EXPLOITING DOMAIN STRUCTURE WITH HYBRID GENERATIVE-DISCRIMINATIVE MODELS

by

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THESIS ABSTRACT

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Machine learning methods often face a tradeoff between the accuracy of discriminative models and the lower sample complexity of their generative counterparts. This inspires a need for hybrid methods. In this paper we present the graphical ensemble classifier (GEC), a novel combination of logistic regression and naive Bayes. By partitioning the feature space based on known independence structure, GEC is able to handle datasets with a diverse set of features and achieve higher accuracy than a purely discriminative model from less training data. In addition to describing the theoretical basis of our model, we show the practical effectiveness on artificial data, along with the 20-newsgroups, MNIST, and MediFor datasets.

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CHAPTER I

INTRODUCTION

Machine learning tasks often involve incorporating information from a variety of sources. For example, it is useful to consider network status information along with email text when attempting to identify spam emails, or to incorporate pixel information and metadata such as a photo's caption or the user's information when searching for falsified or inappropriate images that have been posted on social media. A common approach to integrating these different feature types into one machine learning system is to build complex data pipelines and custom infrastructure for the given dataset (Sculley et al., 2011). Such methods are often well tailored to the problem at hand but do not generalize well to changes in the input feature relationships or different datasets, which can lead to large overhead as code needs to be reorganized for new use over time (Sculley, Holt, Golovin, Davydov, & Phillips, 2015).

In this paper, we present a general framework which can be used to efficiently and effectively integrate domain structure for use with arbitrary classification tasks. Our key observation into this problem is that multi-modal feature spaces create an inherent independence structure. In particular, given a task with a known feature independence structure, we propose the graphical ensemble classifier (GEC), which leverages those independences in order to train smaller models, each over a subset of the original feature space.

As inspiration for the GEC design we look to a simple setting: logistic regression (LR) and naive Bayes (NB). These classic models form a well known generative-discriminative pair of probabilistic models. In particular, for a data set $X \in \mathbb{R}^{n \times m}$ with binary class labels Y, logistic regression discriminatively models the posterior distribution P(Y|X) by learning weights for each feature in X. Naive Bayes, on the other hand, attempts to estimate P(X, Y) under the assumption that the attributes in X are conditionally independent given the class label Y. Discriminative models are typically preferred because they tend to perform better at classification, but their generative counterparts reach asymptotic accuracy after seeing fewer training examples and thus can be useful when data is limited (Raina, Shen, Ng, & McCallum, 2003). The GEC framework that we present represents a class of models which span the space between purely generative and purely discriminative form depending on the true independence structure of the feature space.

Our method has a variety of useful properties. Firstly, it is a linear combination of traditional models, making it simple to implement. Additionally, it is not limited to problems with multi-modal feature spaces; it conveniently generalizes to any task where independence structure between the features is known or can be well approximated. We also explore a variant based on creating an ensemble over randomized partitions for situations where domain knowledge of the feature space is unknown. Finally, we note that because of the hybrid nature of the GEC model, it will have a lower sample complexity than a strictly discriminative method would without sacrificing accuracy (given a perfect partitioning). This makes it particularly useful in domains where the amount of training data is low. As a real-world example, we apply GEC to the DARPA Media Forensics (MediFor) project dataset. The MediFor project aims to create a state-of-the-art, robust system for detecting if alterations have been made to images. Teams from across the country have developed algorithms, each tuned to detect a subset of possible manipulations; our contribution in this paper is using the GEC framework to synthesize the predictions of those models to create a system capable of detecting the full set of manipulations.

The rest of our paper is laid out as follows: In Chapter II we detail related work on combining generative and discriminative models and other ensemble methods. In Chapter III we go on to describe the framework of the classification problem at hand and introduce our novel model in the context of clique trees. In Chapter IV we present results on a synthetic dataset, followed by results on the 20-newsgroup, MNIST, and MediFor datasets showing the real-world applicability and usefulness of our method, before making final conclusions and future remarks in Chapter V.

