HIERACHICAL ACTIVE LEARNING BIOINFORMATICS APPLICATION

by

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I made the classifiers to predict the BioDataset, I made the plots for the Active Passive curves, I made the plots for the Fixed Fine Ratio experiments with various costs.

DEDICATION

This thesis is dedicated to my parents Paul and Vicki Duin and fiancée Anna Spady.

ACKNOWLEDGMENTS

I would like to thank my advisor Dr. Stephen Scott for guidance in selecting this research topic, Yugi Mo for his work in developing the HAL methodology, and Dr. Douglas Downey for his work on this topic. I would like to thank Juan Cui, Jiang Shu, Kevin Chiang for assistance accessing and understanding the protein dataset that is the subject of the paper.

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Chapter 1

Introduction

1.1 Machine Learning

Machine Learning algorithms are defined as computer programs that learn from experience E with respect to some class of tasks T and performance measure P, if their performance at tasks in T, as measured by P, improves with experience E [4]. In the context of this paper, the machine learning algorithm that is used is a support vector machine (SVM) implementation by libSvm [3]. The performance measure is the classification of protein instances according to a label, for example, originated in the mitochondria or not. The experience is the number of training instances in the training set. The dataset is initially partitioned into training and test sets. The algorithm improves its classifier structure based on the features of each instance by iterating through all instances in the training set. When training has been completed, the classifier is then tested on the test set and the number of instances that the classifier correctly or incorrectly labels determines its accuracy, precision and recall scores. In our protein dataset there are 20,098 proteins with 449 features each relating to their structure. In our experiments an SVM classifier is applied to the dataset with the goal of achieving high precision scores for the label mitochondrion, that is, if the protein originates in the mitochondria or not.

1.2 Hierarchical Bioinformatics Data Set

The protein dataset is labeled according to where it originates in the cell. At the root is mitochondrion, then there is the sub level labels for if its native to the mitochondria or if it has a separate target compartment specification. The complete tree along with the number of instances belonging to the each label is included

in *Figure* 1.1.

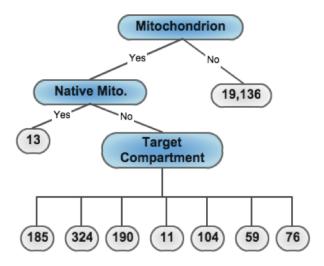


Figure 1.1: The protein dataset is labeled according to where it originates in the cell. At the root is mitochondrion, then there is the sub level labels for if its native to the mitochondria or if it has a separate target compartment specification. The complete tree along with the number of instances belonging to the each label is included in this figure.

1.3 Coarse Grained vs Fine Grained Trade Off

1.1 The classifier that does not take advantage of any of the fine grained labels works off of the root labels for each instance and does not train separate classifiers for the fine grained labels. This classifier is referred to as the coarse grained classifier. The classifier that does use fine grained labels, and trains a separate classifier for each label, then combines them to generate a root level label is referred to as the fine grained classifier. It can be demonstrated through a dummy example that for certain datasets, a fine grained approach to the root level classifier can achieve higher levels of precision for the same level of recall. Such a dataset is shown in ??. The classifiers for this dataset can be thought of as a function of axis parallel rectangular boxes. For the course grained to have high recall and return all of the positive circle instances, it must encompass the entire dataset and incidentally return all of the negative diamond instances as positive also. A fine grained approach is preferable for the dummy dataset pictured. It is the intention of this study to demonstrate that the fine grained classification approach for a root level classifier will achieve higher levels of precision for the same level of recall when applied to the protein dataset.

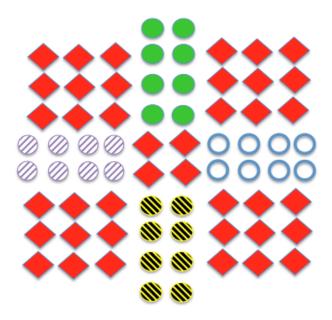


Figure 1.2: Demonstration of a dataset that would benefit from multiple fine grained learners for each circle type. In order for the coarse grain learner to have high recall, precision must be scarified and a large amount of false positives returned. By combining fine grained classifiers the same level of recall can be achieved with a higher level of precision because none of the false positive diamonds will be returned

Chapter 2

Background and Related Work

2.1 Active Learning

Active Learning relates to the coarse grained vs fine grained tradeoff because it is reasonable to assume that fine grained labels may not be as readily available as coarse grained labels, and thus have a higher cost. An active learning approach is used to determine how many fine grained labels to purchase in order to minimize the total cost to train the algorithm an maximize the precision and recall scores. The following equations for precision, recall, and a weighted F score are shown below in equations 1 through 3.

Precisioneqn

Recallegn

F05eqn

The goal in an active learning approach is to maximize the F measure where equals 0.5 [2]. The F-0.5 measure gives more weight to precision, as opposed to recall, so it gives incentive to purchase enough fine grained labels to increase the F-0.5 measure. The coarse grained labels will cost less than fine grained labels, but the increase in the F-0.5 measure justifies the increase in cost up to a certain point. The F-0.5 measure is used in the results section of this paper. ... That's why we use PRauc in the results.

2.2 Other Papers cited by Yugi

Describe some of the other papers that Yugi cited.

2.3 Hierarchical Active Learning

The Hierarchical Active Learning algorithm (HAL) is shown diagrammatically in Figure 3. Multiple fine grained classifiers are trained at each level of the Hierarchy of the dataset. Queries to the oracle are performed purchase the most cost effective labels to add to the training sets of the classifiers. The active learning cycle continues until a cost budget has been reached. The benefit of an active learning approach is to maximize the F-o.5 measure for a given cost budget. It was the goal of this study to apply the HAL algorithm to the protein dataset, however this is not achieved at this time. An existing application of HAL is briefly discussed in the following section.

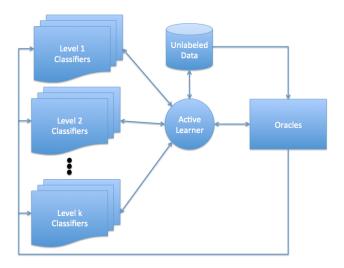


Figure 2.1: Diagram of HAL approach

2.4 Application to Dispatch Dataset

HAL was applied to a Dispatch dataset. This dataset contains 375,026 manually labeled hierarchical names across 1,384 newspaper articles [2]. This is a clear example where fine grained labels have a higher cost since it is easier for a person to manually determine if the article pertains to an organization or not, rather than if it pertains to a railroad or a zoo, which would be sub labels of the organization root. The first analysis step was to determine that the F-0.5 measure is increased by using fine grained classifiers. The results are shown in Figure 4. The highest F-0.5 measure for a given iteration of purchases of training instances is obtained by using the active learning approach with all fine-grained labels. The passive learning curves were generated by selecting batches of instances randomly rather than querying the oracle for a specific

label type that offers that most gain in classifier accuracy. The active learning curves did take advantage of querying for specific labels in order to maximize gain in classifier accuracy. ... add other data sets.



Figure 2.2: Application of HAL demonstrating the benefit of Actively selecting the type of labels to purchase for instances rather than randomly selecting labels to purchase, as in the Passive curves.

The next analysis step is to apply a given ratio of fine grained vs coarse grained labels to purchase at each batch request to the oracle. The results of varying the percentage of fine grained labels purchased are shown in Figure 5. The figure shows that even a small amount of fine grained labels purchased, that is, 20perc provides a significant increase in the F-o.5 measure for a given iteration. ... pr auc results. Add explanation of Bandit approach and results.

