CS4641: Machine Learning
Spring 2019
PS1 Supervised Learning

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1 Introduction

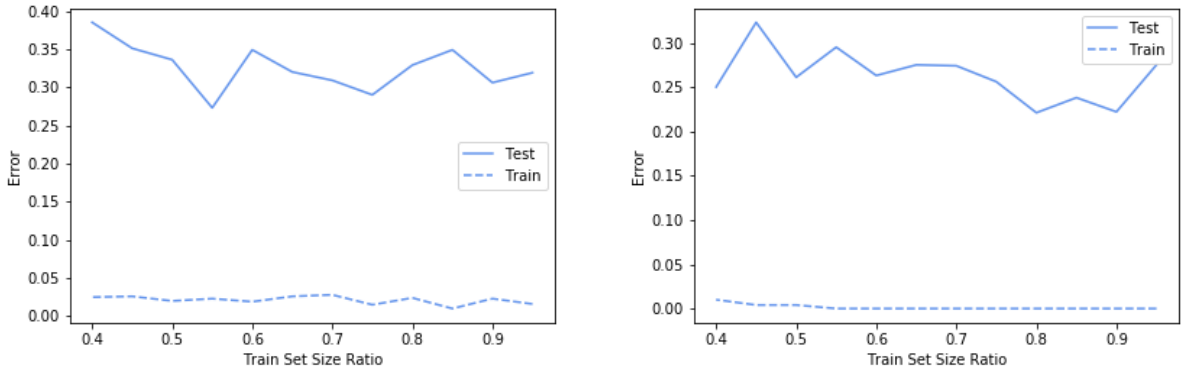
The two datasets used are both publicly available, preferred for their manageable size and clean data. In particular, two datasets of medical measurements for classifying risk of heart disease and risk of diabetes were selected. A critical use of machine learning algorithms is to investigate biological and health domains, where requisite expertise is often prohibitive for data collection and overall throughput of research. Both problems are challenging (or the world would be a better place), but simple enough that these lightweight models can all perform non-trivially, allowing analysis of model configurations. The problem is also good for comparative analysis, as traditional diagnosis can be likened to decision trees or KNN, but other methods explored in this paper may perform better. These datasets are particularly useful for this analysis of model interpretability, as it is essential for any machine learning algorithm in the medical domain to be understood as best as possible.

To detail the two datasets, typical diagnostics are included. For heart disease, the provided information is cleansed down to age, sex, cholesterol, and various heart specific measurements for a total of 13 features. As per standard practice, the provided heart disease status (stage of progression) was collapsed to binary presence of disease. This dataset was pulled from UCI's repository[1], and contains only 303 instances, which causes overfitting that explains some of the noise soon presented.

The other dataset is the Pima Indians Diabetes dataset from Kaggle[2], which has 768 instances and 8 features, along with a binary label of diabetes presence. Its features include more diabetes centered diagnostics such as BMI, blood pressure, and number of pregnancies. The dataset elaborates that a number of NaN entires were filled by 0, but to avoid overengineering the features, this will be regarded as noise. Details of data can be found at cited links.

However, in both feature sets, true NaN values were replaced with average values per feature, and each feature was also independently centered and scaled to unit variance, commonly used to aid algorithms such as KNN as well as neural networks. For analysis, a (consistently) random 80-20 train-test split was used, stratified (class imbalances preserved) to prevent dataset bias interference. Cross validation on generic analysis was omitted as trends were generally clear. 'Optimal' hyperparameters are not used for individual analysis, and so no validation nor cross validation was done, mostly deferring to sklearn's defaults. Models used for comparison are tweaked to the best parameters found through 5-fold cross validation.

Thus after engineering we have two medical binary classification tasks. Results vary largely due to the irreducible noise and small sample sizes, soon to be explained. This paper will examine performances of common algorithms, and then compare them to each other. The main metric used is error, complement of accuracy. A subset of figures were omitted for brevity.



(a) Diabetes (b) Heart Disease

Figure 1: Decision Tree Learning Curves

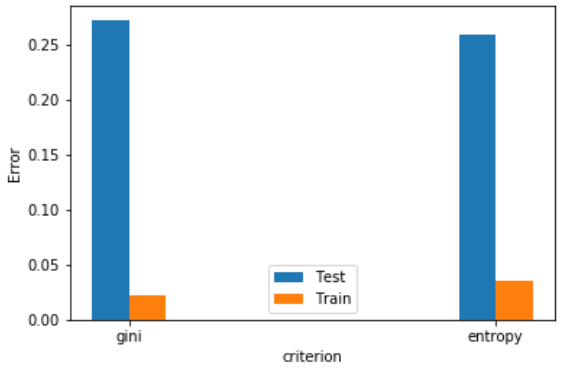
2 Algorithms

Supervised learning algorithms all share the common structure of prediction through labelled data. The five different supervised learning algorithms are as follows: decision trees, neural networks, boosting, support vector machines, and k-nearest neighbors. Implementations are from sklearn.