CHAPTER II

RELATED WORK

The relationship between the asymptotic accuracy and sample complexity of generative and discriminative models was explored in the seminal paper by Ng and Jordan (Ng & Jordan, 2001), who showed that while discriminative models typically out-perform generative ones, the opposite is true when training data is limited. Later work has attempted to bridge this learning gap between generative and discriminative models in a variety of ways (Chang, Yih, & Meek, 2008; Hinton, 2002; Kittler, Hatef, Duin, & Matas, 1998; Raina et al., 2003; Webb, Boughton, Zheng, Ting, & Salem, 2010). For example, in (Raina et al., 2003) Raina et. al. present an algorithm for text classification which trains individual naive Bayes models for each section of the corpus and then combines the predictions of each sub-model using discriminatively learned weights.

The work which is perhaps most closely related to ours is (Chang et al., 2008). They propose a model called partitioned logistic regression (PLR) which combines the predictions of multiple logistic regression classifiers, each trained over an independent subset of the features, using principles of naive Bayes. Their method achieves greater accuracy than either logistic regression or naive Bayes across a varying number of training examples, and continues to perform surprisingly well even when their total independence assumption is weakened. In this paper, we expand their model to explicitly account for some known dependence between partitions, which we expect will allow for even better performance. Further, our model can be applied to a much wider class of problems as we are not limited to the case where features can be neatly partitioned into unrelated sets.

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We also note that our approach has strong connections to dropout (Srivastava, Hinton, Krizhevsky, Sutskever, & Salakhutdinov, 2014). Dropout was presented by Hinton et al. (2014) as a method of increasing the generalizability of deep neural networks, wherein nodes within the neural network are randomly omitted during training (Srivastava et al., 2014). Many papers have gone on to use and explore variations of dropout, including by characterizing dropout as a form of regularization and expanding the method to apply to other models such as logistic regression and support vector machines (Ba & Frey, 2013; Chen, Zhu, Chen, & Zhang, 2014; van der Maaten, Chen, Tyree, & Weinberger, 2013; Wager, Fithian, Wang, & Liang, 2014; Wager, Wang, & Liang, 2013). However, little work has been done exploring the space of dropout where nodes are omitted non-randomly or the connections between dropout and ensemble methods. We argue that the GEC method may be thought of as a Bayesian approach to dropout, aimed at preserving sets of features based on their informativeness.

CHAPTER III

METHODOLOGY

We begin this chapter by briefly defining clique trees in the context of graphical models and go on to present our *graphical ensemble classifier* (GEC) framework which uses clique tree inference over subsets of features to create a general and statistically efficient approach to data classification.

Clique Trees

As a tool for modeling the relationship between features, we look to Markov networks. Let X be a set of continuous or binary random variables, X_1, X_2, \ldots, X_n , with categorical class labels Y. A Markov network (MN), or Markov random field (MRF), is an undirected graph G = (V, E) where each node V represents a feature (Koller & Friedman, 2009). Pairs of features (v_i, v_j) in a MN are dependent if there exists an edge e_{ij} between them and are conditionally independent given a path of edges between them. MNs are thus a useful framework for describing dependence between features in a dataset.

For the remainder of this paper, we will limit ourselves to considering datasets with feature dependence structure described by MRFs which have tree structure: clique trees. A clique tree H over the feature space of $X \in \mathbb{R}^n$ is an undirected, singly-connected graph satisfying the following properties:

- 1. each node *i* in *H* is labeled with a clique of variables, $C_i \subset X$,
- 2. each variable $x_i \in X$ appears in at least one clique, and
- 3. if x_i appears in two cliques, C_i and C_j in the tree, it must also appear on all nodes in between them

(Koller & Friedman, 2009). Conveniently, clique trees have the property that they can be factorized to define the probability distribution:

$$P(X) = \frac{\prod_{c \in C} P(X_c)}{\prod_{s \in S} P(X_s)}$$
(3.1)

for a tree with cliques C and separator sets S (Koller & Friedman, 2009). Limiting our dependence graph to clique trees in this way ensures that we can do exact inference efficiently. However, this work can theoretically be expanded to include arbitrary independence graph structure if some approximations are introduced.