Chapter 3

Bio HAL Application

3.1 Training and Testing Coarse Grain and Fine Grain Classifiers

The first step is to examine the dataset.

Classes	All	All	Folds	0	1	2	3	4	5	6	7	8
0	19136	1	2010	1914	1	19	32	19	1	11	6	7
1	13	2	2010	1914	1	19	32	19	1	11	6	7
2	185	3	2010	1914	1	19	32	19	1	11	5	8
3	324	4	2010	1914	1	19	32	19	1	10	6	8
4	190	5	2010	1914	1	18	33	19	1	10	6	8
5	11	6	2010	1914	1	18	33	19	1	10	6	8
6	104	7	2010	1913	2	18	33	19	1	10	6	8
7	59	8	2010	1913	2	18	33	19	1	10	6	8
8	76	9	2009	1913	2	18	32	19	2	10	6	7
Total	20098	10	2009	1913	1	19	32	19	1	11	6	7
Shape	450	Total	20098	19136	13	185	324	190	11	104	59	76

(a) Classes (b) Folds

Table 3.1: This is what the dataset looks like there are 20098 instances total with 450 features each. This is what the folds of the dataset look like.

Next the dataset is partitioned into 10 folds, each fold contains a representative proportion of each of the classes, the instances are added to each partition at random. The total partitioning looks like Table ??

Then 9 of the folds are compressed into the test set and the fold held out is the test set the totals of each class in the train and test set for fold 1 is shown in Table 3.4.

train Total	all 18088	0 17222	1 12	2 166	3 292	4 171	5 10	6 93	7 53	8 69
test Total	all 2010	0 1914	1 1	2 19	3 32	4 19	5	6	7 6	8 7

Table 3.2: This is what the train and test set look like.

coarse just used marked all positives as 1 and ran a binary classifer. fine grained classifiers trained 8 separate classifiers for the 8 fine grained classes, so for fine grain classifier for 1, all other fine grained classes are marked as 0 in addition to all the coarse instances being marked as 0. Also the Pr auc and Roc auc are the primary metrics for determining the performance of the classifier. The next step is to determine what classifier can be applied to 'learn' the classes of this dataset. Because the experiment will involve running multiple rounds with increasing the instances to be trained on iteratively I tested each classifier against the full dataset and then a reduced dataset with one fifth of the negative instances.

I tried using SVM. Throughout this project I used the python library sci-kit learn [1]. The support vector machine implemented by this library has the following default parameters. SVC C=1.0, kernel='rbf', degree=3, gamma='auto', coefo=0.0, shrinking=True, probability=False, tol=0.001, cache-size=200, class-weight=None, verbose=False, max-iter=-1, decision-function-shape=None, random-state=None.

Classes	All
0	3827
1	13
2	185
3	324
4	190
5	11
6	104
7	59
8	76
Total	4789
Shape	450

All	Folds	o	1 1	2	3	4	5	6	7	8
1	479	383	1 1	19	32	19	1	11	6	7
2	479	383	1	19	32	19	1	11	6	7
3	479	383	1	19	32	19	1	11	6	7
4	479	383	1	19	32	19	1	11	5	8
5	479	383	1	19	32	19	1	10	6	8
6	479	383	1	18	33	19	1	10	6	8
7	479	383	1	18	33	19	1	10	6	8
8	479	382	2	18	33	19	1	10	6	8
9	479	382	2	18	33	19	1	10	6	8
10	478	382	2	18	32	19	2	10	6	7
Total	4789	3827	13	185	324	190	11	104	59	76

(a) Classes Subset

(b) Folds Subset

Table 3.3: This is for the partitions subset.

train all Total 4310	o 0 3444	1 2 160	3 4 5 292 171	5 6 1 10 93	7 8 53 69
test all Total 479	0 383	1 2 1 19	3 4 32 19	5 6 1 11	7 8 7 8

Table 3.4: This is what the train and test set look like for the subset.

coarse-pr	fine-pr	coarse-roc	fine-roc	coarse-acc	fine-acc	coarse-f1	fine-f1
0.807	0.796	0.779	0.768	0.816	0.802	0.214	0.021
0.848	0.822	0.828	0.790	0.825	0.804	0.263	0.041
0.846	0.821	0.810	0.765	0.818	0.802	0.243	0.021
0.860	0.832	0.826	0.775	0.831	0.802	0.319	0.021
0.859	0.829	0.828	0.783	0.833	0.804	0.298	0.041
0.796	0.763	0.748	0.715	0.816	0.806	0.214	0.061
0.838	0.825	0.797	0.792	0.818	0.800	0.243	0.020
0.836	0.816	0.803	0.770	0.823	0.800	0.309	0.020
0.863	0.845	0.833	0.805	0.829	0.797	0.305	0.000
0.844	0.806	0.806	0.758	0.836	0.807	0.339	0.061
avg 0.840	avg 0.815	avg o.806	avg 0.772	avg 0.825	avg 0.802	avg 0.275	avg 0.031

Table 3.5: SVMDef result stats

coarse-tn	fine-tn	coarse-fp	fine-fp	coarse-fn	fine-fn	coarse-tp	fine-tp
379	383	4	О	84	95	12	1
380	383	3	О	81	94	15	2
378	383	5	О	82	95	14	1
379	383	4	О	77	95	19	1
382	383	1	0	79	94	17	2
379	383	4	О	84	93	12	3
378	382	5	1	82	95	14	1
375	382	7	0	78	96	19	1
379	382	3	О	79	97	18	О
379	382	3	О	75	92	20	3
avg 378.8	avg 382.6	avg 3.9	avg 0.1	avg 80.1	avg 94.6	avg 16.0	avg 1.5

Table 3.6: SVMDef conf matrix

title p	r roc	acc	f1	\parallel conf (tn/fn)	\parallel conf (fp/tp)
coarse o. fine o.	840 0.806 815 0.772	0.825	0.275	(378.8 / 80.1) (382.6 / 94.6)	(3.9 / 16.0) (0.1 / 1.5)

Table 3.7: SVMDef

I tried different scaling methods (min max scaler, std scaler), I settled on std scaler.

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.881	0.855	0.799 0.799	0.000	(382.7 / 96.1) (382.7 / 96.1)	(0.0 / 0.0)

Table 3.8: SVMMinMax

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.801	0.791	0.799	0.000	(382.7 / 96.1) (382.7 / 96.1)	(0.0 / 0.0)

Table 3.9: SVMNorm

title	pr	roc	acc	f1	$\parallel conf (tn/fn) \parallel conf (fp/tp)$
coarse fine	0.912	0.882	0.881	0.631	(372.7 / 47.1) (10.0 / 49.0) (382.7 / 91.3) (0.0 / 4.8)

Table 3.10: SVMStandard

I tried different feature select measures, I settled on 75 perc feature select.

