HIERARCHICAL ACTIVE LEARNING (HAL) APPLICATION TO MITOCHONDRIAL DISEASE PROTEIN DATASET

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Introduction

- Identify the source of mutations which give rise to mitochondrial disease.
- Leigh Syndrome, Lebers Hereditary Optic Neuropathy
- Hierarchically-labeled according to location in mitochondria
- Learn mitochondrion concept (Coarse) by combining classifiers for each target compartment (Fine)

You haven't yet defined these terms

For intro, motivate active learning (with respect to some cost model), related to how it can help with this problem. Then, describe how HAL can help even more.

When you use terms such as 'fine' and 'coarse', need to briefly define these in Intro.

- Previous work in text classification and and rich media indexing use hierarchies of labels to improve fine-level classification (McCallum et al. 1998, Jiang et al. 2013)
- Previous work in named entity recognition to target fine-grained entity categories (Fleischman et al. 2002)
- ~~This work is done in conjunction with Yugi Mo, Dr. Scott, and Dr. Downey~~
- First investigation of active learning in a hierarchical setting where label acquisition cost can vary

Not defined

Introduction

Outline?

- Active Machine Learning
- Evaluating Classifier Performance
- Hierarchical Protein Dataset
- Coarse-grained vs Fine-grained Trade-Off
- Active Over-Labeling

Algorithms?

- Application to Protein Dataset

Experimental results?

Machine Learning

Better to use figure(s) to illustrate what ML is. E.g., show labeled training data feeding into a M algorithm, output hypothesis, and then use hyp to label new instances.

- Machine learning (ML) 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 - (Mitchell 1997).
- Support Vector Machine (SVM) - Uses support vectors and kernel functions
- Logistic Regression (Logit) - Uses logistic function

After graphically describing ML, use pictures to show what an SVM looks like, and mention (or graphically show) that logit learns a probabilit distribution

Active Machine Learning

Boldface, or italics

- The learner queries an oracle or supervisor which labels the data at a certain cost
- Active learning solicits new instances that can maximally improve performance of the learned classifier
- Learns the best performing classifier for the minimal amount of labeling cost, or for a given purchase budget

Give examples of domains where active learning is useful: copious unlabeled data, cost associated with acquiring labels.

Evaluating Classifier Performance
Confusion Matrix

Divide data into train and a test set. Analyze test set with the following values:

- True-Negatives (T_n): Correctly classified negatives
- False-Negatives (F_p): Incorrectly classified negatives
- False-Positives (F_n): Incorrectly classified positives
- True-Positives (T_p): Correctly classified positives

Example of a confusion matrix for a test set with 100 negatives and 50 positives:

conf (T_n/F_n)	conf (F_p/T_p)
90	10
20	30

Evaluating Classifier Performance
Precision and Recall

Precision is a measure of result relevancy:

$$P = \frac{T_p}{T_p + F_p} \tag{1}$$

Recall is a measure of how many truly relevant results are returned:

$$R = \frac{T_p}{T_p + F_n} \tag{2}$$

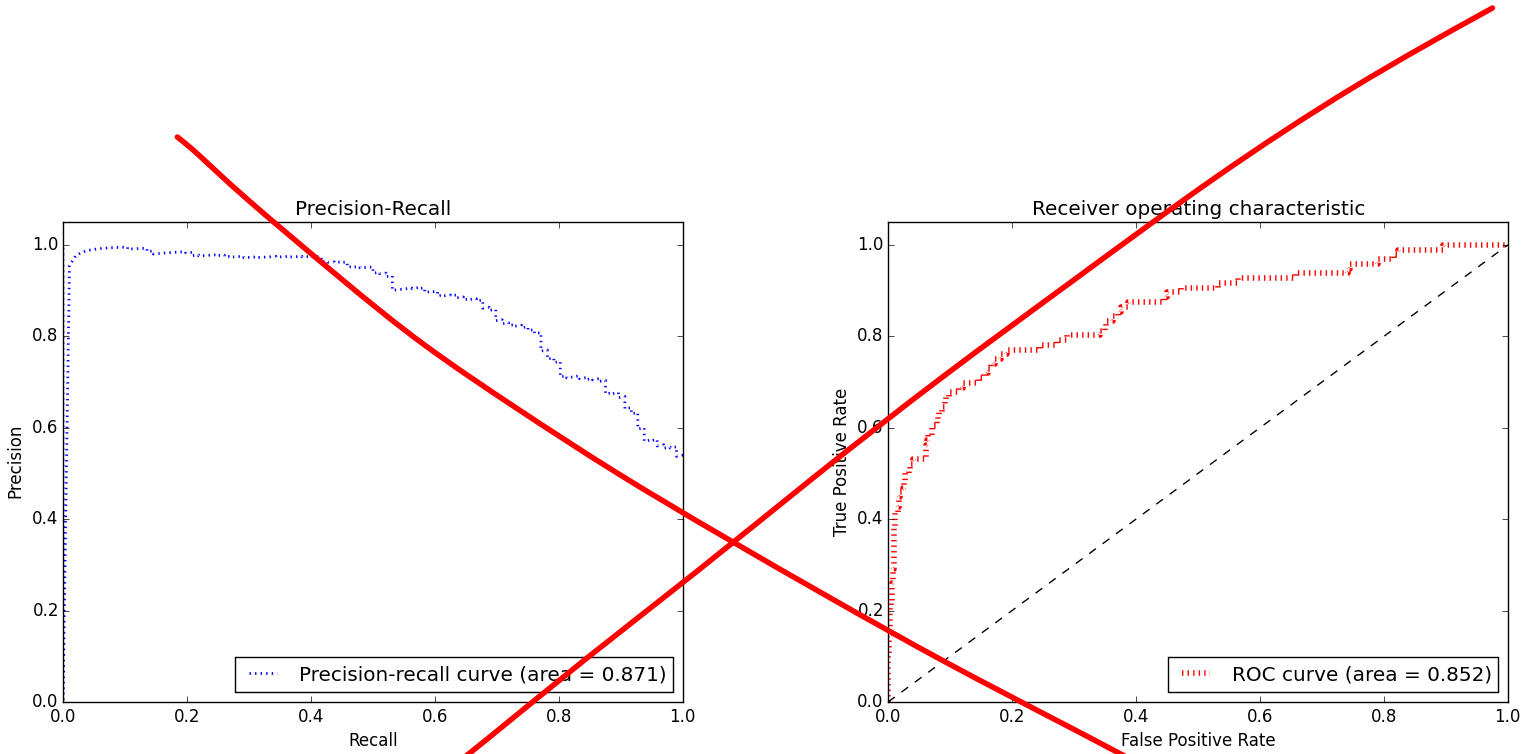
Only describe evaluation methods that you use later in the talk, and only describe them at the time you present results.

Evaluating Classifier Performance
F-Measure

The F-measure or F1-measure (F1) is the harmonic mean of precision and recall:

$$F1 = 2 \cdot \frac{P \cdot R}{P + R} \tag{3}$$

Evaluating Classifier Performance
ROC - PR curves



(a) PR curve. (b) ROC curve.

Figure: Examples of PR and ROC curves with their corresponding AUC values.

Hierarchical Bioinformatics Data Set

Feature Sources

~~Table: Features of the protein dataset along with their respective sources~~:

Type of Properties	Features	Sources Use citations
General sequence features	Amino acid composition, sequence length, etc.	Calculated by Kevin Chiang at UNL, etc.
Physico chemical properties	Hydrophobicity, polarity, etc.	Computed from Cui et al, etc.
Structural properties	Secondary structural content, shape, etc.	SSCP, etc.
Domains and motifs	Signal peptide, transmembrane domains, etc.	SignalP, NetOgly, etc.

Hierarchical Bioinformatics Data Set

Labeling Hierarchy

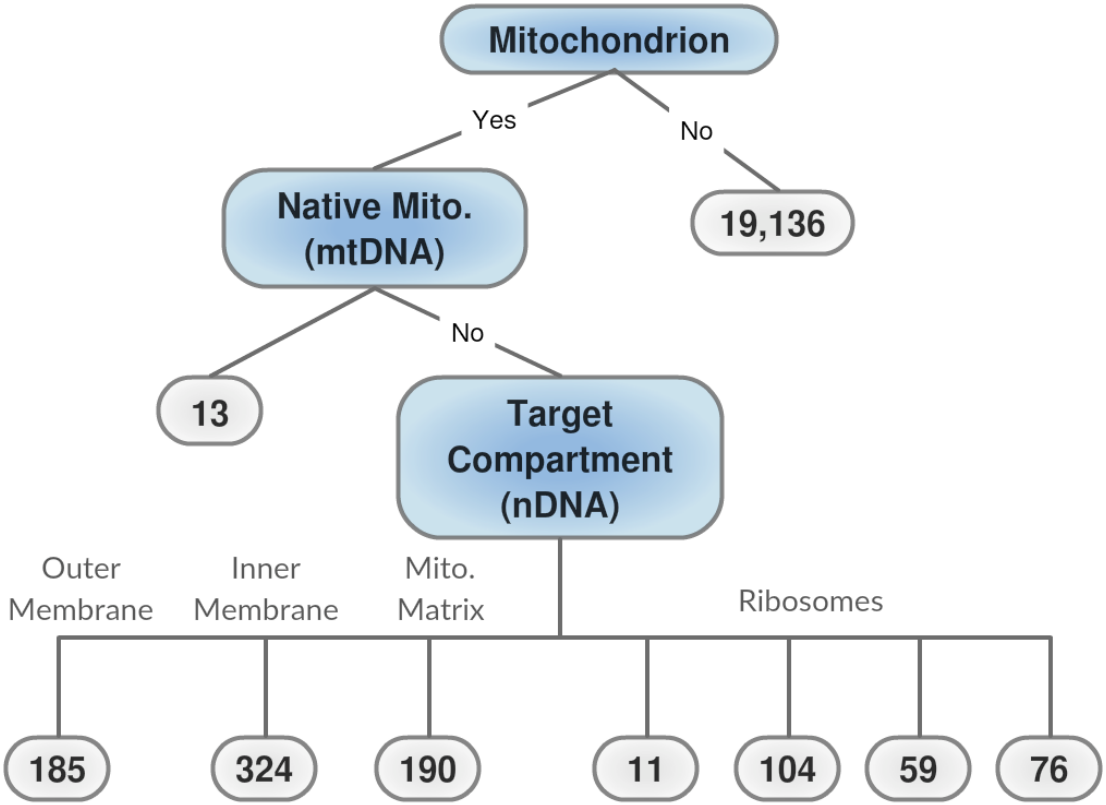
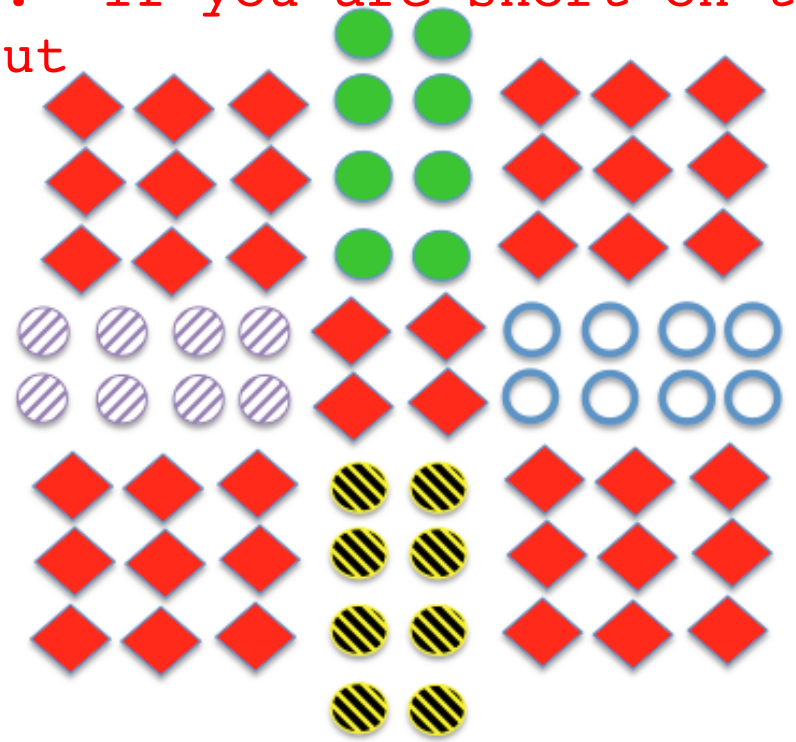