Graphical Ensemble Classifier (GEC)

Using clique trees as our underlying graphical model for describing feature independence structure allows us to handle overlapping groups of variables, for we can then factorize the learning problem according to the factorization of the given clique tree. In particular, let $X \in \mathbb{R}^{n \times D}$ be a dataset with binary class labels $Y \in [0,1]^n$. Let the feature space of X satisfy a clique tree independence structure with cliques C and overlapping (separator) sets S. If X_c represents the data with features limited to those present in the clique $c \in C$ (or X_s for separator $s \in S$), then we have that:

$$P(X) = \frac{\prod_{c \in C} P(X_c)}{\prod_{s \in S} P(X_s)}.$$
(3.2)

For classification problems, we are interested in the discriminative task of predicting P(Y|X). Conditioning the above equation on the class label Y and applying Bayes' rule we obtain that:

$$P(Y|X) \propto P(X|Y)P(Y)$$

$$= \frac{\prod_{c \in C} P(X_c|Y)}{\prod_{s \in S} P(X_s|Y)}P(Y)$$

$$\propto \frac{\prod_{c \in C} P(Y|X_c)/P(Y)}{\prod_{s \in S} P(Y|X_s)/P(Y)}P(Y)$$

$$= \frac{\prod_{c \in C} P(Y|X_c)}{\prod_{s \in S} P(Y|X_s)}P(Y)^{1+|S|-|C|}$$
(3.3)

Using eq. (3.3), we fit linear sub-models $P(Y|X_c)$ and $P(Y|X_s)$ for each partition X_c and each overlapping set X_s , respectively.

The result is the GEC model. Given model weights W_c and W_s trained over each clique c and separator set s, respectively, we have that the log odds are:

$$\hat{lo}(X) = \sum_{c \in C} W_c \cdot X_c - \sum_{s \in S} W_s \cdot X_s$$
$$+ (1 - |C| + |S|) \log \hat{o}$$
(3.4)

where $\hat{o} = \hat{P}(Y=1)/\hat{P}(Y=0)$ is the prior odds.

Relation to Existing Models. To put this into context, we note three interesting cases of this model:

- 1. If there is only one partition so that |C| = 1 and $X_1 = X$, then $S = \emptyset$ and eq. (3.3) trivially reduces to classic logistic regression.
- 2. If each partition X_i contains exactly one variable, then again $S = \emptyset$, |C| = nand $X_i = x_i$ for all $0 < i \le n$. Hence, eq. (3.3) reduces to:

$$P(Y|X) \propto P(Y) \prod_{x_i \in X} \frac{P(Y|x_i)}{P(Y)}$$
$$= P(Y) \prod_{\substack{x_i \in X \\ 8}} P(x_i|Y),$$

which is simply naive Bayes.

3. If the X_C sets consist of a partition into k non-overlapping sets, then the equation reduces to:

$$P(Y|X) \propto P(Y) \prod_{i=1}^{k} \frac{P(Y|X_i)}{P(Y)}$$
$$= P(Y)^{1-k} \prod_{i=1}^{k} P(Y|X_i),$$

which is the case of this problem handled by PLR (Chang et al., 2008).

Thus, depending on the nature of the underlying feature dependencies, the GEC model spans the space between being a generative and being a discriminative model, along with successfully encompassing a broad class of models.

Randomized GEC

While the above GEC framework is especially useful in a setting wherein the feature relationships are known, such information is often not known in practice. Inspired by the success of ensemble methods, we show that even when little to no structure is known, it is possible to leverage ensembles of randomly partitioned features and obtain accurate results without overfitting.

To accomplish this, we propose randomized GEC (Rand-GEC). Since no groupings are known or present, we instead randomly group features into k non-overlapping sets of equal size and run GEC on those random partitions. We then average the results over s such random groups to reduce bias. The procedure is described in Alg. 1.

Algorithm 1 Randomized GEC

1: **procedure** RANDGEC(N, d, k, s)

2: Given data $X \in [0, 1]^{(N,d)}$.

3: **for** trial $t \in \{1, ..., s\}$ **do**

4: Partition d features into k random groups, f_1, \ldots, f_k .

5: Train LR models M_{f_1}, \ldots, M_{f_k} .

6: Sum weights of sub-models using eq. (3.4) to make predictions on test set.

- 7: Calculate test accuracy.
- 8: end for
- 9: Average accuracy of s trials.
- 10: end procedure

CHAPTER IV

RESULTS AND ANALYSIS

To display the capabilities of the graphical ensemble classifier, we present results on artificial data, 20-newsgroups, MNIST, and our Media Forensics (MediFor) dataset. In each case we compare the accuracy of Bernoulli naive Bayes (NB), logistic regression (LR), partitioned logistic regression (PLR), graphical ensemble classifier (GEC), and randomized-GEC as a function of the number of training examples. Since GEC is designed specifically to break the independence assumption of PLR, we additionally consider a model (PLR-split) which takes the set of dependent features and divides them randomly between partitions so as not to count them twice.