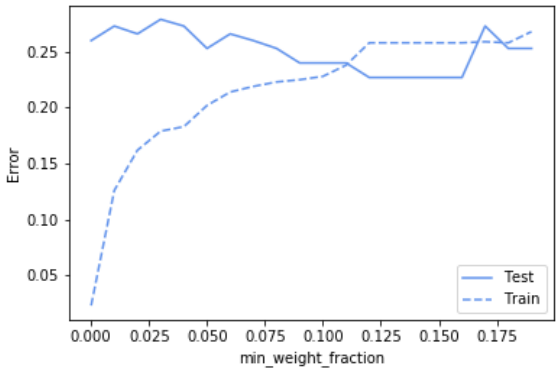
2.1 Decision Trees

Decision trees predict by filtering input examples through several a tree of nodes that split based on feature values. Thus, each branch represents specific values of features, each node representing a decision point. Important hyperparameters mostly play on controlling tree structure, the other main one being the metric used for node creation. Sklearn offers gini impurity and information gain, but both are performance-wise similar (2a). On the training size learning curve (1), there is fairly consistent test error, which indicates the tree is not particularly biased but did not gain much insight into the problems either. The slight downwards trend implies the algorithm would benefit from larger training sets, as no overfitting trends stem from larger training sets. On the other hand, there is near zero training error, as expected, since the tree is built almost deterministically to fit training. The slight bit of training error is caused from imposed max depth of 10 layers. Other than the construction algorithm and input data, the main parameters are pruning parameters, i.e. factors and constants that control how opinionated the tree should be. Sklearn offers similar controls, particularly tweaked were max depth, max leaf nodes, and minimum leaf weight fraction. Both max depth and max leaf nodes restrict how expressive and biased the final tree can be, i.e. the higher they go, the lower train error should be. Minimum leaf weight fraction lower bounds how representative each leaf is, so higher values make trees less biased. Seeing 2b, 2c, 2d, indeed the training error curves vary as expected. For 2c, 2d, test error climbs as the model is more biased, and we see a good tradeoff of bias and variance, as the test error dips to a minimum of around 22%.

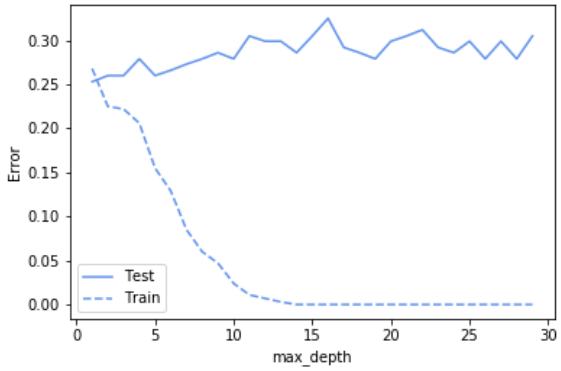
It is also notable to see the performance of decision trees in 2e, 2f. Though the training curve looks similar, the test curve is definitely noisier. This is indicative of the smaller dataset used for heart disease. Since trees fit to our training data is less likely to span the universe of good hypotheses, each perturbation at construction time causes strong performance fluctuations. These pruning methods are few of many, and other methods such as post-pruning as opposed to growth restrictions would result in different curves.



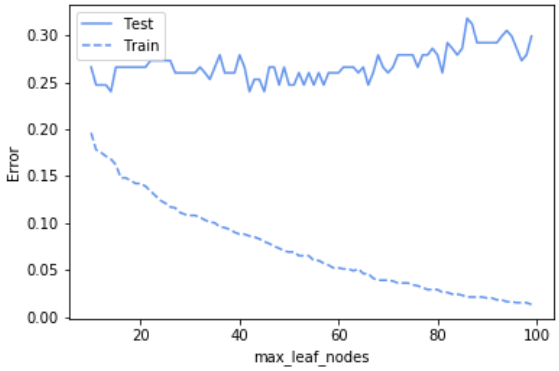
(a) Diabetes Error vs Training Criterion



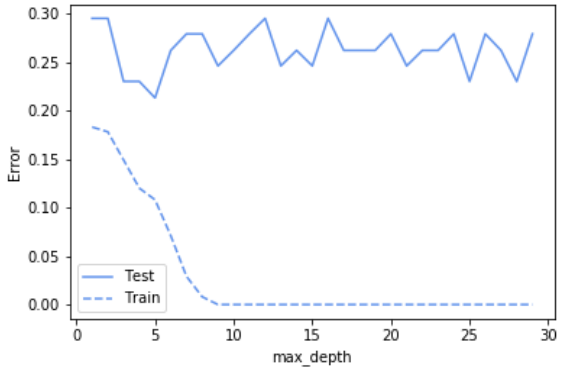
(b) Diabetes Minimum Leaf Fraction Weight



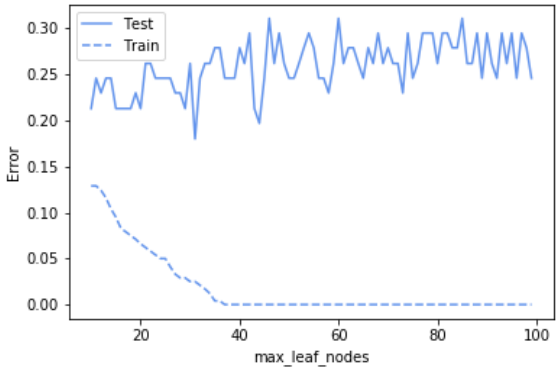
(c) Diabetes Error vs Training Criterion