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse	0.907	0.875	o.877	0.623	(370.7 / 47.1)	(12.0 / 49.0)
fine	0.854		o.806	0.068	(382.7 / 92.7)	(0.0 / 3.4)

Table 3.11: SVMSel25

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.913 0.874	0.885 0.842	0.879	0.632	(371.3 / 46.4) (382.7 / 91.2)	(11.4 / 49.7) (0.0 / 4.9)

Table 3.12: SVMSel50

title	pr	roc acc	f1 conf (tn/fn)	conf (fp/tp)
coarse	0.913	0.883 0.883 0.89	78 0.622 (372.1 / 47.9	(10.6 / 48.2)
fine		0 0.848 0.80	09 0.089 (382.7 / 91.6	(0.0 / 4.5)

Table 3.13: SVMSel75

I tried different C costs, kernels, decision function shape, gamma, tolerance settled on classif = svm.SVC(C=1.0, kernel='rbf',decisionfunctionshape='ovo',gamma=0.0025, tol=0.00001). The default gamma

setting is 0.002967 or (1/num-features) or (1/337). Default cost is actually 1.0, and the default class weight is balanced wiched weights each class by the number of instances it has in the train set. Tolerance default is 0.001.

title pr	roc acc	\parallel f1 \parallel conf (tn/fn) \parallel conf (fp/tp)
coarse 0.913	0.883 0.878	0.621 (372.1 / 48.0) (10.6 / 48.1)
fine 0.880	0 0.847 0.809	0.089 (382.7 / 91.6) (0.0 / 4.5)

Table 3.14: SVM-ovr

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.913	0.883	0.878	0.622	(372.1 / 47.9) (382.7 / 91.6)	(10.6 / 48.2) (0.0 / 4.5)

Table 3.15: SVM-ovo

I left the class weight as balanced for this part, the results did not show much advantage for using the fine grained classifier.

next I tried using a Logistic regression classifier.

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse	0.887	0.862	0.867	0.615	(364.1 / 45.0)	(18.6 / 51.1)
fine	0.854	0.837	0.833	0.395	(364.1 / 45.0) (372.8 / 69.9)	(9.9 / 26.2)

Table 3.16: LogRegDef

title p	r roc	acc f1	conf (tn/fn)	conf (fp/tp)
coarse of offine of offine	864 0.849 833 0.816	0.846 0.5	583 (353.8 / 44. 471 (362.0 / 60.	8) (28.7 / 51.3) 2) (20.5 / 36.0)

Table 3.17: LogRegStandard

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.790	0.761	0.799	0.000	(382.7 / 96.1) (382.7 / 96.1)	(0.0 / 0.0)

Table 3.18: LogRegNorm

title pr	roc acc	$\mid f_1 \mid \mid conf (tn/fn) \mid \mid conf (fp/tp)$
coarse 0.891 fine 0.888	0.867 0.864 0.862 0.812	0.581 (368.6 / 50.9) (14.1 / 45.2) 0.130 (382.1 / 89.3) (0.6 / 6.8)

Table 3.19: LogRegMinMax

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.872 0.869	0.848	0.849 0.804	0.497	(370.8 / 60.3) (382.2 / 93.5)	(11.9 / 35.8) (0.5 / 2.6)

Table 3.20: LogRegSel25

title pr	roc acc	\parallel f1 \parallel conf (tn/fn) \parallel conf (fp/tp)
coarse 0.8 fine 0.8	75 0.849 0.849 72 0.846 0.803	0 0.497 (370.8 / 60.3) (11.9 / 35.8) 8 0.050 (382.2 / 93.6) (0.5 / 2.5)

Table 3.21: LogRegSel50

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.871	0.847	0.848	0.493	3 (370.6 / 60.6 3 (382.0 / 93.7) (12.1 / 35.5)) (0.7 / 2.4)

Table 3.22: LogRegSel75

title	∥ pr	roc	acc	f1	\parallel conf (tn/fn)	conf (fp/tp)
coarse fine	0.886	0.868	0.787	0.60	6 (298.7 / 17.9 7 (361.7 / 47.3	(84.0 / 78.2) (3) (21.0 / 48.8)

Table 3.23: LogRegWtOrig-C1

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	o.88o o.88o	0.861	0.755	0.579	(280.7 / 15.4) (374.2 / 62.7)	(102.0 / 80.7) (8.5 / 33.4)

Table 3.24: LogRegWtOrig-Cp1

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	o.876 o.866	0.855 0.842	0.793 0.835	0.603 0.583	(304.6 / 21.1) (344.8 / 40.9)	(78.1 / 75.0) (37.9 / 55.2)

Table 3.25: LogRegWtOrig-C10

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.883	0.865 0.859	0.690	0.536	6 (245.4 / 10.9 6 (324.2 / 26.7) (137.3 / 85.2)) (58.5 / 69.4)

Table 3.26: LogRegWt10-C1

title	pr	roc	acc	f1	\parallel conf (tn/fn)	conf (fp/tp)
coarse fine	0.879	0.863	0.609	0.486	(203.6 / 7.9) (334.5 / 31.1)	(179.1 / 88.2) (48.2 / 65.0)

Table 3.27: LogRegWt10-Cp1

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.871	0.851 0.837	0.723	0.554 0.585	(264.1 / 13.9 (309.3 / 26.2) (118.6 / 82.2)) (73.4 / 69.9)

Table 3.28: LogRegWt10-C10

title	pr	roc acc	f1	conf (tn/fn)	conf (fp/tp)
coarse	0.884	0.867 0.73	0.56	6 (268.8 / 13.5) (113.9 / 82.6)
fine		0.861 0.84	6 0.62	4 (343.4 / 34.6) (39.3 / 61.5)

Table 3.29: LogRegWt7p5-C1

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse	0.880	0.862	0.668	0.517	(234.8 / 11.1)	(147.9 / 85.0) (25.4 / 53.8)
fine	0.881	0.858	0.859	0.613	(357.3 / 42.3)	(25.4 / 53.8)

Table 3.30: LogRegWt7p5-Cp1

title pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse o.8	873 0.852 863 0.839	0.757	0.578 0.588	(283.2 / 16.7) (323.3 / 31.4)	(99.5 / 79.4) (59.4 / 64.7)

Table 3.31: LogRegWt7p5-C10

title	pr	roc	acc	f1	conf (tn/fn)	\parallel conf (fp/tp) \parallel
fine	0.881	0.858	0.859	0.613	(357.3 / 42.3)	(25.4 / 53.8)
trainCls-1	0.995	0.999	0.998	0.477	(4297.7 / 7.7)	(0.8 / 4.0)
testCls-1	0.722	0.996	0.997	0.100	(477.4 / 1.2)	(0.1 / 0.1)

Table 3.32: LogRegCls1-Wt1

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.880	0.856	0.859	0.613	(357.4 / 42.3)	(25.3 / 53.8)
trainCls-1	0.994	0.998	0.997	0.142	(4298.5 / 10.8)	(0.0 / 0.9)
testCls-1	0.696	0.995	0.997	0.000	(477.5 / 1.3)	(0.0 / 0.0)

Table 3.33: LogRegCls1-Wtp5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.882	0.860	0.859	0.617	(357.1 / 41.7)	(25.6 / 54.4)
trainCls-1	0.995	1.000	0.999	0.854	(4295.8 / 1.0)	(2.7 / 10.7)
testCls-1	0.722	0.997	0.998	0.400	(477.1 / 0.7)	(0.4 / 0.6)

Table 3.34: LogRegCls1-Wt3: this won!