Figure: The protein dataset hierarchy of labels along with the instance count for each label.

Coarse-grained vs Fine-grained Trade Off

This belongs earlier, when you describe active over-labeling. If you are short on time, then this can be cut



~~Figure: Demonstration of a dataset that would benefit from multiple fine-grained learners for each circle type, from Mo et al.~~

Active Over-Labeling

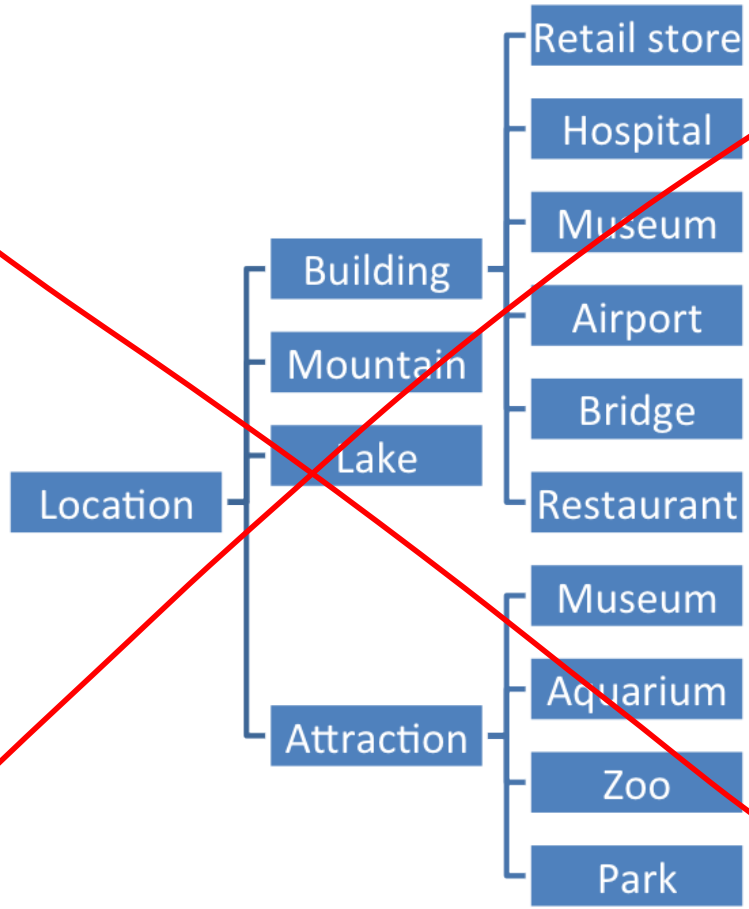
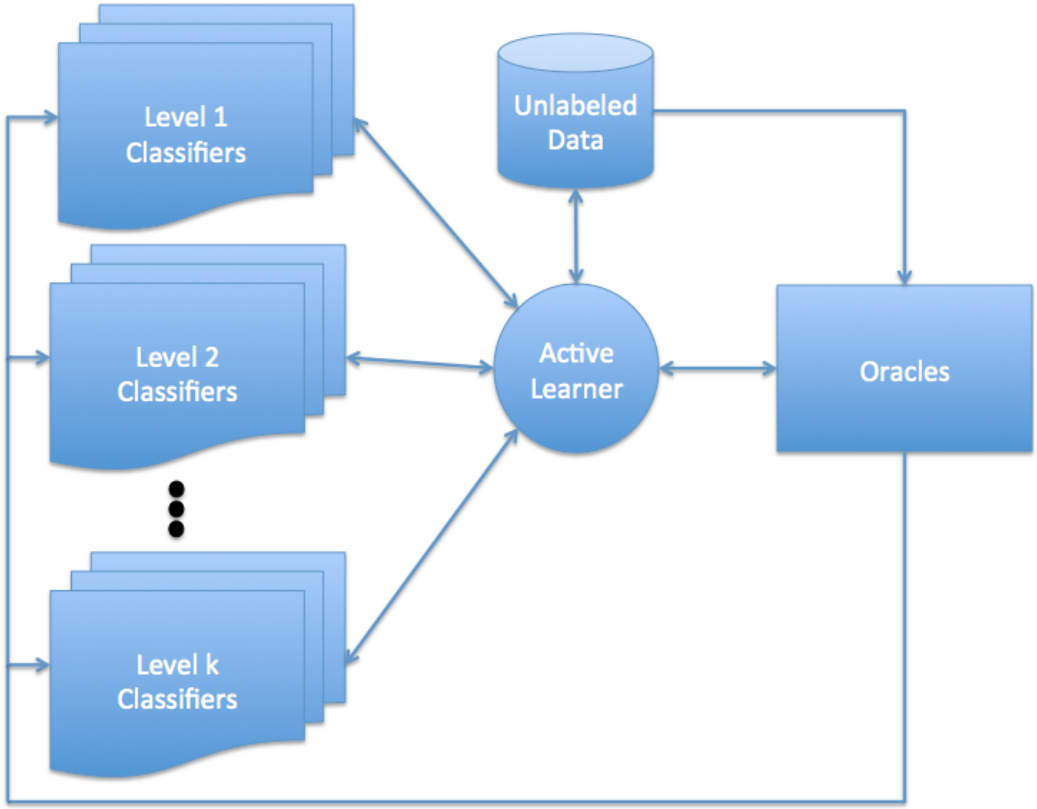


Figure: A labeling tree based on the text categorization dataset RCV1, from Mo et al.

Hierarchical Active Learning

Earlier



~~Figure: Diagram of HAL approach~~

Dynamically Adapting Purchase Proportions

`Can you demonstrate this graphically?`

- HAL is a fixed-fine ratio (FFR) methodology
- Input is a purchase proportion vector p, which allocates budget to purchase labels at a given level in the hierarchy
- The task of choosing the level of granularity to purchase labels is solved using Auer et al.'s ϵ-greedy bandit algorithm
- With probability $1 - \varepsilon_n$ play arm with highest current average reward for round n, otherwise explore

Application to Dispatch Dataset

Analysis and evaluation follow Mo et al.'s work.

- Fine outperforms Coarse in PR-AUC
- Active outperforms Passive in PR-AUC
- HAL ran with variable cost, fine proportions and budget
- BANDIT approach shown to be robust to changes in cost and budget

Not related to your work. After you present HAL, you may briefly summarize results in other domains, but you should avoid detailed descriptions.

Training and Testing Coarse-Grain and Fine-Grain Classifiers

Number of proteins in each class:

Name the classes

Classes	Count	Totals
0	19136	All: 20098
1	13	Coarse: 19136
2	185	Fine: 962
3	324	Features: 449
4	190	
5	11	
6	104	
7	59	
8	76	

Training and Testing Coarse-Grain and Fine-Grain Classifiers

Table: Number of proteins in each partition:

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

Training and Testing Coarse-Grain and Fine-Grain Classifiers

The following variables were varied for both SVM and Logit classifiers:

- Preprocessing Scaling Methods
- Preprocessing Feature Selection
- Class Weight
- SVM Kernel, Cost, and Gamma parameters
- Logit Cost, Fine class weights, Tolerance

SVM and Logit Classifier Performance

Conventional ML

Instead, simply state that you tuned the parameters for the learning algorithms via an independent run of cross-validation.

