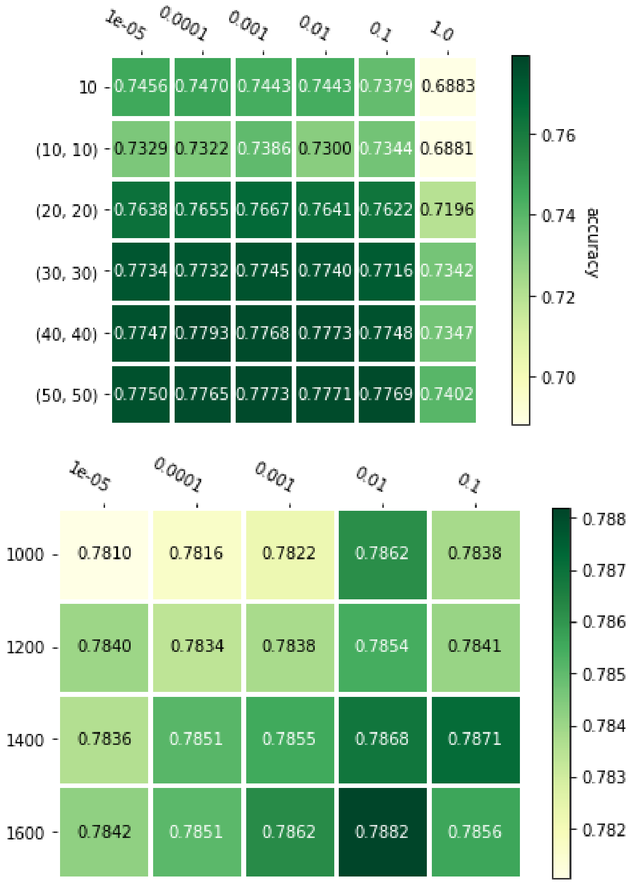
Figure 3: Tuning random forests.



As expected more trees give better results. However, we see that after 100 trees we see a very small increase in accuracy as we add more trees, 0.7492 for 100 trees vs 0.7556 for 1000 trees. Since the time to train random forests grows with the number of trees, we will restrict our selves to 100 trees when we later turn our attention to voting classifiers.

The final single model we have used is neural networks, in the form of scikit learns multilayer perceptron classifier. Here there are two parameters to tweak, the network structure in the form of number of layers and number of notes in each layer, as well as a regularization parameter called α. The regularization done by α is like the ridge (or ℓ^2) type, that have been discussed in past projects. While we tested more settings, the below figures give all the relevant information.

Figure 4: Tuning multilayer perceptron classifier.



We see that most setting actually end up in a very similar space. Increasing the number of nodes does improve the accuracy, but as for the forests, we will for computation reasons restrict ourselves. This time to the setting of a single layer network with 1000 hidden nodes and $\alpha = 0.01$.

3.2 Voting Classifiers

We explored various combinations of the classifiers described above, and bundled them intok a single voting classifier. Since there is no good way to break ties for a hard voting scheme with only two classifiers voting, we are not investigating them. Instead we looked at soft voting for all pairs of classifiers that give probabilities, that is logistic regression, random forests and multilayer preceptrons. We also looked at soft voting for all three at once, and two cases of hard voting. The results of the cross validation are show in Table 1 (soft voting) and Table 2 (hard voting). Since logistic regression and support

Table 1: Soft voting

Voting scheme	Average accuracy
logistic v forest	0.793308
logistic v mlp	0.785866
forest v mlp	0.798361
forest v mlp v logistic	0.796149

Table 2: Hard voting

Voting scheme	Average accuracy
svm v forest v mlp	0.798084
svm v forest v mlp v logistic	0.790843

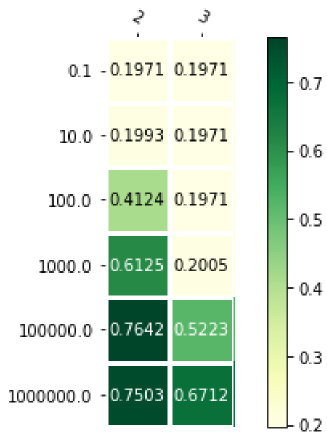
vector machines often act very similiar **??** we did not consider triples like svm v forest v logistic with hard voting.

The first thing we observe is that all most all the voting classifiers are slightly better than the single model classifiers and that they all give very similar accuracies. The three highest accuracies are for soft voting with forest v mlp (0.7893), soft voting with forest v mlp v logistic (0.7961), and hard voting with svm v forest v mlp (0.7890). These are so close, that recommending one over another based only on these number seems very hard. Instead we think soft voting with forest v mlp v logistic is likely to be the best option. This is based on a preference for soft voting over hard voting, and for having more classifiers casting their vote.

3.3 Kernels and feature transformation

As we discussed in Section 2.3.3, kernel tricks for support vector machines provide a relative cheap (in memory usage and computation time) way to look at something close to a transformed feature space. We used cross validation to test the performance of a polynomial kernel, a sample of our finding are in Figure 5.

Figure 5: Average accuracies for poly kernel SVM



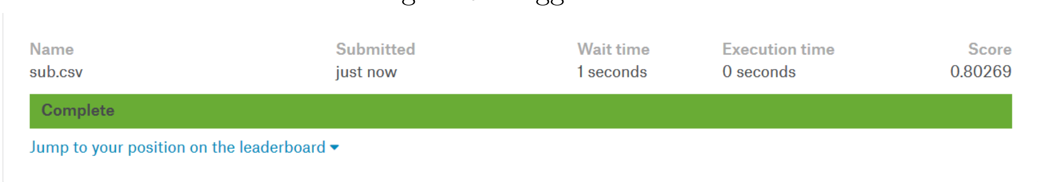
Our take away is that the polynomial kernel does not increase the performance of support vector machines. We take this as evidence that using a polynomial transformation of the features is unlikely to improve the other methods. Note also that the only interesting polynomial terms would be the interaction terms. This is because our data points are mainly vectors with entries from $\{0, 1\}$.

