Scalable Multilabel Prediction via Randomized Methods

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Abstract
Modeling the dependence between outputs is a fundamental challenge in multilabel classification. In this work we show that a generic regularized nonlinearity mapping independent predictions to joint predictions is sufficient to achieve state-of-the-art performance on a variety of benchmark problems. Crucially, we compute the joint predictions without ever obtaining any independent predictions, while incorporating low-rank and smoothness regularization. We achieve this by leveraging randomized algorithms for matrix decomposition and kernel approximation. Furthermore, our techniques are applicable to the multiclass setting. We apply our method to a variety of multiclass and multilabel data sets, obtaining state-of-the-art results.

1. Introduction
In multilabel classification the learner is given an example and is asked to output a subset of the labels that are relevant for that example. Multilabel problems come up often in web applications where data of interest may be tagged with zero or more tags representing, for example, the objects in an image, the topics of a news story, or the relevant hashtags of a tweet. A simple approach to multilabel prediction is to learn one classifier per label and predict each label independently. Why should we expect that we can improve upon this procedure? One answer is because in many real world multilabel problems the labels are correlated. A blog post about cooking has a higher chance of also being related to nutrition than to finance.

In this paper we propose a simple and efficient technique for multilabel classification, in which the dependencies between predictions are modeled with a flexible link function. This corresponds to the rich literature of using a stacking architecture (Wolpert, 1992) in the multilabel context to combine independent predictions to produce a joint prediction (Godbole & Sarawagi, 2004). However, many modern multilabel (and multiclass) problems are characterized by increasingly large output spaces. Such large output spaces present both computational and statistical challenges. The former is easily understood: a straightforward approach will scale at least linearly with the number of outputs both during training and inference. The latter also presents several challenges: naive models can have too many parameters, while certain labels and features can be extremely rare. Predicting each label must therefore borrow strength from other labels to avoid overfitting.

Our approach to mitigating statistical difficulties is via regularization; specifically we are interested in enforcing both low-rank and smoothness. To mitigate the computational burden of this regularization, we leverage randomized algorithms for embedding (Mineiro & Karampatziakis, 2014) and kernel approximation (Rahimi & Recht, 2007). Fortunately, these procedures can be combined in a manner which avoids expensive intermediates and scales to the largest public benchmark data sets. The technique also applies to multiclass classification, which is just a special case of multilabel prediction where exactly one of the labels must be output. To illustrate this our experiments include both multilabel and multiclass data.

In the rest of the paper we overview a randomized algorithm for embedding (Section 2), we introduce our technique as fitting a flexible link function (Section 3), and we argue that statistical (Section 4) and computational (Section 5) improvements are possible if we use randomized embedding on the inputs to the link function. We present related work on Section 6 and experiments on Section 7.

2. Background and Notation
Here we will introduce notation and review randomized embedding, a technique we leverage and adapt in the sequel. For additional background on randomized linear algebra, we refer the reader to (Halko et al., 2011).

2.1. Notation
Vectors are denoted by lowercase letters $x$, $y$ etc. and matrices by uppercase letters $W$, $Z$ etc. We are given $n$ examples as matrices $X \in \mathbb{R}^{n \times d}$ and $Y \in \mathbb{R}^{n \times c}$. We assume
Algorithm 1 Randomized Embedding

1: **Input:** $X, Y, k, \ell, q$
2: $Q \leftarrow \text{randn}(c, k + \ell)$
3: for $i \in \{1, \ldots, q\}$ do
   4: $Z \leftarrow \arg \min_{Z \in \mathbb{R}^{d \times (k+i)}} \|YQ - XZ\|_F^2.$
   5: $Q \leftarrow \text{orthogonalize}(Y^T X Z)$
5: end for
6: $F \leftarrow (Y^T X Q)^T (Y^T X Q)$
7: $(\hat{U}, \Sigma^2) \leftarrow \text{eig}(F, k)$
8: $U \leftarrow Q \hat{U}$
9: Return $U$

that the labels $Y$ are sparse: each example is typically associated with only a handful of labels. We use $\|X\|_F$ for the Frobenius norm, $E[\cdot]$ for the expectation operator.

2.2. Randomized Embedding

Algorithm 1 is a recipe for approximating, via randomized linear algebra techniques, the label projection matrix associated with the optimal rank-constrained least squares prediction of the labels given the features (Mineiro & Karampatziakis, 2014). The inputs are the data matrix $X \in \mathbb{R}^{n \times d}$, the label matrix $Y \in \mathbb{R}^{n \times c}$, the desired rank $k$, and hyperparameters $\ell$ and $q$. The algorithm is insensitive to the parameters $\ell$ and $q$ as long as they are large enough (in our experiments we use $\ell = 20$ and $q = 1$). We start with a set of $k + \ell$ random vectors and use them to probe the range of $Y^T \Pi_{X,L} Y$, where $\Pi_{X,L}$ is the projection onto the left singular subspace of the data matrix. We compute an orthogonal basis for the range and refine it by repeating $q$ times. This can also be thought as orthogonal (aka subspace) iteration for finding eigenvectors with early stopping (i.e., $q$ is small). Afterwards we use our approximation of the principal subspace to optimize fully over that subspace (lines 7 and 8) and back out the solution (line 9). These last few steps are cheap because we are only working with a $(k + \ell) \times (k + \ell)$ matrix, and in practice the most expensive step is the least squares fit to compute $Z$ (line 4). Note the least squares fit is a regression problem in $k + \ell$ outputs, independent of $c$, whose computation beneficially exploits the sparsity of $Y$.