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.881	0.859	0.860	0.618	(357.0 / 41.5)	(25.7 / 54.6)
trainCls-1	0.995	1.000	0.999	0.850	(4294.3 / 0.0)	(4.2 / 11.7)
testCls-1	0.722	0.997	0.998	0.513	(476.9 / 0.5)	(0.6 / 0.8)

Table 3.35: LogRegCls1-Wt5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.882	0.860	0.859	0.617	(357.1 / 41.7)	(25.6 / 54.4)
trainCls-2	0.800	0.804	0.952	0.200	(4076.9 / 140.5)	(66.8 / 26.0)
testCls-2	0.655	0.689	0.944	0.081	(450.7 / 17.3)	(9.6 / 1.2)

Table 3.36: LogRegCls2-Wt1: this won!

title	pr	roc	acc	l fı	conf (tn/fn)	conf (fp/tp)
fine	0.882	0.857	0.862	0.618	(359.1 / 42.5)	(23.6 / 53.6)
trainCls-2	0.785	0.787	0.961	0.052	(4139.4 / 161.9)	(4.3 / 4.6)
testCls-2	0.656	0.694	0.960	0.009	(459.4 / 18.4)	(0.9 / 0.1)

Table 3.37: LogRegCls2-Wtp5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.877	0.857	0.855	0.620	(352.5 / 39.3)	(30.2 / 56.8)
trainCls-2	0.806	0.814	0.924	0.263	(3924.1 / 108.1)	(219.6 / 58.4)
testCls-2	0.652	0.684	0.914	0.123	(434.8 / 15.6)	(25.5 / 2.9)

Table 3.38: LogRegCls2-Wt1p5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.882	0.860	0.859	0.617	(357.1 / 41.7)	(25.6 / 54.4)
trainCls-3	0.846	0.852	0.882	0.401	(3628.6 / 120.7)	(390.0 / 170.9)
testCls-3	0.795	0.803	0.873	0.360	(401.2 / 15.4)	(45.2 / 17.0)

Table 3.39: LogRegCls3-Wt1: this won!

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine trainCls-3 testCls-3	0.870 0.838 0.792	0.852 0.838 0.798	0.839	0.445	(370.9 / 65.1) (3942.0 / 229.7) (437.2 / 26.5)	(11.8 / 31.0) (76.6 / 61.9) (9.2 / 5.9)

Table 3.40: LogRegCls3-Wtp5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.879	0.855	0.832	0.626	(331.2 / 28.9)	(51.5 / 67.2)
trainCls-3	0.849	0.859	0.813	0.351	(3288.4 / 74.5)	(730.2 / 217.1)
testCls-3	0.795	0.805	0.804	0.318	(363.3 / 10.6)	(83.1 / 21.8)

Table 3.41: LogRegCls3-Wt1p5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.882	0.860	0.859	0.617	(357.1 / 41.7)	(25.6 / 54.4)
trainCls-4	0.937	0.942	0.960	0.531	(4038.6 / 72.9)	(100.6 / 98.1)
testCls-4	0.882	0.902	0.952	0.433	(447.1 / 10.2)	(12.7 / 8.8)

Table 3.42: LogRegCls4-Wt1

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.875	0.852	0.855	0.590	(359.2 / 45.9)	(23.5 / 50.2)
trainCls-4	0.928	0.932	0.965	0.397	(4108.1 / 120.9)	(31.1 / 50.1)
testCls-4	0.878	0.898	0.962	0.320	(456.0 / 14.6)	(3.8 / 4.4)

Table 3.43: LogRegCls4-Wtp5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.883	0.861	0.856	0.624	(352.4 / 38.8)	(30.3 / 57.3)
trainCls-4	0.941	0.947	0.936	0.462	(3918.1 / 53.2)	(221.1 / 117.8)
testCls-4	0.886	0.903	0.926	0.382	(432.5 / 8.0)	(27.3 / 11.0)

Table 3.44: LogRegCls4-Wt1p5: this won!

title	pr	roc	acc	f1	\parallel conf (tn/fn)	conf (fp/tp)
fine	0.880	0.859	0.853	0.627	(348.9 / 36.7)	(33.8 / 59.4)
trainCls-4	0.943	0.950	0.917	0.429	(3817.7 / 36.5)	(321.5 / 134.5)
testCls-4	0.886	0.903	0.906	0.352	(421.8 / 6.8)	(38.0 / 12.2)

Table 3.45: LogRegCls4-Wt2

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine trainCls-5	0.883	0.861	0.856	0.624	(352.4 / 38.8) (4300.2 / 10.0) (477.8 / 1.0)	(30.3 / 57.3)

Table 3.46: LogRegCls5-Wt1

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.883	0.861	0.856	0.624	(352.4 / 38.8)	(30.3 / 57.3)
trainCls-5	0.911	0.912	0.998	0.000	(4300.2 / 10.0)	(0.0 / 0.0)
testCls-5	0.389	0.672	0.998	0.000	(477.8 / 1.0)	(0.0 / 0.0)

Table 3.47: LogRegCls5-Wtp5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.883	0.861	0.856	0.624	(352.4 / 38.8)	(30.3 / 57.3)
trainCls-5	0.957	0.958	0.998	0.000	(4300.2 / 10.0)	(0.0 / 0.0)
testCls-5	0.396	0.687	0.998	0.000	(477.8 / 1.0)	(0.0 / 0.0)

Table 3.48: LogRegCls5-Wt1p5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.883	0.861	0.856	0.624	(352.4 / 38.8)	(30.3 / 57.3)
trainCls-5	0.990	0.990	0.998	0.374	(4299.8 / 7.6)	(0.4 / 2.4)
testCls-5	0.401	0.694	0.998	0.000	(477.7 / 1.0)	(0.1 / 0.0)

Table 3.49: LogRegCls5-Wt5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.883	0.861	0.855	0.623	(352.1 / 38.8)	(30.6 / 57.3)
trainCls-5	0.996	0.997	0.998	0.609	(4293.4 / 2.7)	(6.8 / 7.3)
testCls-5	0.402	0.696	0.996	0.000	(476.8 / 1.0)	(1.0 / 0.0)

Table 3.50: LogRegCls5-Wt10: this won!

title	pr	roc	acc	f1	$\parallel conf (tn/fn) \parallel conf (fp/tp)$
fine	0.881	0.860	0.854	0.622	(351.6 / 38.7) (31.1 / 57.4)
trainCls-5	0.998	0.998	0.992	0.355	(4265.8 / 0.5) (34.4 / 9.5)
testCls-5	0.381	0.616	0.989	0.000	(473.5 / 1.0) (4.3 / 0.0)

Table 3.51: LogRegCls5-Wt20

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.883	0.861	0.855	0.623	(352.1 / 38.8)	(30.6 / 57.3)
trainCls-6	0.945	0.962	0.976	0.303	(4182.5 / 70.8)	(34.1 / 22.8)
testCls-6	0.892	0.936	0.972	0.191	(463.9 / 8.8)	(4.5 / 1.6)

Table 3.52: LogRegCls6-Wt1

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.882	0.860	0.855	0.622	(352.1 / 38.9)	(30.6 / 57.2)
trainCls-6	0.938	0.956	0.978	0.006	(4216.5 / 93.3)	(0.1 / 0.3)
testCls-6	0.881	0.928	0.978	0.000	(468.3 / 10.4)	(0.1 / 0.0)

Table 3.53: LogRegCls6-Wtp5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.884	0.861	0.855	0.627	(350.8 / 37.6)	(31.9 / 58.5)
trainCls-6	0.950	0.967	0.949	0.380	(4023.8 / 26.4)	(192.8 / 67.2)
testCls-6	0.897	0.939	0.945	0.292	(447.0 / 5.0)	(21.4 / 5.4)

Table 3.54: LogRegCls6-Wt2: this wins!