(d) Diabetes Minimum Leaf Fraction Weight

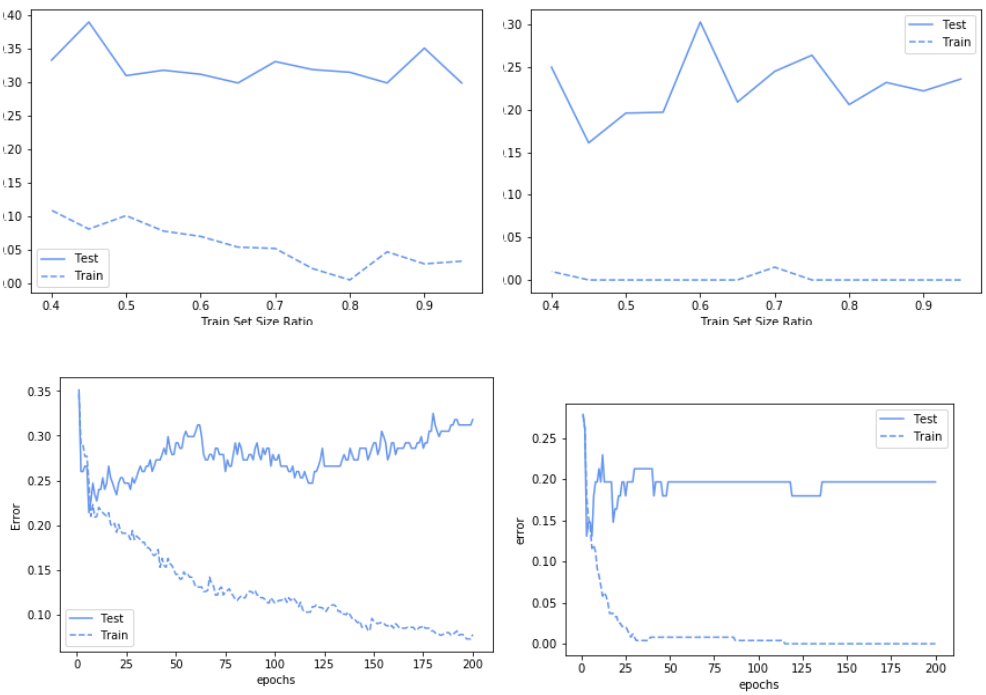


(e) Heart Disease Error vs Training Criterion



(f) Heart Disease Minimum Leaf Fraction Weight

Figure 2: Decision Tree Metrics



(a) Diabetes

(b) Heart Disease

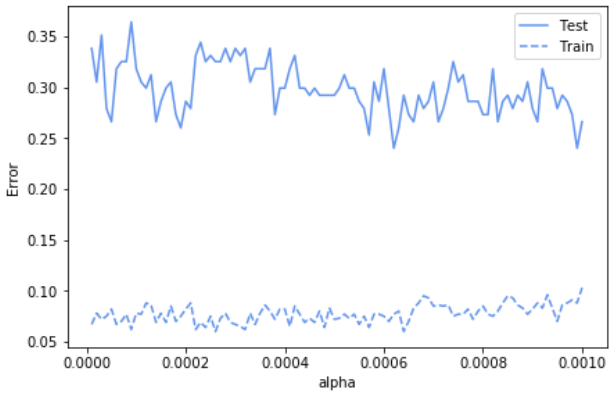
Figure 3: Neural Network Learning Curves

2.2 Neural Networks

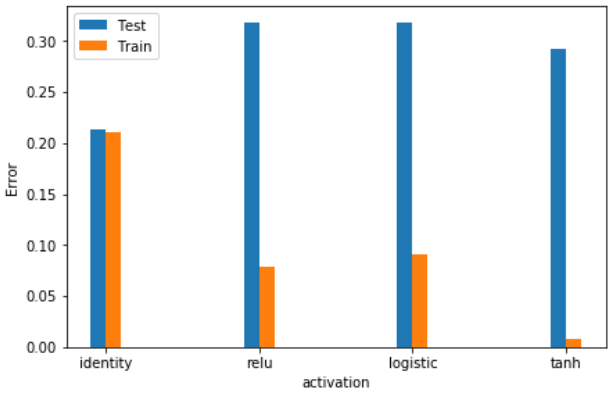
Neural networks are the most heavyweight algorithm in this analysis, and in their general form should be able to get very competitive results. For this analysis, sklearn's multilayer perceptron was used, meaning that the input data is fed into a series of fully connected hidden layers, each activated by a nonlinear function; weights are updated via backpropagation to improve hypotheses. There are many hyperparameters to tweak with neural networks, but the ones experimented with were architecture, activation function, iterations, and alpha, a regularization term.

For most of the curves the net ran until convergence. The learning curves flatline on test and training error with respect to train set size. At this point we might conclude that more training data would definitely aid the diabetes problem, but questionably so for heart disease. Notably the network doesn't have perfect accuracy on the diabetes training curve, and this is a little inexplicable. Smaller training sets should be easy to learn, but probably the network converged too optimistically, getting stuck in a local loss minimum because the loss surface is so noisy. Looking at error vs iterations, we see heart disease should be a simpler problem as the network converges to perfect accuracy, but even after 200 epochs, the diabetes train set did not converge (note that sklearn's convergence tolerance was dramatically reduced for this experiment). In both cases, we still have a good example of how training convergence means overfitting, as this validation experiment should we should have stopped in around 10 epochs for both problems, retaining simple hypotheses. Note that at convergence the test error flatlines as well, as the weight updates are infinitesimal.

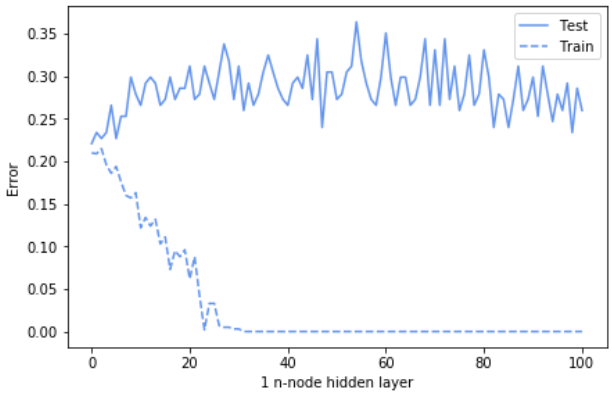
Analyzing the neural network metrics shed light on the nature of the problems. For example, per 4a, the most consistent activation function is actually the linear identity map, implying a simple linear combination of the inputs yields the best hypothesis on the diabetes dataset. More regularization slightly lowers error over time, but neither width nor depth of hidden layers has any