Table: Logit results after parameter tuning:

Title	PR	ROC	Acc	F1	conf (tn/fn)	conf (fp/tp)
coarse	0.870	0.871	0.787	0.268	(1503.2 / 17.8)	(410.4 / 78.3)
fine	0.875	0.871	0.913	0.403	(1776.5 / 37.3)	(137.1 / 58.8)

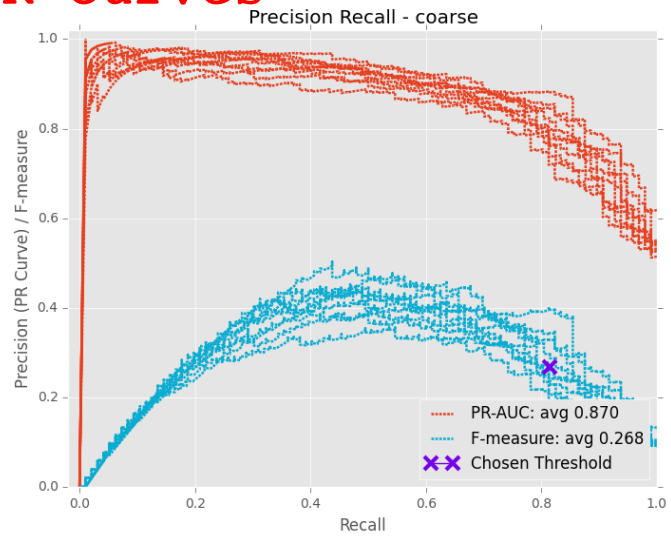
Table: SVM results after parameter tuning:

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)
fine	0.898	0.882	0.942	0.485	(1839.0 / 41.5)	(74.6 / 54.6)

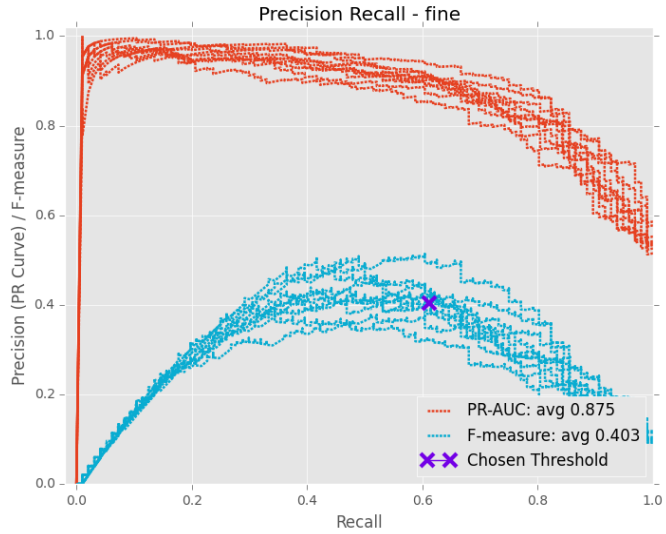
SVM and Logit Classifier Performance

F-measure Analysis

On the prior slide, define precision, recall, and P-R curves



(a) Log Reg Pr Curves - Coarse

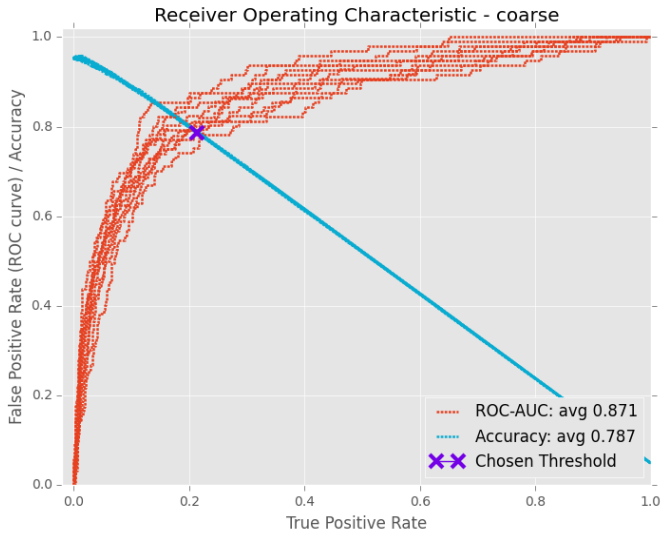


(b) Log Reg Pr Curves - Fine

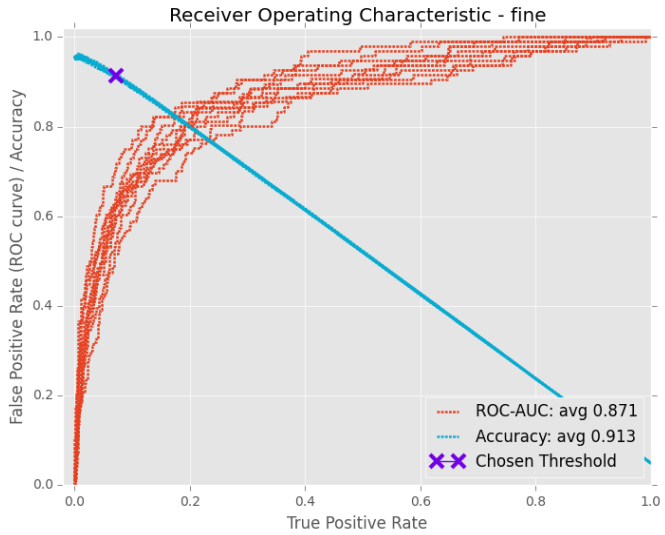
~~Figure: The fine default threshold occurs at a point on the PR curve associated with a higher F-measure score compared to the coarse curves~~.

SVM and Logit Classifier Performance

F-measure Analysis



(a) Log Reg ROC Curves - coarse



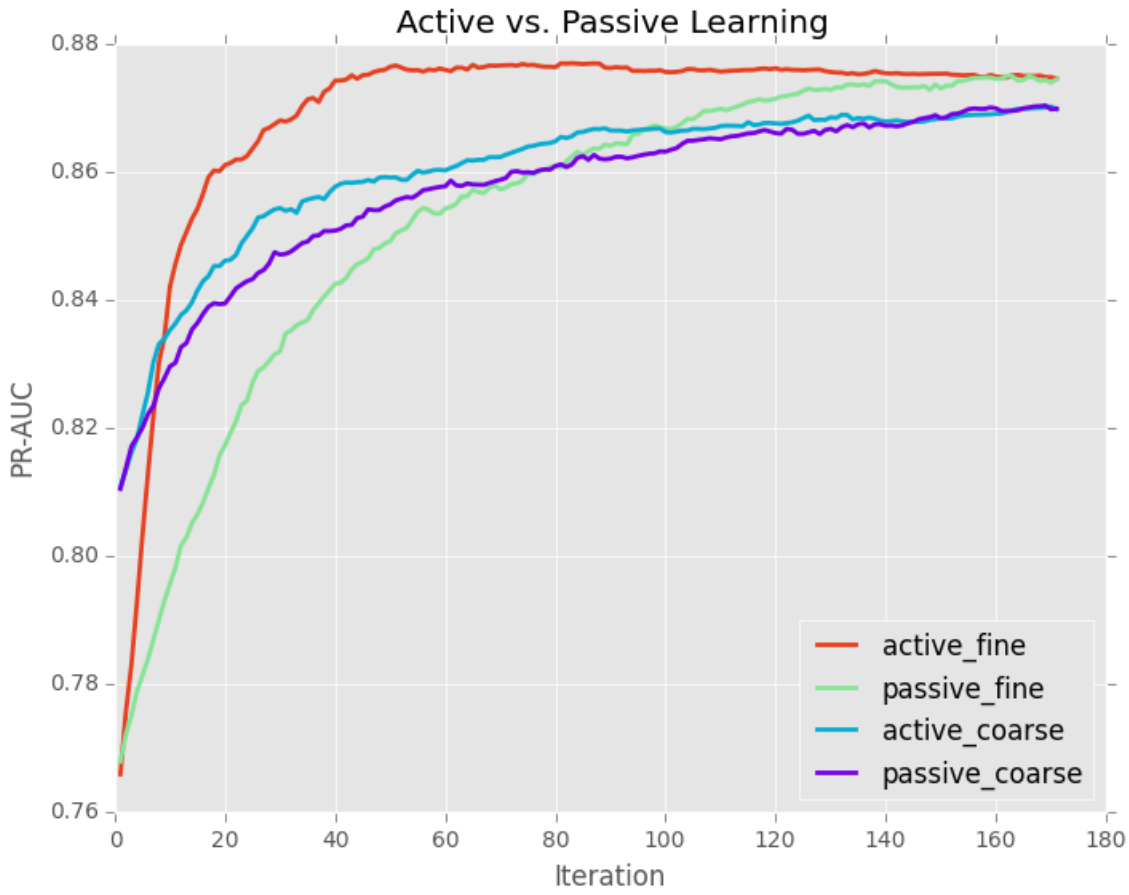
(b) Log Reg ROC Curves - fine

~~Figure: Fine has a higher accuracy than coarse at the default threshold for the Logit classifier~~.

Active vs. Passive Curve Analysis

Logit PR-AUC curves

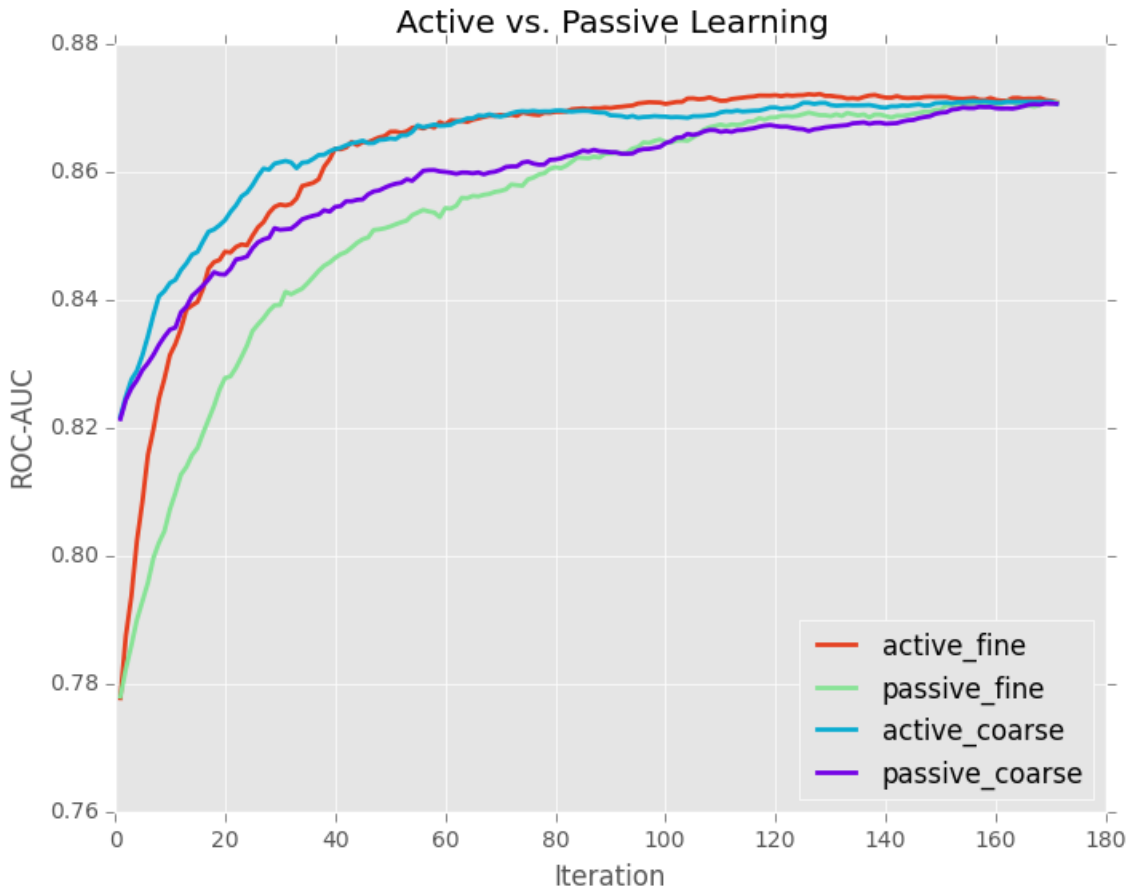
Define 'iteration' and 'AUC'