Artificial data

In this section we present results and analysis of the GEC model on an artificial dataset. We first describe the process we use to generate this data and then go on to show results on that artificial data.

Data Generation. Since our model assumes known clique tree structure over features, we create an artificial dataset to test the GEC model under a controlled setting where the data's feature independence structure is known and controllable. Our artificial data generation ensures that we can purposefully vary the feature independence tree and amount of dependence between partitions. We base this generation process on the methodology presented in (Chang et al., 2008). Let $Y \in \{0, 1\}$ be the class label of a random example $X \in \{0, 1\}^d$. For a given number of partitions k we generate random examples X using:

$$Y \sim \text{Bernoulli}(0.5)$$

$$\hat{X} = (\hat{X}_1, \dots, \hat{X}_k) \sim N(\vec{\mu}_y, \Sigma_y)$$
$$X = (X_1, \dots, X_k) = \left(f(\hat{X}_1), \dots, f(\hat{X}_k)\right)$$

such that $N(\vec{\mu}_y, \Sigma_y)$ is a multivariate normal with parameters based on the class label $y \in Y$. In particular, $\vec{\mu}_0 = \{-\sqrt{d}\}^d$ and $\vec{\mu}_1 = \{\sqrt{d}\}^d$. To simulate kindependent partitions, we generate each Σ_y by first creating a Gram matrix G_y and then zeroing out the covariance terms between the classes, as described below. For example, when k = 2:

$$G_y = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \text{ becomes } \Sigma_y = \begin{bmatrix} A & 0 \\ 0 & C \end{bmatrix}$$

This process ensures that variables from each partition X_i are independent from variables in different partitions X_j for $i \neq j$.

Each Gram matrix G_y is formed from k * d vectors of size 10 with entries drawn uniformly at random between -1 and 1. After zeroing out the covariance terms, this creates a unique, positive semi-definite $d \times d$ covariance matrix for each class label, which we use in the generation of $\hat{X} \sim N(\vec{\mu}_y, \Sigma_y)$.

After generating \hat{X} using the process described above, we expand the real valued samples from \hat{X} into a binary representation. Using a sign bit and the bits corresponding to 2^2 , 2^1 , 2^0 , 2^{-1} , and 2^{-2} we obtain the expanded samples $X = (X_1, \ldots, X_k)$ of size 6n. This expansion process makes some features more informative than others. We use $f(\hat{X}_i)$ to denote this expanded set of features.

The above process results in a dataset consisting of k independent partitions, and mirrors the data generation process presented in (Chang et



Figure 1. A visual representation of the process of creating the overlapping sets in the artificial data generation process, where the size of overlapping sets, o, is 1. In this case, the model has k = 3 partitions (X_1, X_2, X_3) over 3 features each and ends up with two separator set models (X_{12}, X_{13}) over o = 1 feature each.

al., 2008). We introduce a final step in the data generation to create a chain structure of dependence between the partitions. For each original pair of partitions (X_i, X_{i+1}) we pair o features from each and create dependence between them. Concretely, let $x_j^{(i)}$ denote the jth element in partition i. Then, we pair sets $O_i = \{x_{6n-o}^i, \ldots, x_{6n}^i\} \subset X_i$ and $O_{i+1} = \{x_1^{(i+1)}, x_2^{(i+1)}, \ldots, x_o^{(i+1)}\} \subset X_{i+1}$, to create the overlapping partition $X_{i(i+1)}$ where each element $x_j^{i(i+1)}$ is the maximum of the jth elements of O_i and O_{i+1} . This process is visually depicted in Fig. 1 for clarity. This allows us to control the level of dependence between partitions, varying from complete independence (o = 0) to full overlap (o = d).