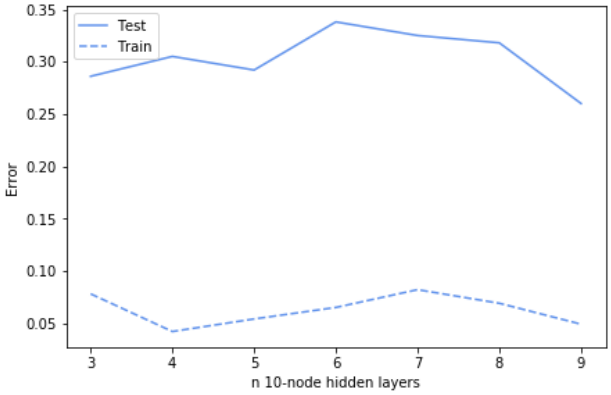
(a) Diabetes α



(b) Diabetes Activation Function



(c) Diabetes, 1 hidden layer



(d) Diabetes, n hidden layers

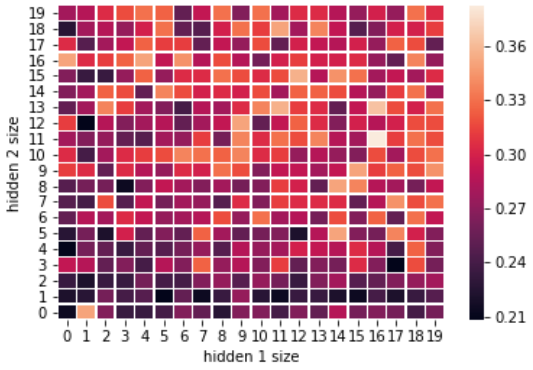
noticeable impact on the error. A 2 hidden layer analysis reveals some interesting properties. On the training side, the top right region show the threshold for perfectly overfit networks. Comparing this with heart disease, we see it's immediately possible to overfit heart disease, on top of almost patternless 5c, implying the network derived a general heuristic but cannot improve much further than that. From this we would probably expect to see similar limits in performance across other algorithms. In 5a we note the slight improvement in test error when the second hidden layer size is small, again validating that simpler hypotheses work better. These parameters generally all outperform the other architectures of 4c, 4d.

Quickly noting the training time, important for more complicated use cases of neural nets. 6a,6b shows approximately linear time complexity with respect to epochs, fitting our simply linear network.

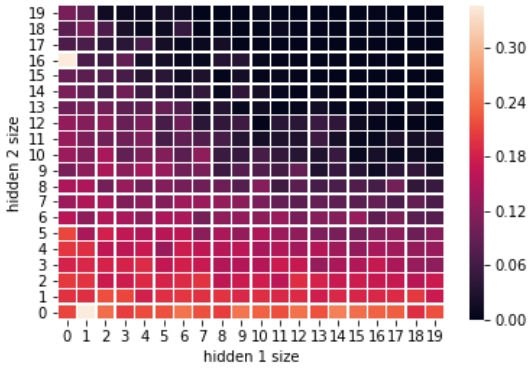
2.3 Boosting

Boosting is a meta-learning technique that capitalizes on individual weak learners to build a collective algorithm that predicts well. The ada-boosting algorithm from sklearn was used. Typically the input weak learners are expected to do only slightly better than random, and the meta-learning delegates classification to the individual learners, weighted by the learners' track records. This method might be expected to perform better because it is more resistant to overfitting.

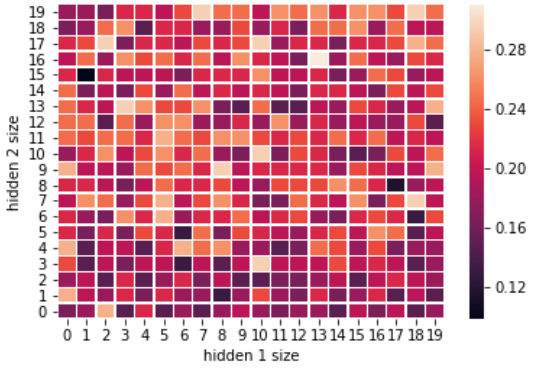
The learning curves 7a, 7b indicate that boosting has different training behavior that others learners. Given a small train set, our weak learners do relatively poorer, presumably because they