~~Figure: The PR-AUC curves for rounds with the Logit classifier conforms to expectations~~

Active vs. Passive Curve Analysis

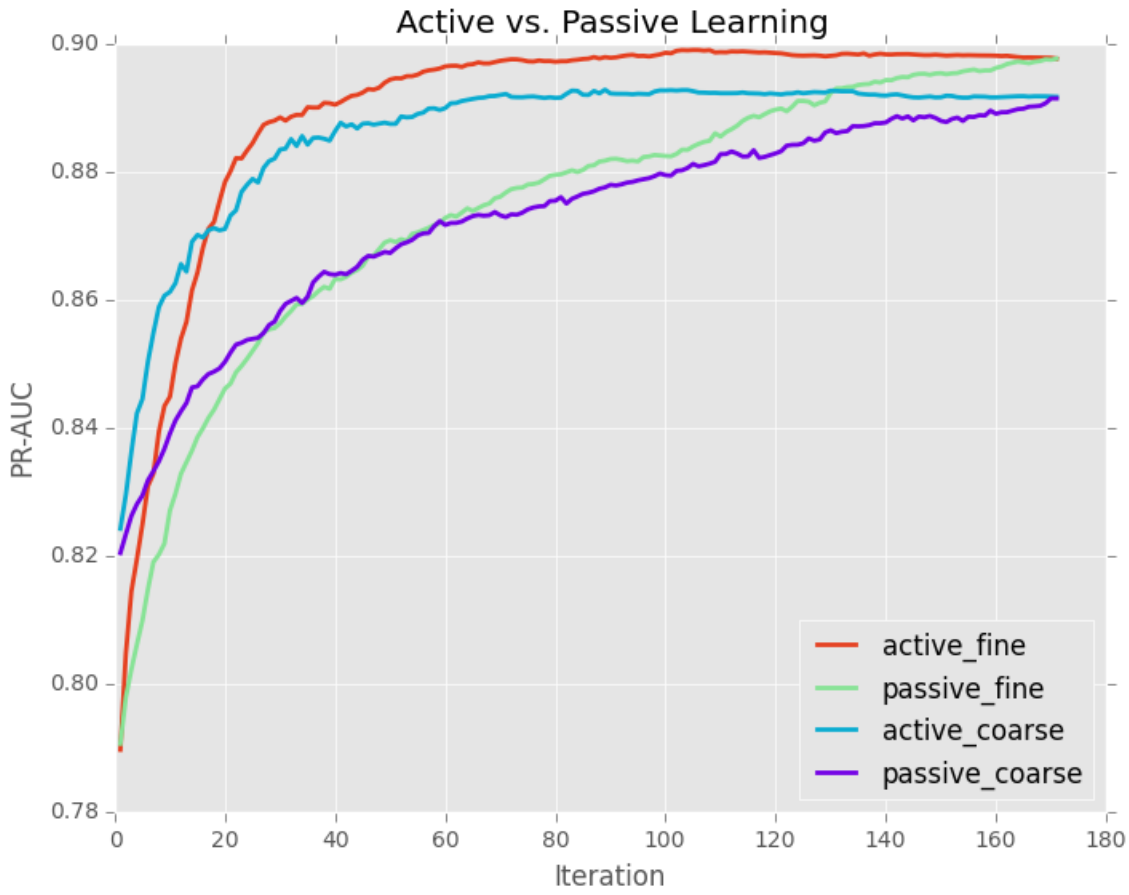
Logit ROC-AUC curves



~~Figure: The ROC-AUC curves for rounds with the Logit classifier; active curves beat out the passive curves for both coarse and fine.~~

Active vs. Passive Curve Analysis

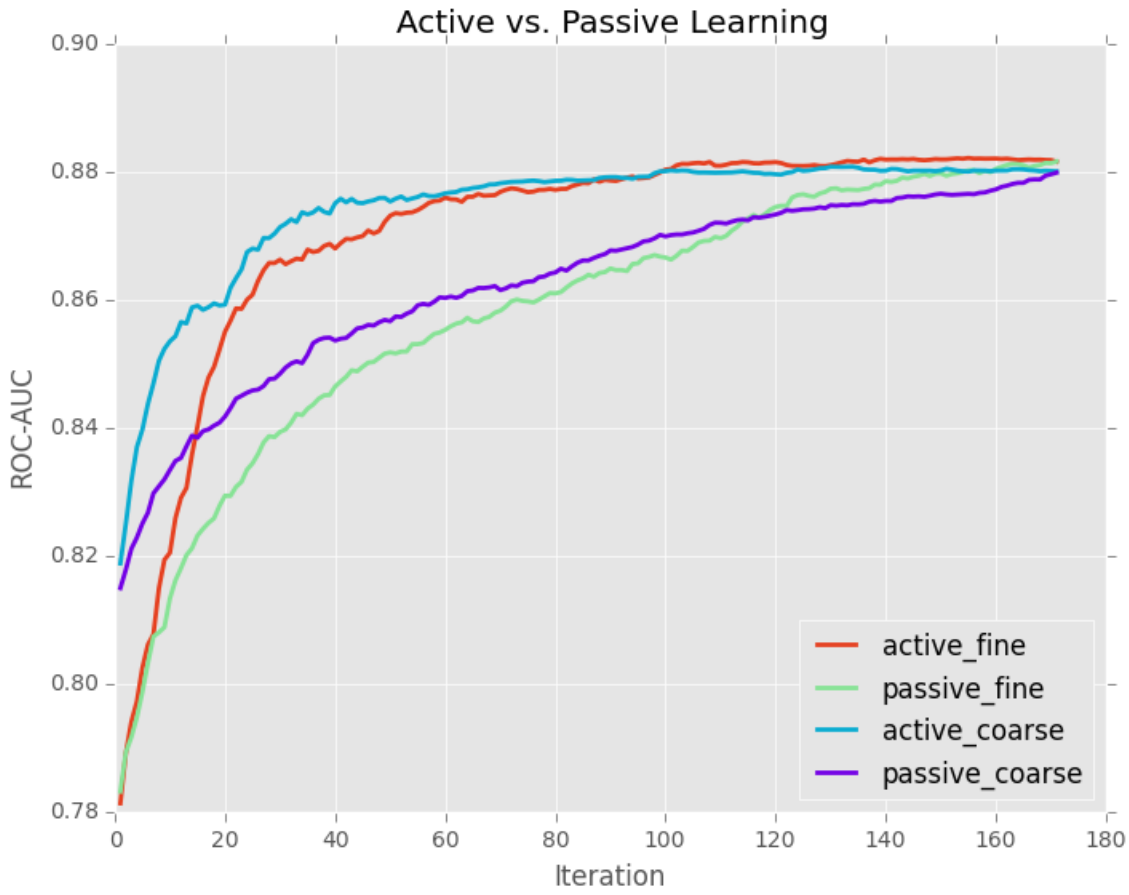
SVM PR-AUC curves



~~Figure: The PR AUC curves for SVM show a slight advantage for active fine, similar to the Logit results.~~

Active vs. Passive Curve Analysis

SVM ROC-AUC curves

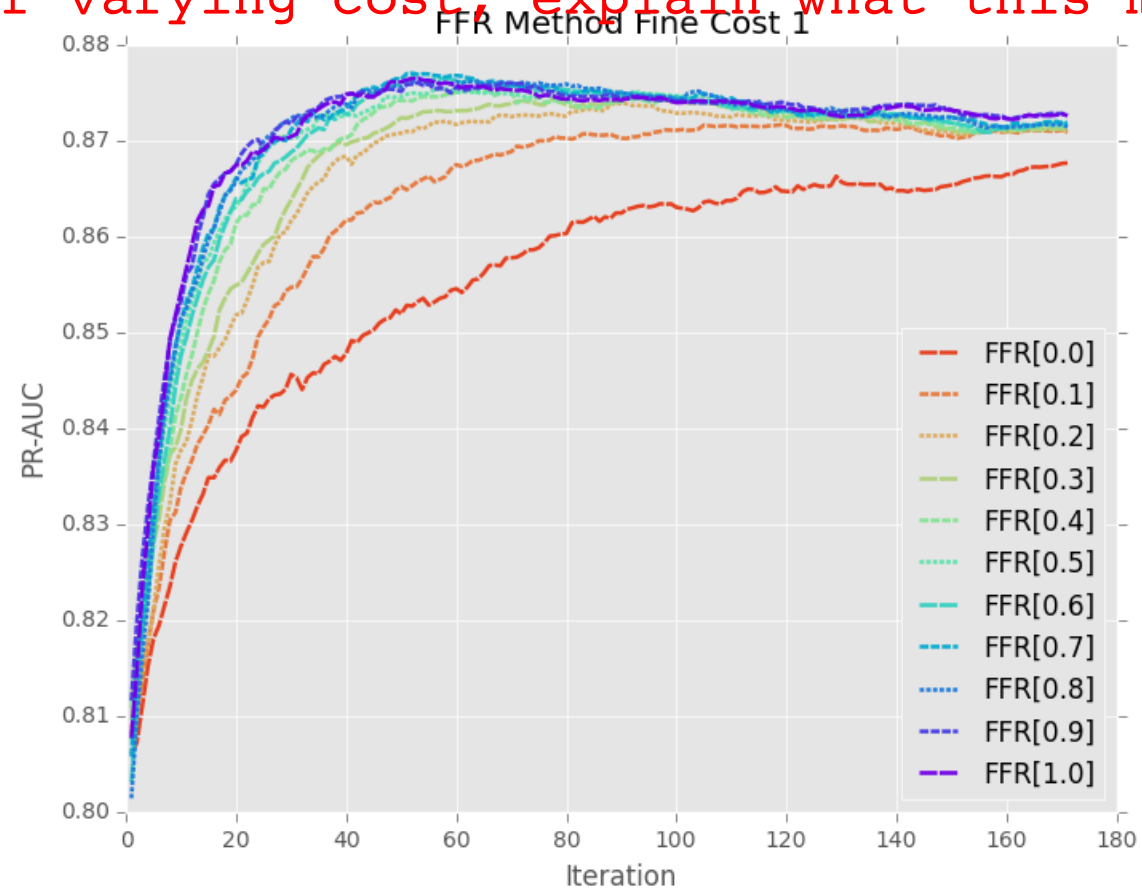


~~Figure: The ROC AUC curves for SVM match the Logit results, the convergence of active fine to active coarse takes slightly longer~~.