For each experiment we run 5-fold cross validation on the training data in order to choose the ℓ_2 -regularization constant, C, for logistic regression. For simplicity, we choose $C \in [0.01, 0.1, 1, 10, 100]$ to be the same for each sub-model of a given model. (In preliminary experiments, we find that the results are not very sensitive to this tuning process.) For the randomized splits, we randomly divide features into k groups and average the results over s of these random splits to reduce bias. Results are averaged over 10 random datasets, with randomized groupings additionally averaged over s = 3 random splits per dataset.

Artificial Results. Our first experimental setting is designed to compare the effectiveness of GEC and PLR when there are known groups and some overlap (Fig. 2). In the case of no overlap (Fig. 2a), we observe as expected that PLR, PLR-Split, and GEC are all equivalent and significantly out-perform the other models in most cases. As the amount of dependence between the two groups increases (Figs. 2b, 2c, 2d), we see that PLR does not remain as competitive. Interestingly, PLR-split continues to succeed, particularly in the mid-range of number of training examples. However, in nearly all cases our GEC method obtains higher accuracy on held-out test data after seeing enough examples.

Next, we analyze the impact of the number of random partitions, k, on accuracy when an underlying group structure is not present. Fig. 3 shows a heatmap of accuracy for training set size versus number of partitions, k. Results are again averaged over 10 random datasets of dimension d = 600 with no forced independence structure (one group). Each model is averaged over 3 random groupings. It is clear from this figure that given enough training data, logistic regression (1 group) is the superior choice. When the number of training examples gets smaller ($\sim 100 - 1500$), it becomes progressively better to use larger numbers of partitions. This reflects the notion that logistic regression over n features needs O(n) samples to converge to asymptotic accuracy (Ng & Jordan, 2001); splitting into more groups allows each partition to be over a smaller number of features, decreasing the effective sample complexity to O(n/k) for each partition.

20 Newsgroups

The 20-newsgroups text dataset, as used in (Wang & Manning, 2012), consists of thousands of text documents relating to 20 different topic groups. We consider the task of distinguishing the topic pairs *alt.atheism* versus *soc.religion.christianity*, *rec.sport.hockey* versus *rec.sport.baseball*, and *comp.windows.x* versus *comp.graphics*. Since this text data has no particular natural grouping, we choose to group words by their parts of speech for PLR. We



Figure 2. Accuracy versus number of training examples on artificial data for varying dependence between groups on a semi-log scale. Each partition originally contains d = 240 features. From top left to bottom right, the number of dependent features: (a) 0, (b) 60, (c) 120, (d) 180.



Figure 3. Heatmap comparing accuracy of number of random splits for varying number of training examples on artificial data with d = 600 features.

only consider randomized GEC for this set of experiments, and omit PLR-split since there is no overlap in part of speech tagging.

In Fig. 4 we select the top 3000 most common words in the given training set as features and average all results over 10 random train-test splits. An important takeaway from this set of figures is that the answer of which model is best is very dependent on the data. Looking at Fig. 4a, *alt.atheism* versus *soc.religion.christianity*, we observe that using smaller numbers of groups is preferable to using more groups, but in Fig. 4b, *rec.sport.hockey* versus *rec.sport.baseball*, we see the opposite trend. The reasoning behind this stark difference comes from the fact that the task of differentiating the topics atheism and Christianity is harder than of hockey and baseball, as seen in an about 10% lower accuracy for the former. Some of the most common words for atheism versus Christianity include "god" and "believe," which on their own do not give much information to distinguish between the categories. For hockey and baseball,



Figure 4. Accuracy versus number of training examples on the 20-newsgroups data. Newsgroup pairings from left to right: (a) *alt.atheism* versus *soc.religion.christianity*, (b) *rec.sport.hockey* versus *rec.sport.baseball*, (c) *comp.windows.x* versus *comp.graphics*.

however, standalone words such as "pitcher" for baseball or "goalie" for hockey can alone be strong evidence for classification. Datasets which require modeling of more complex relationships between features will often see better results with smaller numbers of groups, so that those interactions are not lost. It is thus important to be aware of the expected properties of a dataset before choosing what number of random GEC groups to use.