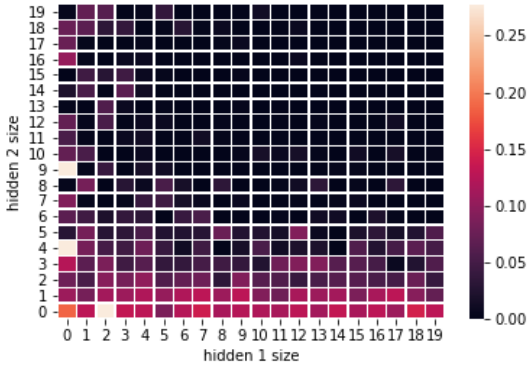
(a) Diabetes, 2 layers test error



(b) Diabetes, 2 layers training error

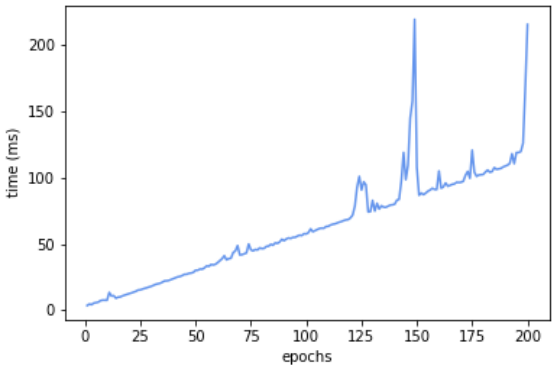


(c) Heart Disease, 2 layers test error

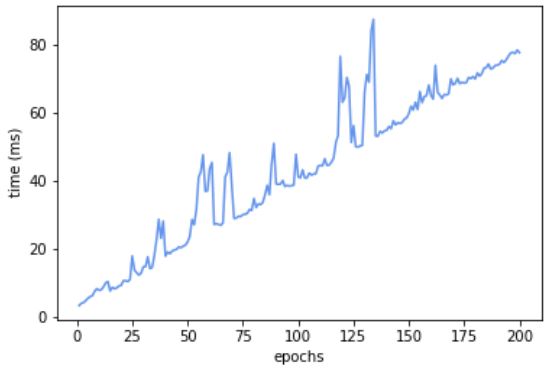


(d) Heart Disease, 2 layers training error

Figure 5: Neural Network 2d error

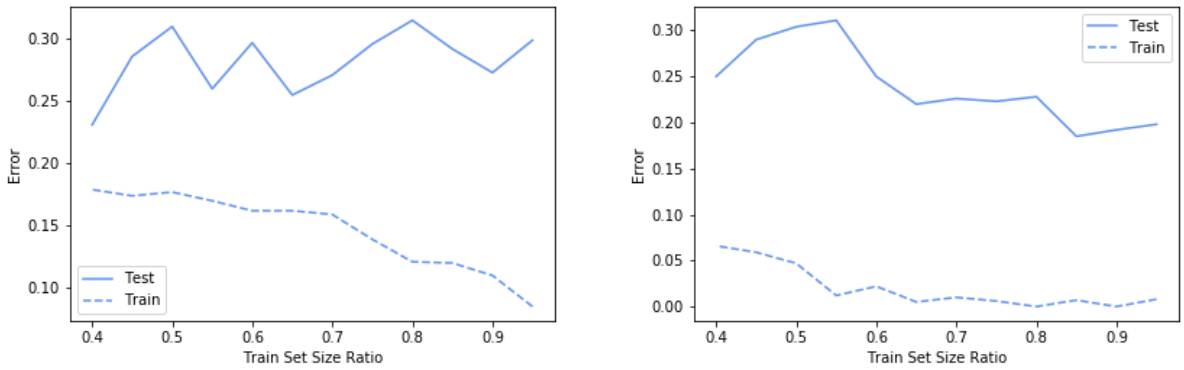


(a) Diabetes



(b) Heart Disease

Figure 6: Neural Network Train Timeâ¨â¨



(a) Diabetes

(b) Heart Disease

Figure 7: Boosting Learning Curves

cannot see a good sprawl of data to have diverse learners, but given a greater variety in a larger training set, the learners cover all bases and reduce training error. Promisingly, there is a visible downward trend in 7b, which means the algorithm is capitalizing on the greater training information without overfitting to it. 7a does not behave the same way, but this could be an artifact of noise.

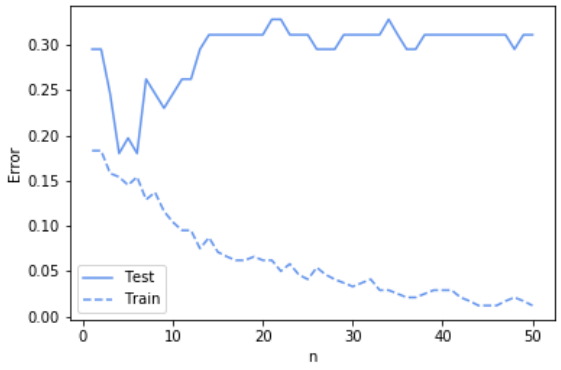
The hyperparameters for adaboosting investigated are number of learners (n), base classifiers, and max depth (when using decision trees). Note the inconsistency between 8b and 8c is due to a difference in boosting algorithms (SAMME was used for the latter, a discrete boosting algorithm over SAMME.R, a continuous one). The default one used for experimentation is more consistent and typically gets lower test error, thus better to benchmark (our validation) with. As number of learners increase in 8a, test error sinks briefly and then rises back up, seen before in plots of analogous bias increasing hyperparameters. For reference, number of estimators can be seen as number of iterations of the boosting algorithm. Max depth was only kept from 1 to 4, to prevent the weak learners from overfitting data, and there is at least some value in allowing more than a decision stump as a learner. There is no conclusive winner for which base classifier does better in general (which is why it is a hyperparameter to be tweaked).

2.4 Support Vector Machines

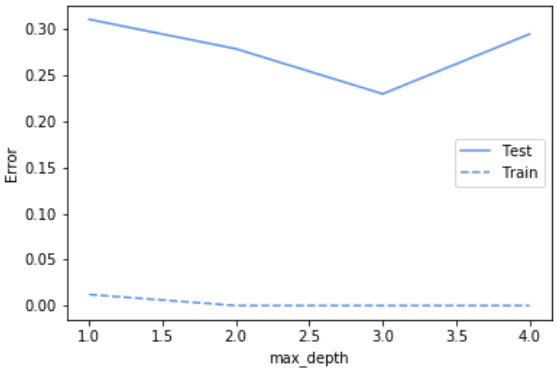
SVMs are known to be good models for data that is approximately linearly separable in some dimension. It is mainly useful for tasks with a few important features, due to curse of dimensionality. Though both tasks here are conveniently binary, SVM generalizes, in one vs one scheme in sklearn SVC, which is the model used. SVM finds the feature space in which the data is linearly separable via the kernel trick, so the kernel used is an important hyperparameter. These kernels themselves are tuneable, and on top of this the main hyperparameter of interest is the regulatory term C, which controls error penalty.

First considering the learning curves, we see generally the same trends as with boosting. With a smaller train set, the diabetes problem suffers from uninformative, inseparable spaces, i.e. there is simply not enough data to create a meaningful boundary given all the noise. What's different is that overall, the SVM is unable to fit perfectly on the training sets regardless of size, which is likely good, as we force a simpler construct with low bias onto these problems.