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.884	0.860	0.850	0.629	(346.6 / 35.5)	(36.1 / 60.6)
trainCls-6	0.952	0.969	0.921	0.335	(3885.8 / 8.3)	(330.8 / 85.3)
testCls-6	0.898	0.940	0.915	0.281	(430.5 / 2.6)	(37.9 / 7.8)

Table 3.55: LogRegCls6-Wt3

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.884	0.862	0.855	0.628	(350.8 / 37.5) (4257.1 / 53.1) (472.9 / 5.9)	(31.9 / 58.6)
trainCis-7	0.892	0.893	0.988	0.000	(4257.1 / 53.1)	(0.0 / 0.0)

Table 3.56: LogRegCls7-Wt1

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.884	0.861	0.855	0.627	(350.8 / 37.6)	(31.9 / 58.5)
trainCls-7	0.859	0.857	0.988	0.000	(4257.1 / 53.1)	(0.0 / 0.0)
testCls-7	0.636	0.708	0.988	0.000	(472.9 / 5.9)	(0.0 / 0.0)

Table 3.57: LogRegCls7-Wtp5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.885	0.863	0.855	0.632	(350.1 / 36.7)	(32.6 / 59.4)
trainCls-7	0.930	0.939	0.986	0.344	(4234.1 / 37.3)	(23.0 / 15.8)
testCls-7	0.667	0.739	0.983	0.105	(470.1 / 5.4)	(2.8 / 0.5)

Table 3.58: LogRegCls7-Wt3: this won!

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.883	0.860	0.847	0.628	(344.0 / 34.4)	(38.7 / 61.7)
trainCls-7	0.941	0.953	0.956	0.265	(4086.0 / 18.9)	(171.1 / 34.2)
testCls-7	0.674	0.744	0.948	0.099	(452.3 / 4.5)	(20.6 / 1.4)

Table 3.59: LogRegCls7-Wt5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.886	0.864	0.855	0.632	(350.1 / 36.6)	(32.6 / 59.5)
trainCls-8	0.967	0.978	0.982	0.453	(4199.8 / 36.1)	(42.0 / 32.3)
testCls-8	0.896	0.952	0.978	0.308	(465.7 / 5.2)	(5.5 / 2.4)

Table 3.60: LogRegCls8-Wt1: this won!

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.885	0.862	0.855	0.630	(350.4 / 37.0)	(32.3 / 59.1)
trainCls-8	0.961	0.972	0.984	0.253	(4229.6 / 56.7)	(12.2 / 11.7)
testCls-8	0.893	0.952	0.982	0.135	(469.5 / 6.8)	(1.7 / 0.8)

Table 3.61: LogRegCls8-Wtp5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
fine	0.886	0.864	0.855	0.632	(349.5 / 36.4)	(33.2 / 59.7)
trainCls-8	0.967	0.980	0.978	0.478	(4169.7 / 24.3)	(72.1 / 44.1)
testCls-8	0.892	0.947	0.973	0.376	(462.2 / 3.9)	(9.0 / 3.7)

Table 3.62: LogRegCls8-Wt1p5

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.880 0.886	0.863	0.668 0.855	0.517	(234.8 / 11.1 2 (350.1 / 36.6) (147.9 / 85.0)) (32.6 / 59.5)

Table 3.63: LogRegAftFineTune

title pr	roc acc	f1 conf (tr	n/fn) conf (fp/tp)
coarse 0.880	0.862 0.66	8 0.518 (234.9	/ 11.1) (147.8 / 85.0)
fine 0.885	0.863 0.85	5 0.632 (350.1	/ 36.7) (32.6 / 59.4)

Table 3.64: LogRegOrig-0001

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.885	o.865 o.866	0.671	0.520	(236.3 / 11.1 (350.4 / 36.3) (146.3 / 85.0)) (32.2 / 59.8)

Table 3.65: LogReg-00001: this won!

title pr	roc acc f1	conf (tn/fn)	conf (fp/tp)
coarse 0.880	0.862 0.668 0.517	7 (234.8 / 11.1)	(147.9 / 85.0)
fine 0.885	0.863 0.855 0.632	2 (350.1 / 36.7)	(32.6 / 59.4)

Table 3.66: LogReg-000001

title 1	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse c	0.867	o.868 o.868	0.803 0.919	0.280 0.404	(1537.6 / 19.2) (1792.3 / 41.0)	(376.0 / 76.9) (121.2 / 55.1)

Table 3.67: LogRegAllOrig-Wt2op887

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.870	0.871	0.787	0.268	(1503.2 / 17.8) (1776.5 / 37.3)	(410.4 / 78.3) (137.1 / 58.8)

Table 3.68: LogRegAll-Wt23: this won!

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse	0.867	o.868	0.772	0.256	(1473.0 / 17.3)	(440.6 / 78.8)
fine	0.871	o.868	0.905		(1758.8 / 35.6)	(154.8 / 60.6)

Table 3.69: LogRegAll-Wt25

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.901	0.874	0.847	0.653	(336.6 / 27.2) (371.1 / 50.2)	(46.1 / 68.9) (11.6 / 45.9)

Table 3.70: SVM-OrigWithFtune

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.901	0.874 0.865	0.846	0.651	(336.0 / 27.2) (371.1 / 50.1)	(46.7 / 68.9) (11.6 / 46.0)

Table 3.71: SVM-C1-Gp0029674

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.903	0.873 0.857	0.866	0.672	2 (348.9 / 30.4 4 (373.8 / 55.8	(33.8 / 65.7) (8.9 / 40.3)

Table 3.72: SVM-C2-Gp0029674

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.892	0.869	0.664	0.518	(231.5 / 9.8) (363.5 / 43.8)	(151.2 / 86.3) (19.2 / 52.3)

Table 3.73: SVM-Cp1-Gp0029674

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	0.883	0.860 0.853	0.591	0.474	(194.9 / 8.0) (370.1 / 55.5) (187.8 / 88.1) (12.6 / 40.6)

Table 3.74: SVM-Cpo5-Gpo029674

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse	0.896	0.873 0.874	0.714	0.553 0.640	(257.5 / 11.6 (362.1 / 41.1) (125.2 / 84.5)) (20.6 / 55.0)

Table 3.75: SVM-Cp15-Gp0029674: this won!

\mid title $\mid\mid$ pr	roc acc	f1 conf ((tn/fn) \parallel conf (fp/tp)
coarse 0.899	0.875 0.755	0.584 (279.	6 / 14.0) (103.1 / 82.1)
fine 0.903	0.875 0.871	0.640 (362.	1 / 41.2) (20.6 / 54.9)

Table 3.76: SVM-Cp2-Gp0029674

title p	r roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse of	894 0.87 906 0.87	71 0.706 77 0.869	0.545	(253.6 / 11.7 (358.3 / 38.5) (129.1 / 84.4)) (24.4 / 57.6)

Table 3.77: SVM-Cp15-Gp002: this won!

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse	0.883	0.864	0.664	0.516	(232.1 / 10.3) (358.5 / 39.2) (150.6 / 85.8)) (24.2 / 56.9)

Table 3.78: SVM-Cp15-Gp001

I tried different scaling methods, min max scaler, std scaler, I settled on min max scaler.

I tried different feature select measures, decided to use all of the features.

I tried different C costs, tolerances, and class weights. I settled on C=0.1, tol = 0.00001, and weight equal to the balanced, adjusted via a scaling line.