Plots for Fine Fixed Ratio Results

Fine Cost 1

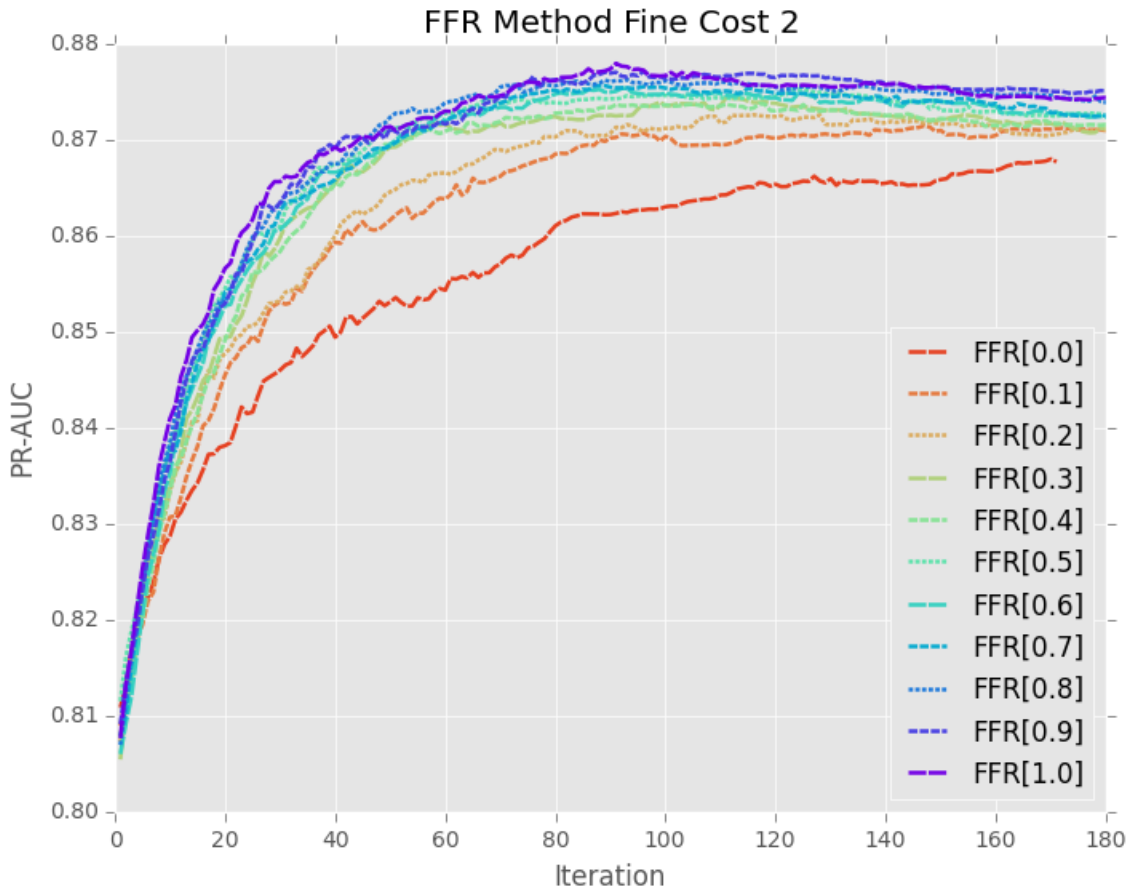
On each slide, describe what you are comparing. E.g., for varying cost, explain what this means.



~~Figure: The fine and coarse grain labels both have a cost of 1.~~

Plots for Fine Fixed Ratio Results

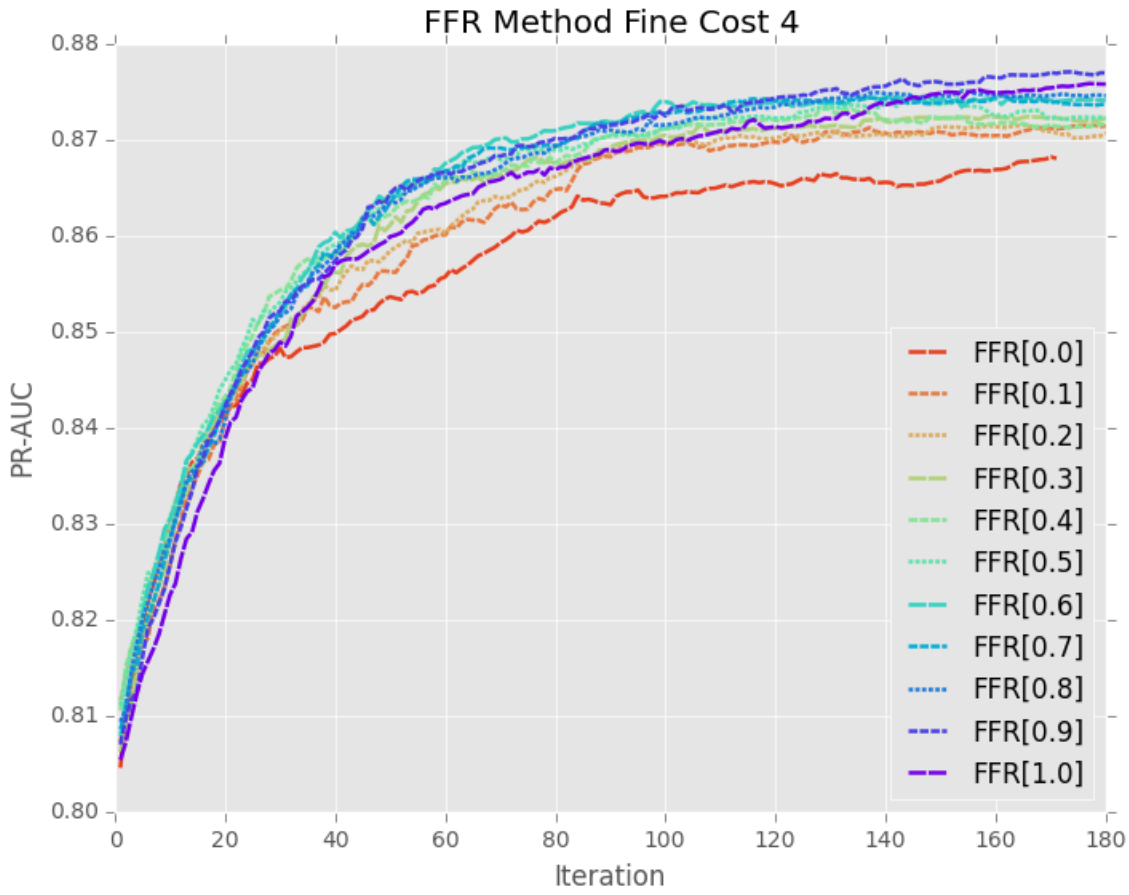
Fine Cost 2



~~Figure: At fine cost 2, advantage of the higher FFR values decreases but the ordering of the curves remains unchanged~~.

Plots for Fine Fixed Ratio Results

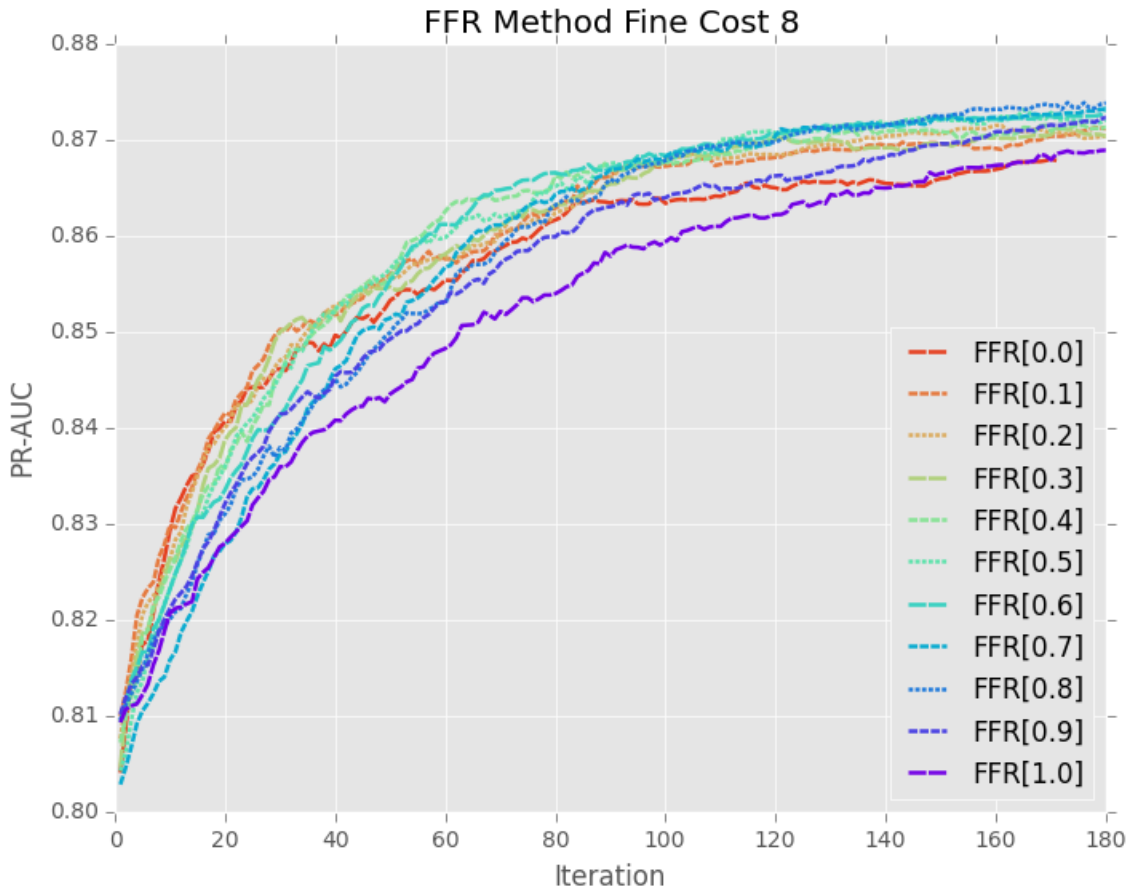
Fine Cost 4



~~Figure: At fine cost 4, the highest FFR 1.0 is no longer preferred. Purchasing a greater number of coarse instances is a better strategy.~~