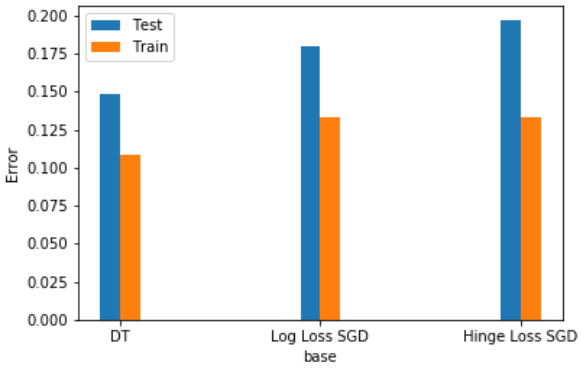
The depicted metrics in 10 are kernel used, gamma, a hyperparameter of rbf kernel, and C, the aforementioned penalty term. Both gamma and C are shown on log axis, as their values typically



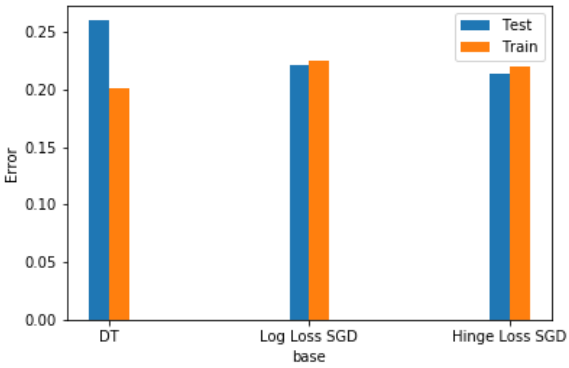
(a) Heart Disease n



(b) Heart Disease max depth

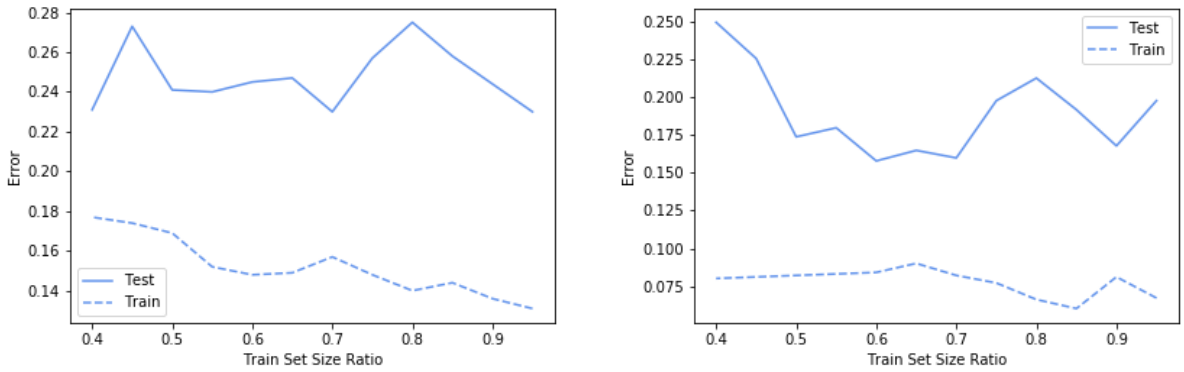


(c) Heart Disease base classifier



(d) Diabetes base classifier

Figure 8: Boosting Metrics



(a) Diabetes

(b) Heart Disease

Figure 9: SVM Learning Curves

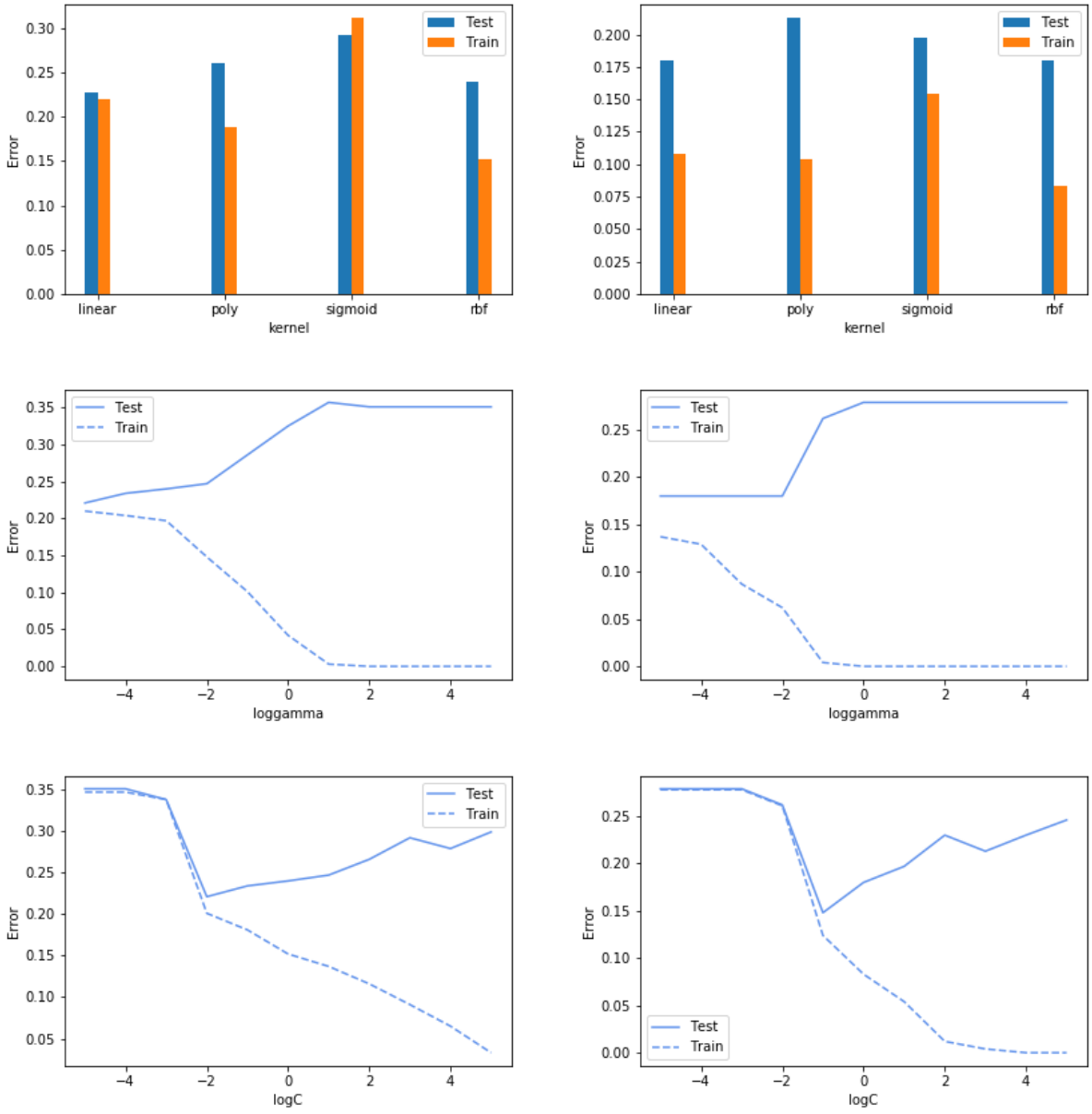
scale as such. From the kernel graphs, we note the same conclusion as from neural nets using linear activation, in that a linear kernel gets best test time results. However, rbf (which stands for radial basis function), it's notable that test error is only slightly worse than linear, and the data is fit significantly better. Gamma is a parameter that tweaks the influence radius of local data, where low gamma means each point has large radius. High gamma means local influence is emphasized, causing the overfitting seen. The regulatory term displays another typical bias variance tradeoff.