Another thing to note in Figure 5 is that the average accuracy is the same for $C = 0.1, 1, 10$ with a third degree polynomial. This might be because those C values end up given the exact same support vectors. But by increasing the number of points we allow inside the margin and to cross it, the classifier can depend on more data points and therefore get better accuracy. Mostly it is odd though.

4 Results and discussion

As mentioned in the introduction our data set comes from a kaggle competition. The competition is over, but allows late submissions, so submitted our best classifier using the script one can see at `github/somewhere`. The results are not public, so below is a screen shot of our result.

Figure 6: Kaggle result

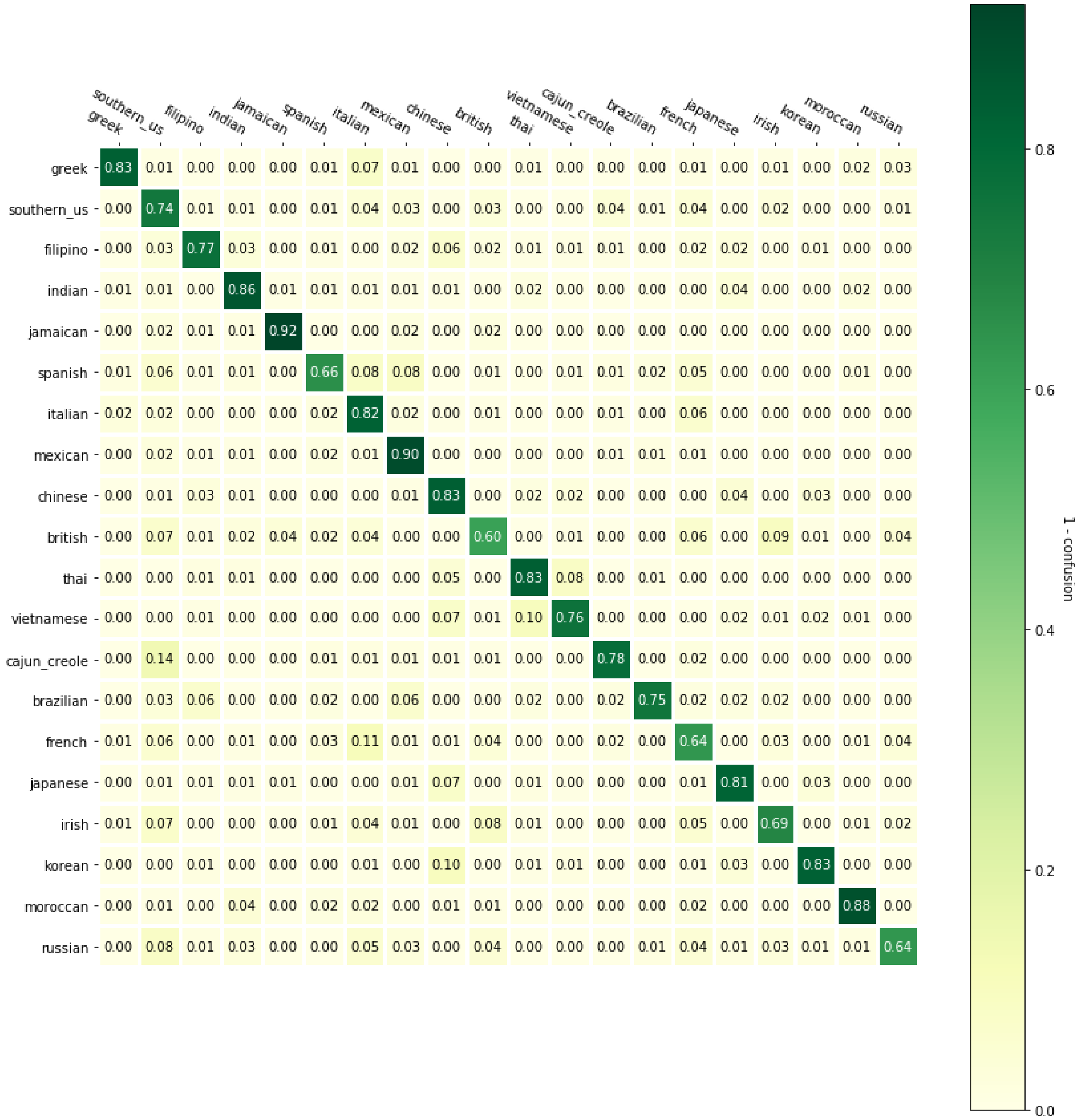


We got an accuracy of 0.80269. Which would have given us a somewhat unimpressive 231st place in the competition. It is worth noting the the highest accuracy achieved in the competition is 0.82783, so we are only off by about 2% worth of accuracy.

There are something one could do to do better in the competition: We could base our `CountVectorizer` on the test set, so we only consider ingredients that we will be tested on as features. Since there is no submission limit, we could also just have submitted various attempt and seen which one got a better score. But these are competition solutions.

To get an understanding on where our classifier fails, we split or training data into 2, trained on one part and then tried to to predict the other. Figure 7 shows the confusion matrix for this test.

Figure 7: Confusion matrix



5 Conclusion

We did good.

References

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