Plots for Fine Fixed Ratio Results

Fine Cost 8

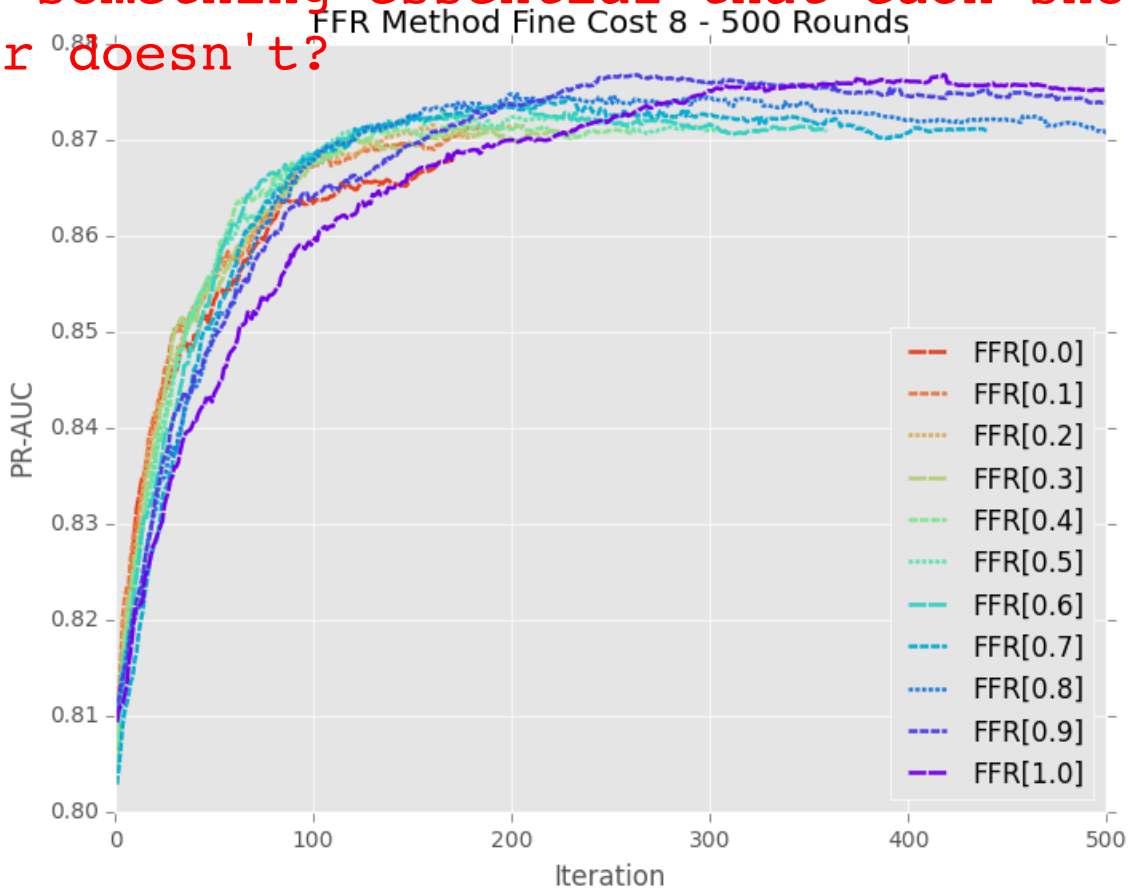


~~Figure: At fine cost 8 the middle FFR values outperform the extreme values for rounds 0 to 180.~~

Plots for Fine Fixed Ratio Results

Fine Cost 8 - Rnds to 500

Is there a reason to display both cost-8 curves? Is there something essential that each shows that the other doesn't?

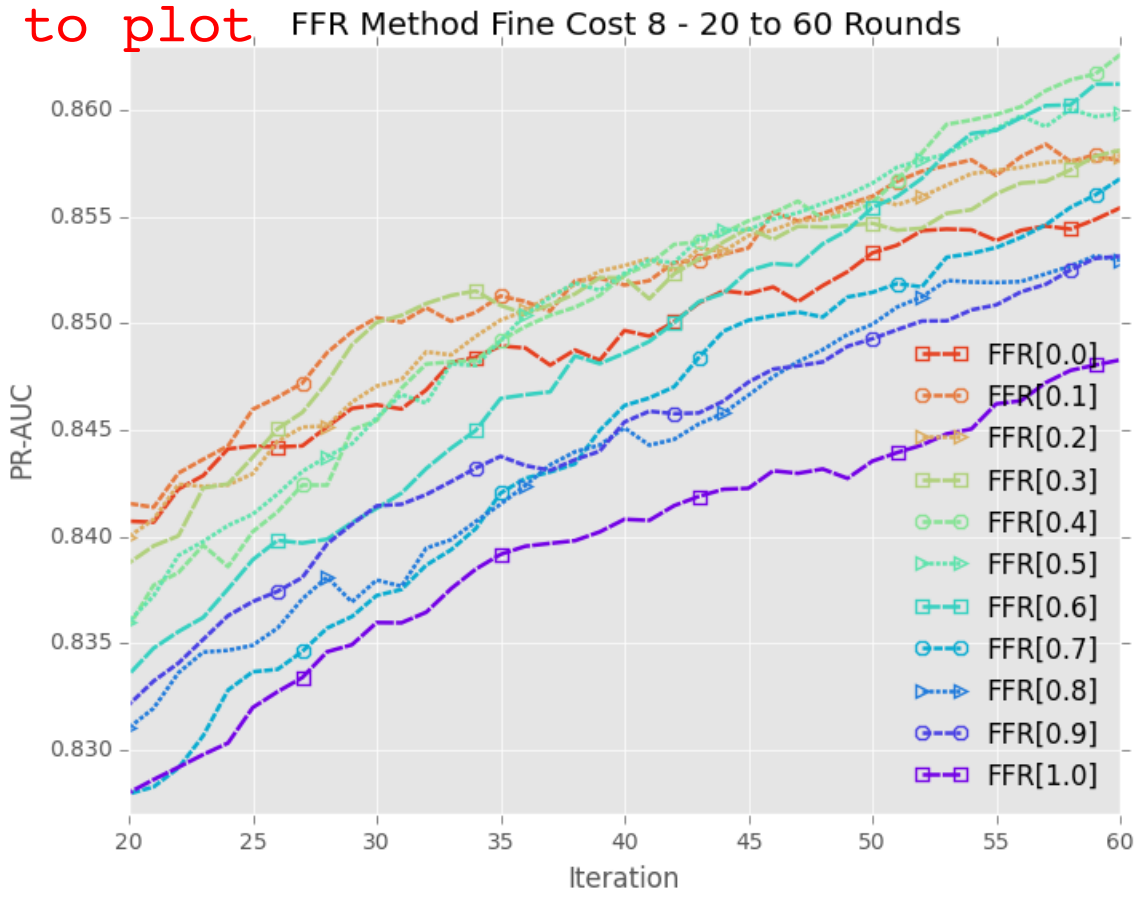


~~Figure: This shows the iterations continuing through round 500, the curves with the higher fine rates settle to the same end point.~~

Plots for Fine Fixed Ratio Results

Fine Cost 8 - Rnds 20 to 60

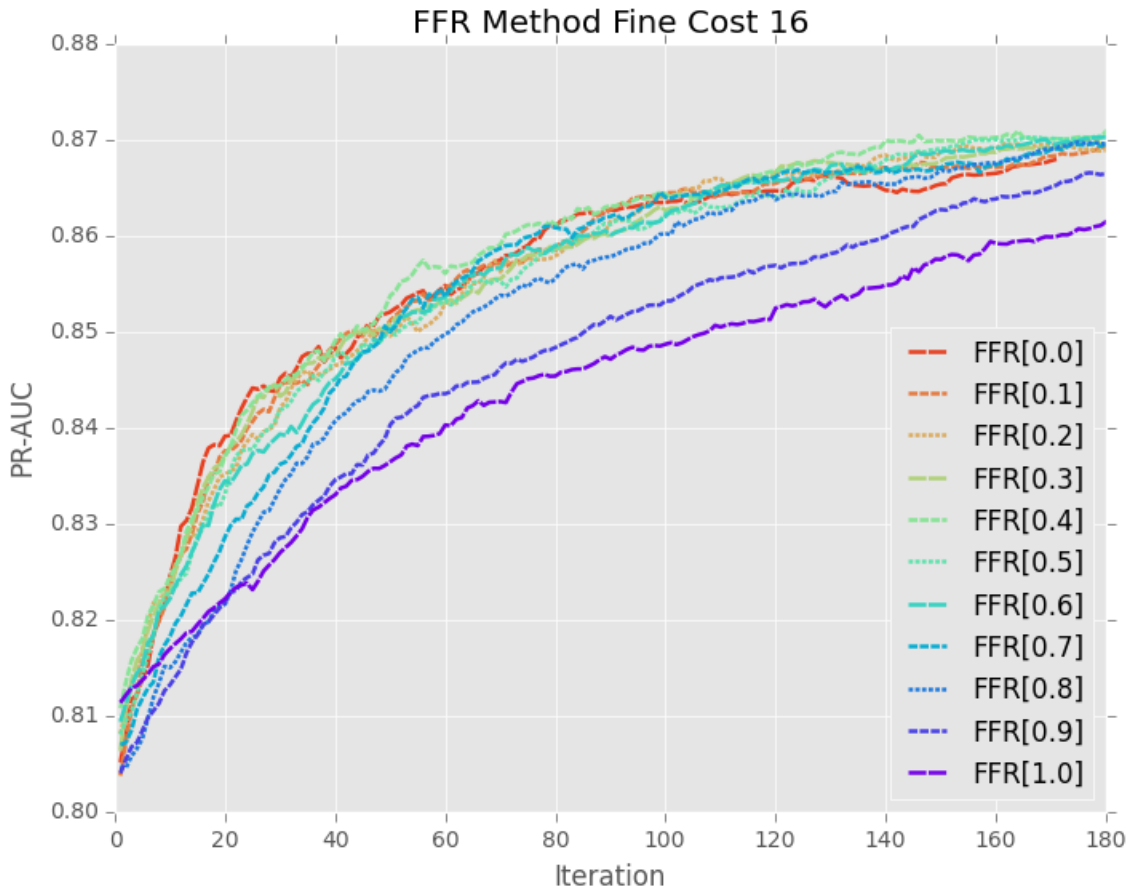
Same comment as earlier: be judicious of which curves to plot