2.5 K-Nearest Neighbors

K nearest neighbors classifies each input using the labels of the input's closest K neighbors. KNN is unique for its nonparametric nature, causing constant traintime but linear runtime. The parameters considered are k, p, and weighting function. k is the number of neighbors to consider when taking the classification vote. On the low end, this encourages overfitting, matching exactly nearest neighbor, while on the high end, it encourages underfitting, considering only the majority class. The weighting function can intervene in this process, as it decides how the votes of each neighbor is weighted, (if at all). Thus more distant neighbors have reduced influence, this should help with smoothing our hypothesis. p is the exponent on the Minkowski distance (where p=2 implies Euclidean distance). Higher values of p make Minkowski distance tend toward Manhattan distance, which encourages listening to neighbors that are more similar on fewer axes (but it's not too clear how this affects error).

Examining the learning curve, we see the first learning curve on heart disease error that matches what we would expect, a rising training error. The space becomes harder to characterize simply, and this was always true for the diabetes problem. Test error on the other hand is mostly unperturbed as sklearn models usually are not particularly biased on default parameters.

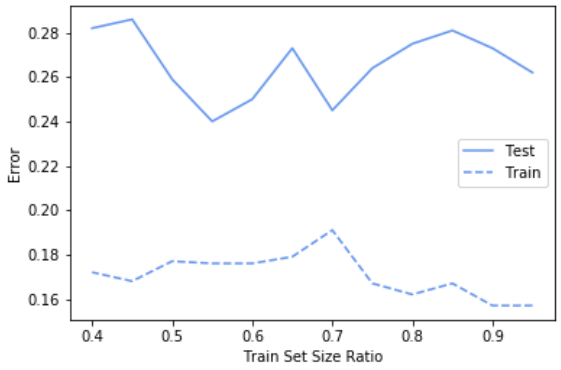
Looking at the effects of each metric, weighting turns out to be extremely unimportant, with no effects in either dataset, though its interesting that using distance as weight causes immeidate overfitting and zero training error. This is likely due to the 7-8 dimensional input features. The k graph shows progression towards perfect fitting of train and suggests a model error limit of about 16%. The effect of p on diabetes data is similar.