I also further tuned the fine grained classifiers starting from the initial scaling from the line an then multiplying that by a ratio. I got this vector of ratios [0.87, 0.4, 0.78, 0.65, 3.48, 0.78, 1.74, 0.87]

3.2 Passive SVM Rbf kernel vs Logistic Reg

This shows the advantage to fine grained labels to justify the experiment.

coarse-pr	fine-pr	coarse-roc	fine-roc	coarse-acc	fine-acc	coarse-f1	fine-f1
0.898	0.905	0.905	0.899	0.767	0.912	0.259	0.404
0.870	0.871	0.846	0.852	0.803	0.918	0.272	0.406
0.897	0.908	0.895	0.902	0.793	0.919	0.287	0.449
0.864	0.860	0.852	0.852	0.778	0.908	0.256	0.391
0.855	0.864	0.859	0.857	0.795	0.920	0.269	0.423
0.867	0.863	0.874	0.864	0.785	0.913	0.263	0.411
0.871	0.882	0.873	0.879	0.784	0.910	0.269	0.404
0.835	0.842	0.843	0.841	0.794	0.910	0.258	0.357
0.869	0.878	0.868	0.875	0.785	0.914	0.265	0.418
0.873	0.873	0.891	0.890	0.786	0.906	0.279	0.365
avg 0.870	avg 0.875	avg 0.871	avg 0.871	avg 0.787	avg 0.913	avg 0.268	avg 0.403

Table 3.79: Here are the results for the logistic regression passive 10 folds.

coarse-tn	fine-tn	coarse-fp	fine-fp	coarse-fn	fine-fn	coarse-tp	fine-tp
1460	1773	454	141	14	36	82	60
1540	1790	374	124	22	40	74	56
1509	1782	405	132	12	30	84	66
1486	1767	428	147	19	37	77	59
1521	1790	393	124	20	37	76	59
1501	1774	413	140	19	35	77	61
1496	1769	417	144	17	36	80	61
1524	1780	389	133	25	47	72	50
1498	1773	415	140	17	33	78	62
1497	1767	416	146	13	42	83	54
avg 1503.2	avg 1776.5	avg 410.4	avg 137.1	avg 17.8	avg 37.3	avg 78.3	avg 58.8

Table 3.80: Here are the results for the logistic regression confusion matrices. The main source of the advantage for fine is from the decreased amount of false negatives.

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse fine	o.870 o.875	0.871 0.871	0.787	0.268	(1503.2 / 17.8) (1776.5 / 37.3)	(410.4 / 78.3) (137.1 / 58.8)

Table 3.81: LogRegAll-Wt23

coarse-pr	fine-pr	coarse-roc	fine-roc	coarse-acc	fine-acc	coarse-f1	fine-f1
0.894	0.914	0.890	0.900	0.862	0.944	0.351	0.525
0.896	0.902	0.886	0.888	0.870	0.948	0.359	0.514
0.885	0.889	0.856	0.859	0.865	0.941	0.333	0.482
0.893	0.893	0.881	0.874	0.859	0.942	0.331	0.496
0.886	0.884	0.872	0.872	0.865	0.932	0.340	0.445
0.879	0.887	0.863	0.870	0.868	0.943	0.342	0.472
0.902	0.899	0.892	0.886	0.868	0.945	0.342	0.488
0.879	0.896	0.859	0.875	0.860	0.943	0.332	0.491
0.911	0.913	0.904	0.903	0.871	0.943	0.360	0.482
0.891	0.901	0.898	0.890	0.874	0.940	0.375	0.452
avg 0.892	avg 0.898	avg o.880	avg 0.882	avg 0.866	avg 0.942	avg 0.347	avg 0.485

Table 3.82: Here are the results for the SVM passive 10 folds.

coarse-tn	fine-tn	coarse-fp	fine-fp	coarse-fn	fine-fn	coarse-tp	fine-tp
1658	1836	256	78	21	34	75	62
1676	1851	238	63	23	41	73	55
1670	1837	244	77	28	41	68	55
1657	1837	257	77	26	39	70	57
1668	1818	246	96	26	41	70	55
1676	1845	238	69	27	45	69	51
1676	1846	237	67	28	44	69	53
1658	1841	255	72	27	42	70	55
1676	1841	237	72	22	42	73	53
1680	1838	233	75	20	46	76	50
avg 1669.5	avg 1839.0	avg 244.1	avg 74.6	avg 24.8	avg 41.5	avg 71.3	avg 54.6

Table 3.83: Here are the results for the SVM confusion matrices. Here the fine returns less false negatives than the coarse, but not as many true positives compared to coarse.

title	pr	roc	acc	f1	conf (tn/fn)	conf (fp/tp)
coarse	0.892	0.880	0.866	0.347	(1669.5 / 24.8)	(244.1 / 71.3) (74.6 / 54.6)
fine	0.898	0.882	0.942	0.485	(1839.0 / 41.5)	(74.6 / 54.6)

Table 3.84: SVM-All

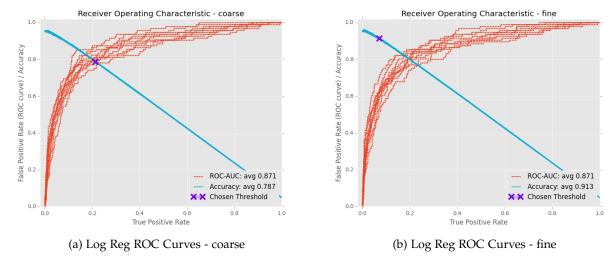


Figure 3.1: Fine has a higher accuracy than coarse at the default threshold.

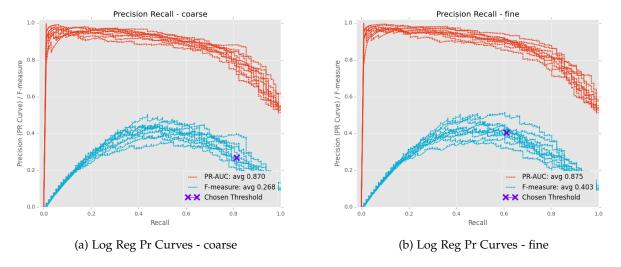


Figure 3.2: The fine threshold occurs at a point on the pr-curve associated with a higher f-measure than the coarse curves.

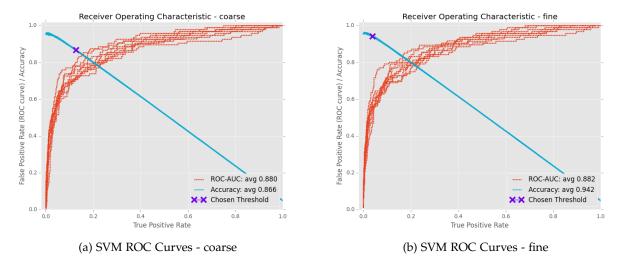


Figure 3.3: SVM results are similar between coarse and fine.

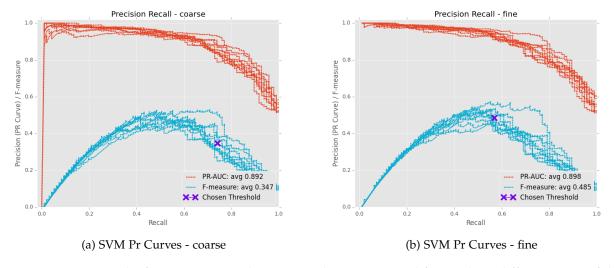


Figure 3.4: SVM results for PR-curves and F-measure have coarse and fine picking different parts of the curves for their respective thresholds, coarse f1 avg is slightly higher at 0.468 compared to 0.457 for fine.

3.3 Active vs Passive curves

The following plots were obtained with a round batch size of 100 and a starter set of 1040 instances out of the total 2098 instances. The plots are the average of 10 folds, for each fold a test set of 2010 containing representatives of each class was held out, out of the remaining 18088, the starter set was selected which again contained representatives of each class. Coarse and fine classifiers share the same starter set. During

each round coarse and fine classifiers are trained on their corresponding sets, metrics are outputted on the held out test set, then confidence estimates are ran on the remaining eligible instances. Eligible instances are kept in separate sets for coarse and fine, 100 of the most uncertain instances are removed from each eligible set and added to its corresponding coarse or fine set to be trained on for the next round.