~~Figure: The fine cost 8 curves shown expanding the rounds 20-60. If a round budget of 40 occurs than the recommended FFR would be 0.2.~~

Plots for Fine Fixed Ratio Results

Fine Cost 16



~~Figure: The fine cost is increased to 16. The fine cost is to high to offset the decreased number of instances purchased~~.

BANDIT Approach Results

Varying Cost Analysis

You have not defined BANDIT, why it's important, or given an example of how it works. You should do that when you describe your original approaches

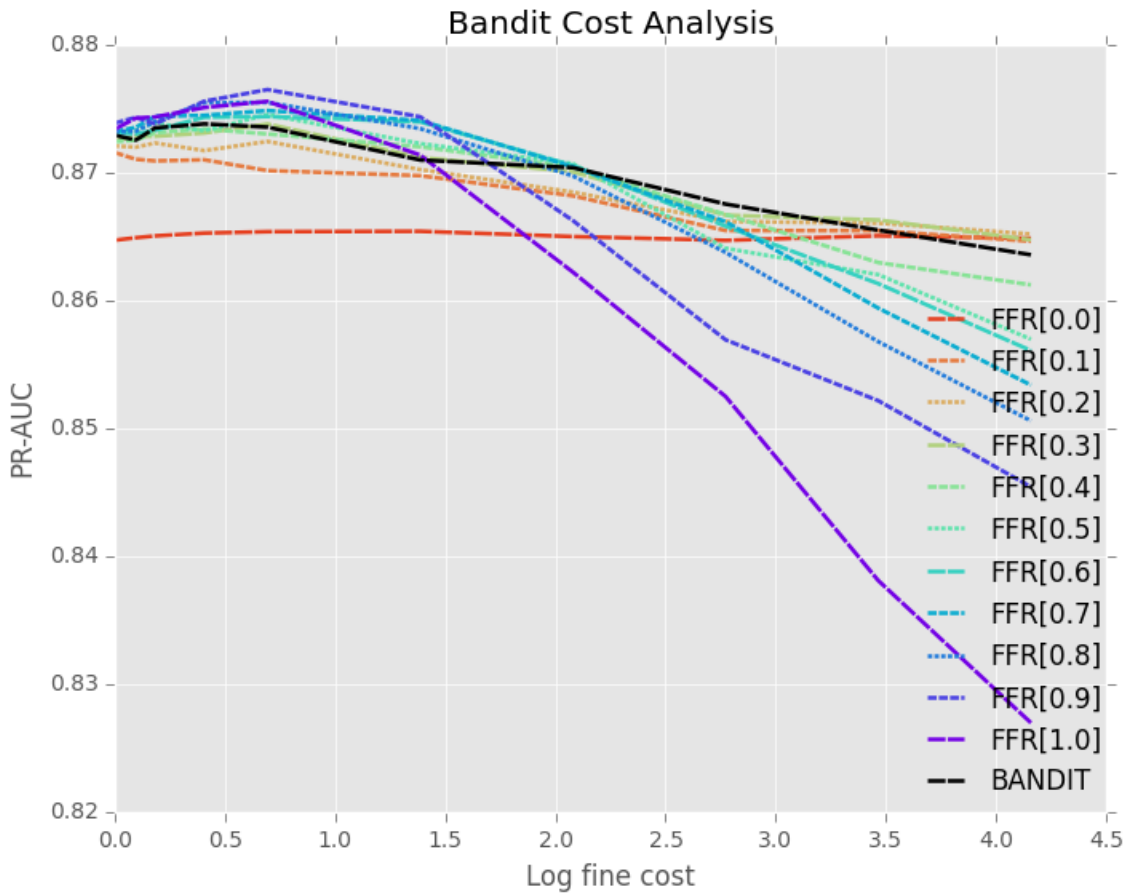
- The BANDIT approach is compared to the previous FFR curves for the following fine-grain costs $\{1.0, 1.1, 1.2, 1.5, 2.0, 4.0, 8.0, 16.0, 32.0, 64.0\}$
- Budget held fixed at round 120.
- The metric *diff* is the learner's absolute difference in PR-AUC from the top learner for a given cost.

Define before experimental results presented

- The metric *rank* is the learners 0 indexed ranking in terms of PR-AUC for a given cost.

BANDIT Approach Results

Varying Cost Analysis - Plot



~~Figure: BANDIT log fine cost analysis with budget fixed~~.

BANDIT Approach Results

Varying Cost Analysis - Rank and Diff Metrics

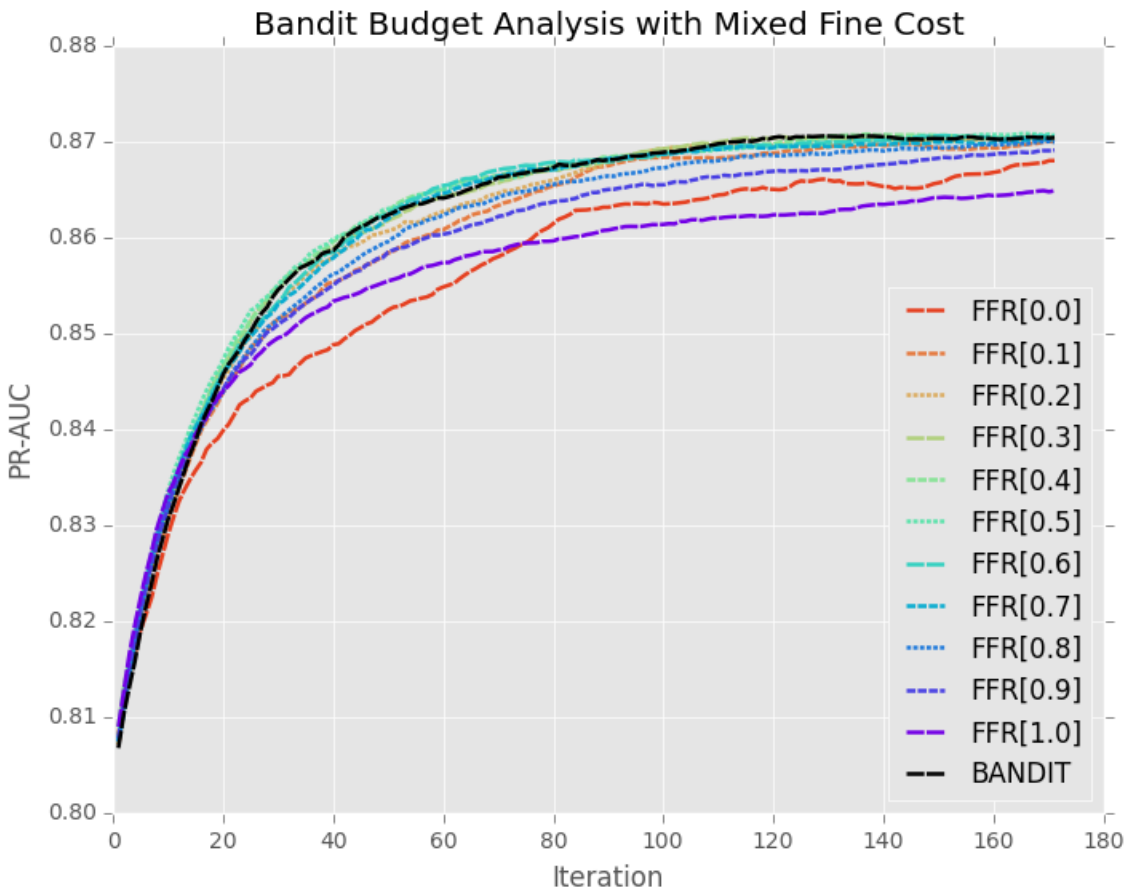
~~Table: Aggregated PR AUC for the protein dataset~~

Remember to explain what these terms mean, even if you do not define them on your slides

	diff				rank			
	min	max	mean	std	min	max	mean	std
algorithm								
BANDIT	0.000	0.003	**0.001**	0.001	0	8	4.8	2.315
FFR[0.0]	0.000	0.011	0.007	0.004	1	11	8.8	3.429
FFR[0.1]	0.001	0.006	0.003	0.002	3	10	8.0	2.793
FFR[0.2]	0.000	0.004	0.002	0.001	0	9	6.5	3.500
FFR[0.3]	0.000	0.003	0.001	0.001	0	8	5.1	2.663
FFR[0.4]	0.000	0.004	0.002	0.001	1	8	5.6	2.200
FFR[0.5]	0.000	0.008	0.002	0.002	0	8	4.6	2.200
FFR[0.6]	0.000	0.009	0.002	0.003	1	7	4.6	1.855
FFR[0.7]	0.000	0.012	0.002	0.004	0	8	**3.3**	2.571
FFR[0.8]	0.000	0.015	0.003	0.005	1	9	4.8	3.027
FFR[0.9]	0.000	0.020	0.005	0.007	0	10	4.3	4.605
FFR[1.0]	0.000	0.038	0.009	0.013	1	11	5.6	4.630