MNIST

Next, we explore the classic hand-written digit recognition task, MNIST (LeCun, Bottou, Benigo, & Haffner, 1998). The MNIST dataset consists of 60000 training examples of black-and-white hand-written digits 1-9, sized to 28x28 pixels each. For our experiments, we consider the binary task of differentiating two given numbers. We choose the pair4&9, which is classically more difficult to differentiate than most other pairs due to the visual similarity of the two numbers. Our hypothesis for this dataset is that partitioning the image into smaller regions will allow our model to out-perform logistic regression. Since the numbers are centered in each image, we focus on the middle region as our overlapping set. We consider three different partitioning schemes: focal, diagonal, and 9-grid, as depicted in Fig. 5.

An interesting point in the results of Fig. 6 is that PLR does not get much higher accuracy than random splits into a few groups, and GEC does worse than either. This indicates that in many cases it is better to use a series or random groups than to attempt to use this method with a poorly designed group.

MediFor

The Media Forensics (MediFor) project is an ongoing effort into improving our capability and accuracy at detecting if manipulations have been made to images. This issue has become of critical importance over the past few years as



Figure 5. Visual representation of partition schemes used for PLR and GEC on MNIST dataset. From left to right: focal, diagonal, and 9-grid.



Figure 6. Accuracy versus number of training examples on MNIST data. Solid, dashed, and dotted lines represent focal, diagonal, and grid groupings, respectively.

social media has become increasingly prevalent and influential across the world, making it easier to spread false information and images. The MediFor project consists of a group of industry and university teams who have been independently developing methods for detecting certain image manipulations, such as crops, recaptures, blurs, and splices. Rather than develop another algorithm for directly detecting alterations, we are interested in the task of synthesizing the outputs of the existing algorithms, with the hope of getting better overall accuracy than any individual algorithm. We thus create a dataset whose features are the output confidence scores of each algorithm for the given image. Since our inputs are the outputs of each algorithm, we then group features using domain knowledge of algorithm similarity.

Since current information about each algorithm is limited, we have manually chosen a sequence of groupings to represent a variety of possible relationships between the algorithms. We begin with each algorithm in it's own group (equivalent to naive Bayes) and sequentially choose the two most similar groups to merge until all of the algorithms make up one group (equivalent to logistic regression). The hierarchy of groupings we have chosen are displayed in the dendrogram in Fig. 7.

In Fig. 8 we present results of accuracy and area under the receiver operating characteristic curve (AUC ROC) as we increase number of partitions (following the groupings described in the dendrogram) when training on 20% and 80% of the dataset. As before, random groupings are averaged over 5 trials, and all values represent an average over 5-fold cross validation.

In this setup we find that logistic regression (one group) is the best option for this task, with accuracy dropping off as we increase the number of groups. We can also see that the partitions made manually with knowledge of algorithm similarity achieve higher accuracy and AUC ROC than random partitions do. These two observations both indicate that using the relationships between the algorithms is a better approach than assuming that they are all independent.



Figure 7. Dendrogram describing groupings chosen for MediFor dataset.



Figure 8. Accuracy and AUC ROC versus number of groups when training on 20% and 80% of the MediFor data. Green lines represent manual partitions based on domain knowledge, and red lines represent random groupings. From left to right: (a) accuracy, (b) AUC ROC.

CHAPTER V

CONCLUSION

In this paper we presented the graphical ensemble classifier as a hybrid between logistic regression and naive Bayes and showed that it can obtain higher accuracy than baseline methods when an overlapping set structure is present in the data. In addition to requiring less data to fit an accurate model, GEC is simple to implement, for it is a simple linear combination of traditional logistic regression models. This means that it can be applied to a wide range of datasets with low implementation overhead. We believe that this method shows promise and may be of use with datasets where structured domain information is known.

It should be noted that GEC is very sensitive to the chosen partitioning, as seen in the 20-newsgroup and MediFor results. If a given grouping fails to capture key relationships in the features, the accuracy of GEC may decrease substantially as compared to a traditional logistic regression model. Averaging over models trained on random partitions (as in randomized GEC) is a simple and surprisingly effective method for counteracting that property, and is favorable to settling for one inaccurate partition. Nevertheless, our artificial data results indicate that using a proper grouping with GEC is more effective than random splits.

In future work, we hope to develop a strategy for automatically finding possible partitions based on feature correlations or other similarities. In addition, we aim to extend our method to accept different, non-linear underlying discriminative models, such as support vector machines or even feed-forward neural networks. The super-linear complexity of such models should mean that reducing the size of the feature space will allow for even greater accuracy gains than we see with logistic regression.

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