3.3.1 Plots for Logistic Regression Active vs Passive curves

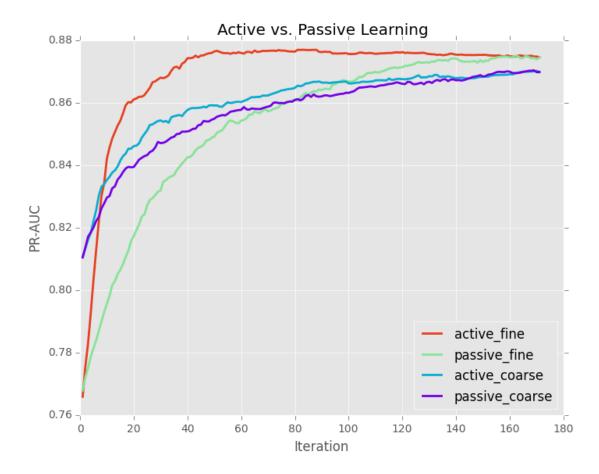


Figure 3.5: The PR AUC curves for rounds with the Logistic Regression classifier conforms to expectations, with active-fine having the highest performance. Active-coarse outperforms passive-coarse. Passive-fine doesn't outperform the coarse classifiers until rnd 100.

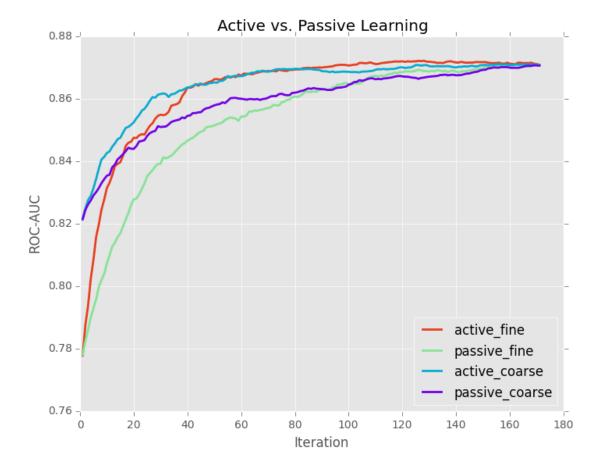


Figure 3.6: The ROC AUC curves for rounds with the Logistic Regression classifier. The active curves beat out the passive curves for both coarse and fine. Coarse roc starts with an advantage over fine as in the PR curves. Both converge to the same rate after roc auc level after 80.

3.3.2 Plots for SVM Active vs Passive curves

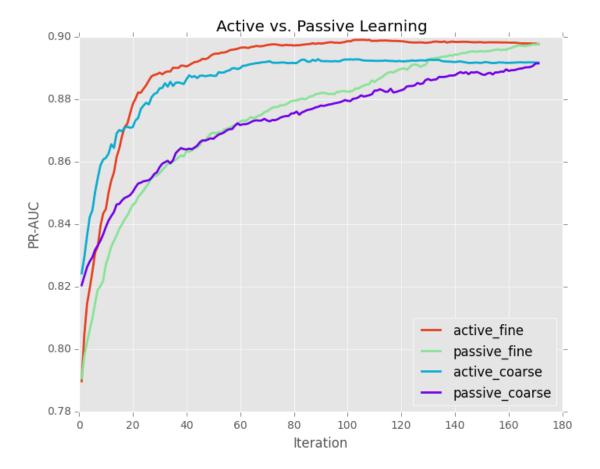


Figure 3.7: The PR AUC curves for rounds with SVM show little advantage for fine. The results are slightly different than the ones shown on 2/14 due to fixing a bug with the code that wasn't performing the preprocessing scaling for the SVM case at the same stage as it was being done for the logistic regression classifier.

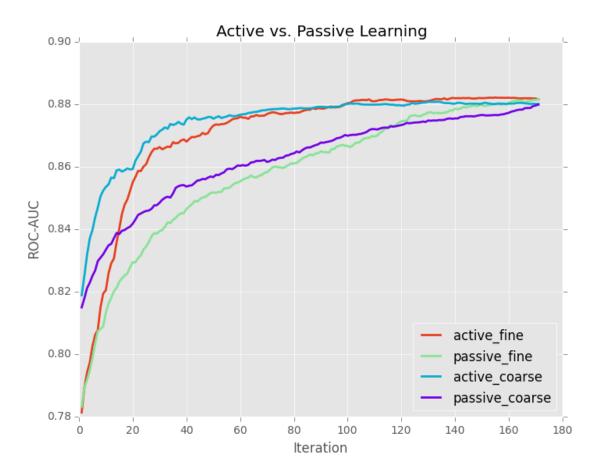


Figure 3.8: The ROC curves show more of an advantage for coarse classifiers.

3.4 Plots for FFR experiments

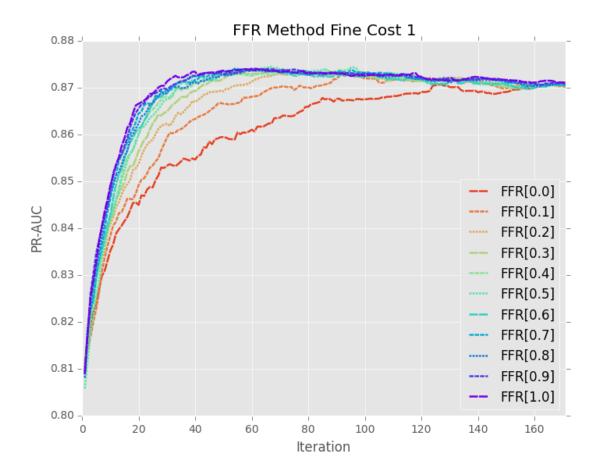


Figure 3.9: The strategy is changed from purchasing a set number of instances per round to having a set budget per round and spending a portion of that budget on fine and coarse grained labels. For this curve the fine and coarse grain labels both have a cost of 1. The purple 1.0 curve shows that if only fine grained labels are purchased, the highest performing PR-AUC can be obtained. The results are an average of 10 folds.

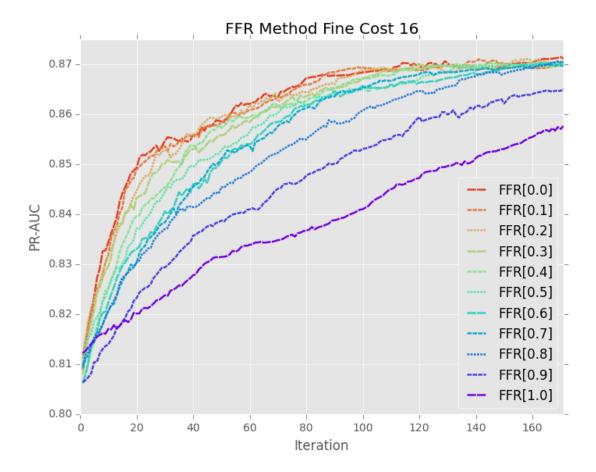


Figure 3.10: The fine cost is increased to 16. The budget for each iteration is 100, and for the case of the 0.5 curve, 50 instances are bought for coarse and 3.125 instances are bought for fine. The remainder 0.125 is then turned into a 0.125 chance for any round to purchase an extra fine label. The round size for the FFR 1.0 curve is very small, with only 7 labels purchased per iteration. The cost is to high for the fine label advantage to offset the decreased number of instances purchased.