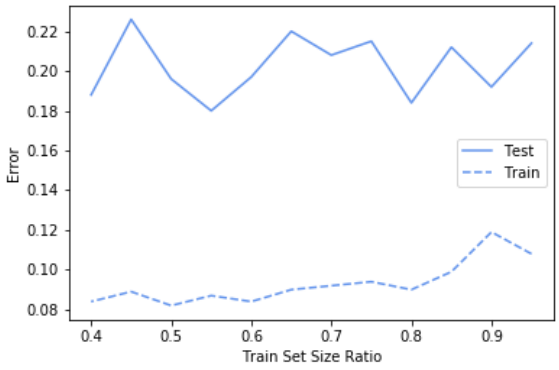
(a) Diabetes

(b) Heart Disease

Figure 10: SVM Metrics

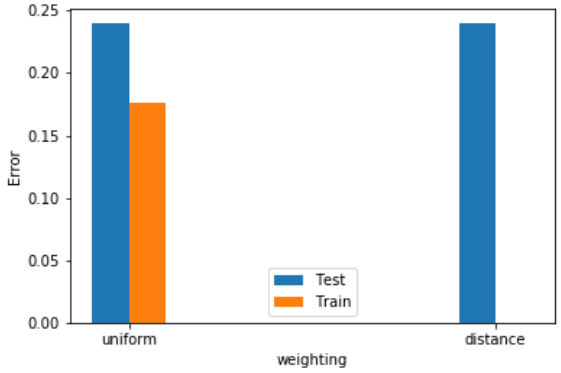


(a) Diabetes

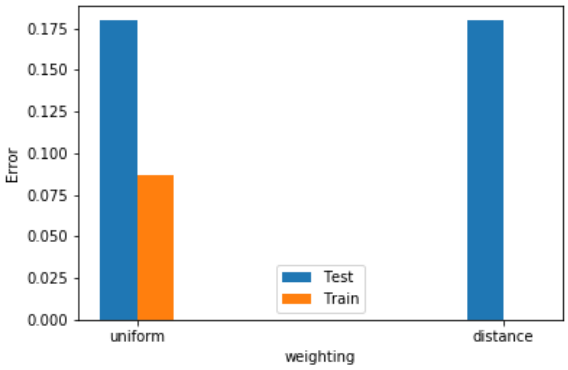


(b) Heart Disease

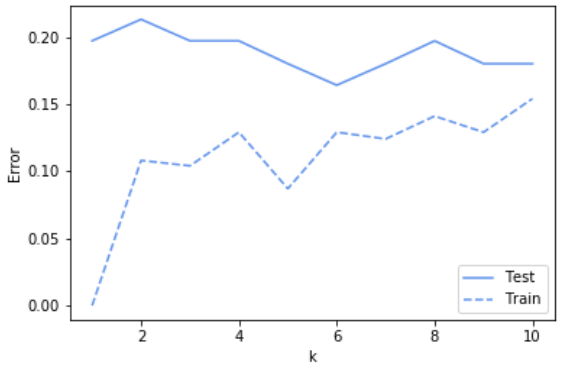
Figure 11: KNN Learning Curves



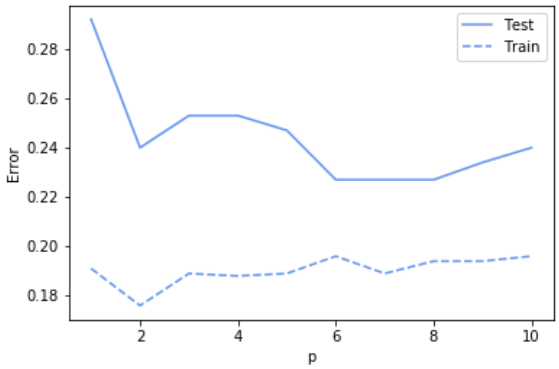
(a) Diabetes Weighting



(b) Heart Disease Weighting

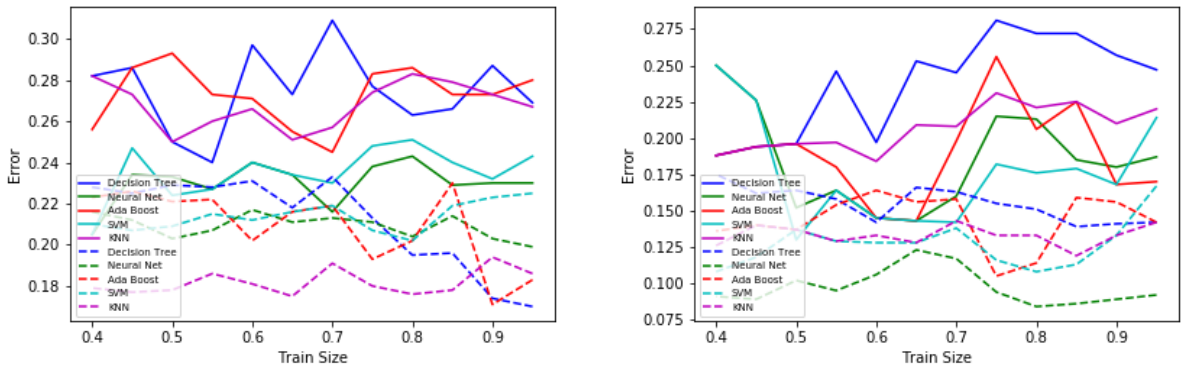


(c) Heart Disease k



(d) Diabetes p

Figure 12: KNN Metrics



(a) Diabetes

(b) Heart Disease

Figure 13: Learning Curves Summary

3 Comparison of Algorithms and Conclusion

Individual analyses help illuminate the effects of hyperparameters, while comparative analysis will help detail quirks of the dataset. In general it is difficult to see the effects of train set size on the error. There is high variance in the dataset as test and training error never begin to converge, and the irreducible error in the dataset looks to about 21 percent for diabetes, and 14 percent for heart disease. These irreducible errors could stem from lack of suitable hypotheses in the models we tried, but more likely are caused by the inherent noise in the dataset, and lack of true hard rules in reality. In the medical domain, there are absurdly many factors that can influence a condition, and oftentimes the best heuristics doctors can use is by following known heuristics (i.e. SVM). As the graphs demonstrate, SVM models pull out slightly ahead of the others, while possibly overcomplex models such as the net and overly simplistic decision trees. However, all the models get fairly similar performance, within 5-8% ranges for test error, as they were all optimized to minimize variance. This is why the testing and training errors are fairly closely aligned, especially easily regularized structures such as SVM and neural net. In most scenarios, the neural net bias is high due to its natural flexibility, but having tweaked the regularization parameter to excessively high even that variance gap can be reduced. Notice that overall our error "curves" lay mostly flat. In some problems we expect training error to rise with set size in properly regularized models (as noise seeps into the train set), but in this case our dataset is too small to see this pattern. Our regularized models are restricted to the point that more data does not particularly lower test error either. Performance of the models between the datasets is relatively consistent, which makes sense considering the similarity of the domains. The general best performer is a toss-up between KNN and neural nets, leaning towards KNN for their interpretability.

References

[1] Andras Janosi, William Steinbrunn, Matthias Pfisterer, Robert Detrano, *Heart Disease Dataset.* 1988.

[2] Pima Indians Diabetes Database
`https://www.kaggle.com/uciml/pima-indians-diabetes-database/home`