BANDIT Approach Results

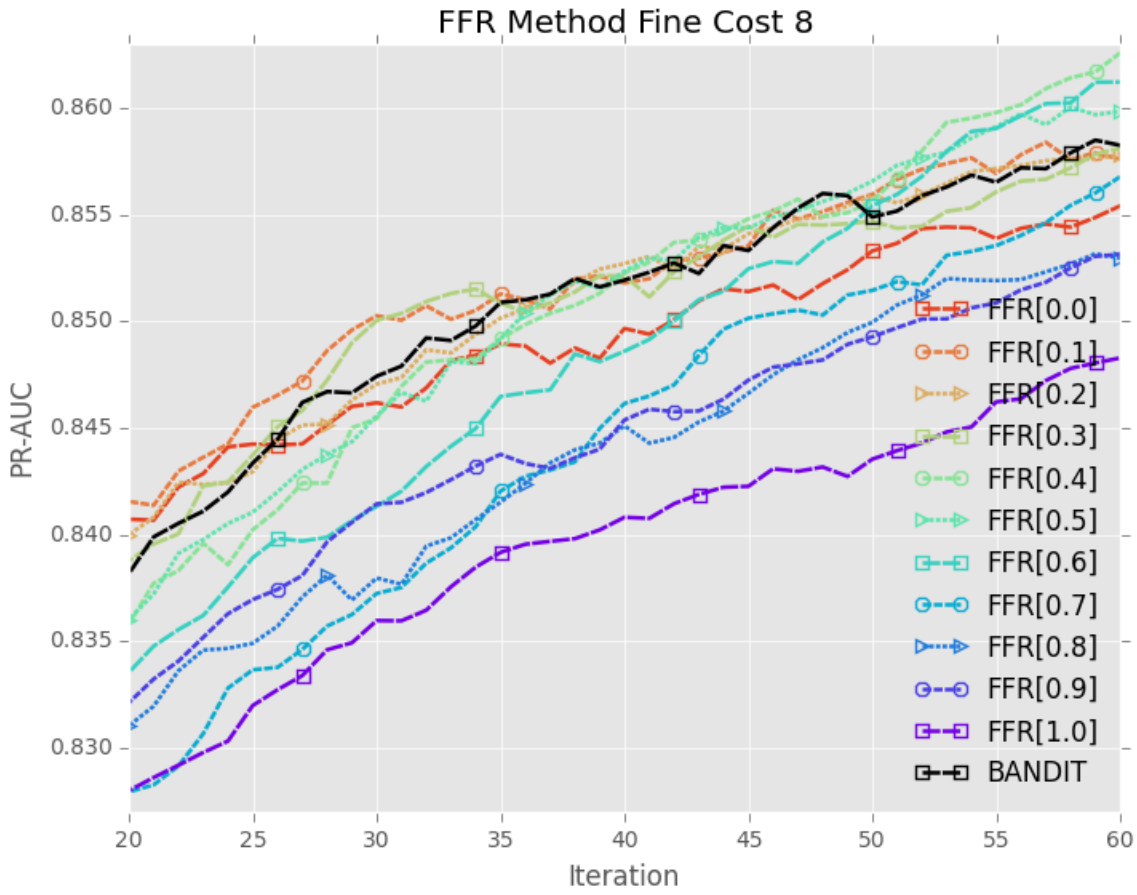
Varying Budget Analysis - Mixed Cost



~~Figure: BANDIT mixed fine cost plot.~~

BANDIT Approach Results

BANDIT - Rnds 20 to 60



~~Figure: The fine cost 8 curves shown expanding the rounds 20-60. With the BANDIT approach plotted~~.

Conclusions

- Demonstrated fine-grained labels can be used to improve a coarse-grained classifier for the protein dataset
- Demonstrated a prominent advantage for active fine with the Logit classifier
- HAL is implemented and applied to the protein dataset for various FFR proportions and fine label costs
- The BANDIT approach is shown to be robust to both labeling cost and budget

Future Work

- Future work is to apply the active over-labeling approach to other datasets with more complex hierarchical label trees; datasets derived from Gene Ontology research could be investigated

Questions

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- etc.

Active vs. Passive Curve Analysis

Logit Accuracy

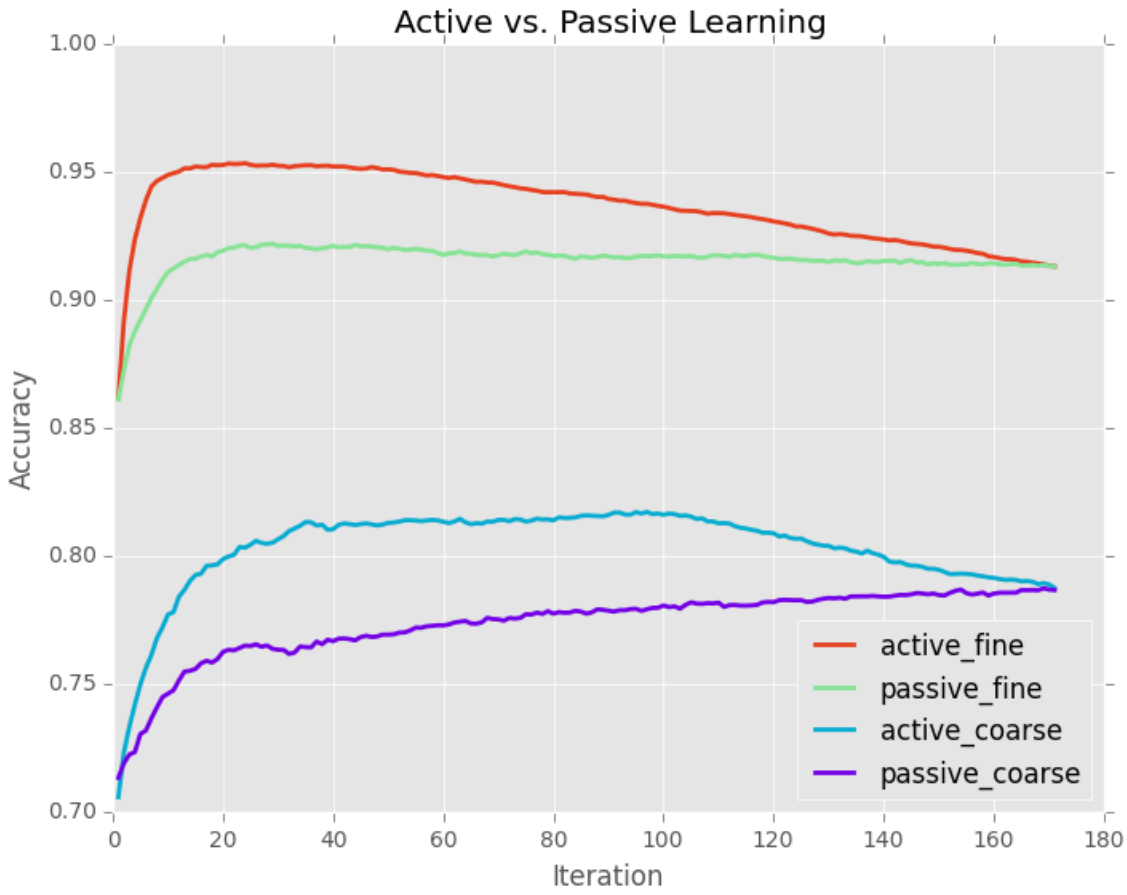

Figure: The accuracy of the classifiers stays at roughly the same rate throughout the rounds; this is due to an effective weighting scheme.

Active vs. Passive Curve Analysis

Logit F-measure

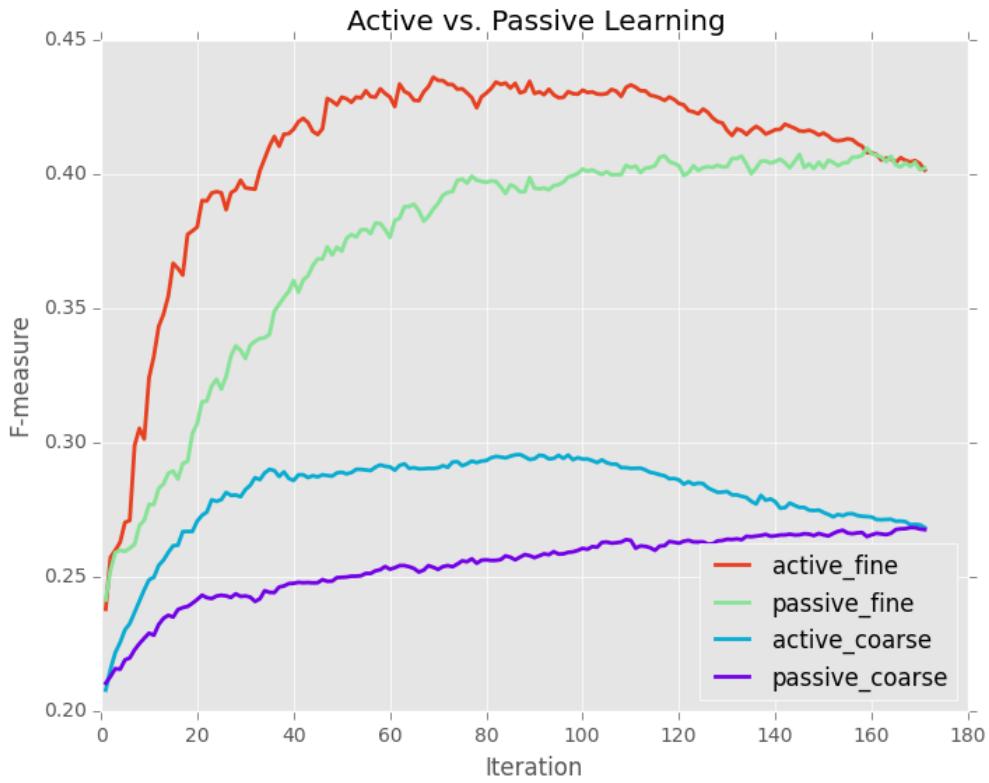

Figure: Both curves show a dominance of fine over coarse and Active over Passive.