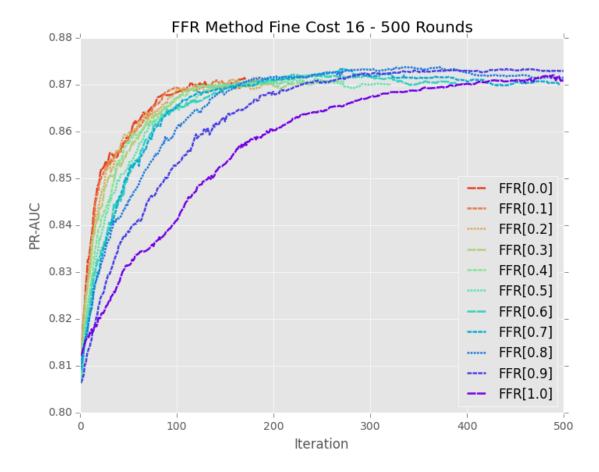


Figure 3.11: This shows the iterations continuing through round 500, the curves with the higher fine rates eventually settle to the same end point that the curves with the high rates of coarse labels purchased achieved at previous iterations.

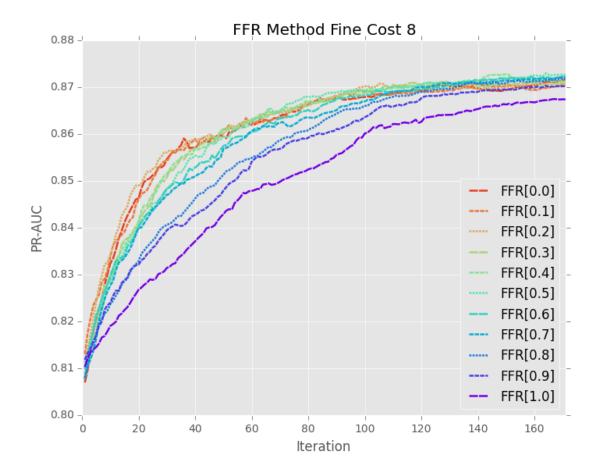


Figure 3.12: At fine cost 8 the FFR 0.0 rate is no longer the best option, 0.1 generally outperforms 0.0 slightly.

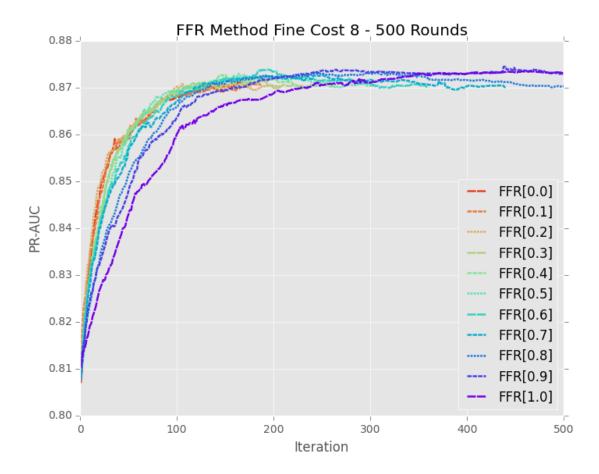


Figure 3.13: The extended picture of the FFR cost 8. The round size for FFR 1.0 is small, only 13 instances purchase per iteration.

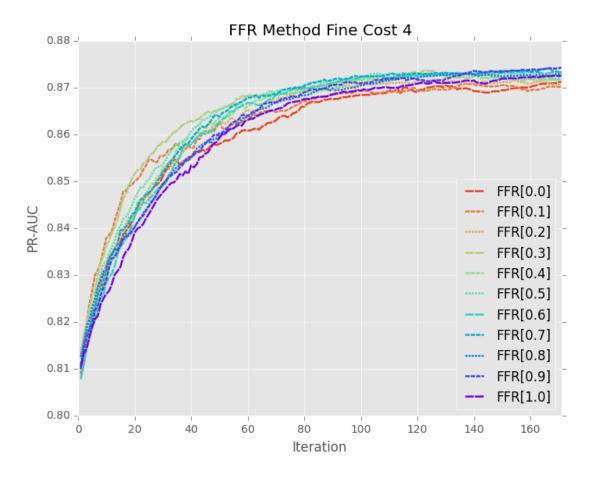


Figure 3.14: At fine cost 4, FFR 0.3 appears to be the highest performing rate.

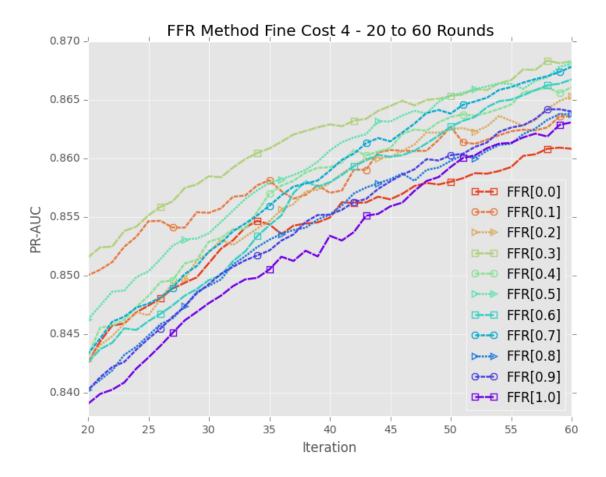


Figure 3.15: The fine cost 4 curves shown expanding the rounds 20-60.

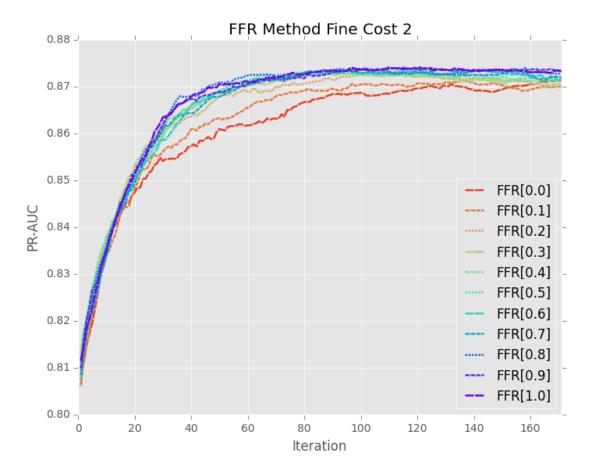


Figure 3.16: At fine cost 2, the preferred rate jumps up to 0.8, similar to the cost 1 results.

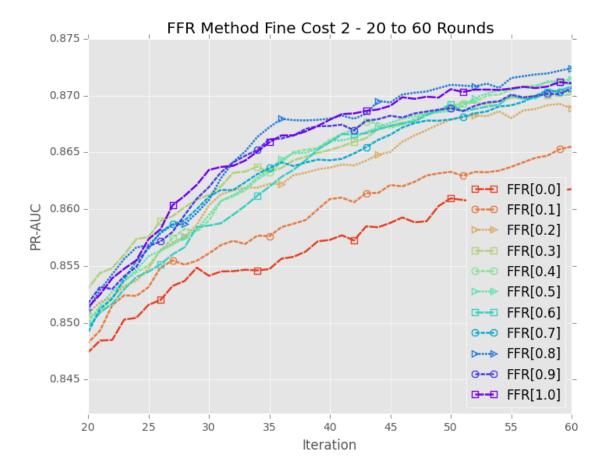


Figure 3.17: The fine cost 2 curves shown expanding rounds 20-60.

Chapter 4

Conclusions and Future Work

I should probably do the Bandit experiments.

Appendix A

Tuning the fine grained classes

All the data and results for tuning the fine grained classes.

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