Note once the label projection operator has been obtained, the feature projection operator can be computed with a final least squares fit using the projected labels as targets.

3. A Flexible Link Function

We begin with the premise that in many multilabel problems certain label combinations frequently co-occur. We would like to take advantage of such co-occurrence patterns, but we cannot jump directly into modeling the output space because the classifier can only reach that space through the features it uses. Therefore, we will try to model correlations among the predictions. The simplest way to do this is to introduce a link function as an operator that maps a vector of activations $p$ to a vector of predictions $\hat{y} = C p$. A very popular operator in the setting of multiclass classification is the softmax: $g(p) = \nabla \log \sum_y \exp(p_i)$. This is an oblivious operator whose effect is to boost the largest activation while ensuring the predictions form a probability distribution. In multilabel classification, we would like to introduce a non-oblivious operator, because we do not know a priori which labels frequently occur together.

A first possibility is a linear operator i.e. $C$ is a $c \times c$ matrix. A natural choice in this case is

$$C = \frac{1}{n} \sum_{i=1}^{n} y_i y_i^T$$

and with $g_0(p) = C p$ we see that the link function is taking a weighted combination of training labels weighted by the inner product between the activation and each label. Though intuitive, this link function does not do much: the predictions are a fixed linear transformation of the activations with no adjustable parameters. This can be easily fixed by introducing a non-negative scalar $\alpha_i$ for each label:

$$g_1(p) = \sum \alpha_i y_i y_i^T p,$$

so that labels with a large $\alpha_i$ influence the prediction more towards themselves. This link function is now evidently a linear kernel machine with $\alpha$ playing the role of dual variables. Our next step is to generalize the link function by replacing the inner product in input space with a kernel function, an inner product in a reproducing kernel Hilbert space:

$$g_2(p) = \sum \alpha_i y_i K(y_i, p).$$

In practice we will approximate the kernel function with a finite sum of basis elements. There are several techniques for doing this, including the Nyström method (Williams & Seeger, 2001), Incomplete Cholesky Factorization (Fine & Scheinberg, 2002), and Random Fourier Features (RFFs) (Rahimi & Recht, 2007). Here we will use RFFs which are especially easy to work with shift invariant kernels (i.e. $K(y, p) = \kappa(y - p)$) and have the advantage that they can be generated in an oblivious way, without knowing how the activations $p$ look like. This will prove important for the efficiency of the final algorithm.

Although it is not yet obvious, for our final algorithm we believe (and present some empirical justification) that shift-invariant kernels are broadly applicable in this context. Recall that applying $\ell_2$ regularization on a kernel machine with a shift-invariant kernel, such as the Gaussian kernel, is the same as penalizing the derivatives of all orders of the functions that the kernel machine can represent (Smola & Schölkopf, 1998). Such a smoothness prior is
very appropriate for our link function: we are applying kernels to the activations (or, later, to projected activations), not to the feature space.

Recall that for shift invariant kernels

$$K(y, p) \propto \mathbb{E}_{r \sim q \times U(0,2\pi)} \cos(r^T y + b) \cos(r^T p + b)$$

where the distribution $q$ depends on the kernel and $U(a, b)$ is the uniform distribution in $(a, b)$. Therefore we can approximate $g_2$ by

$$g_3(p) = \sum_{i=1}^{n} \alpha_i y_i \frac{1}{s} \sum_{j=1}^{s} \cos(r_j^T y_i + b_j) \cos(r_j^T p + b_j)$$

We now replace $\frac{1}{s} \sum_{i=1}^{s} \alpha_i y_i \cos(r_j^T y_i + b_j)$ by optimization variables $v_j$ and arrive at

$$g(p) \overset{\text{def}}{=} \sum_{j=1}^{n} v_j \cos(r_j^T p + b_j)$$

At this point we have the two-stage procedure outlined in Algorithm 2. For multilabel problems, the loss function in the final fit can be either least squares or the sum over classes of per-class logistic loss. The latter usually requires a smaller $s$ to attain the same result, while the former admits a fast fitting procedure (Vincent, 2014) that is independent of the size of the output as long as the output is sparse. As we argue in the next sections, Algorithm 2 is actually quite wasteful both statistically and computationally. In the following sections we will address these problems using randomized embedding.

### 4. Dealing with Statistical Issues

Though we started with assuming that certain combinations of labels (and activations) are more correlated than others we have not yet clarified what is the exact property we will be exploiting. Correlations between activations are captured in their empirical second moment and our assumption is that this matrix is low rank and therefore can be described by $k \ll c$ eigenvectors:

$$\mathbb{E}[pp^\top] \overset{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} p_i p_i^\top = \sum_{i=1}^{k} \lambda_i u_i u_i^\top.$$ Empirically we have found this assumption to hold for many multilabel problems. Furthermore, similar ideas, such as assuming that the second moment of the labels is low rank, have been employed in other techniques for multilabel problems, e.g., (Tai & Lin, 2012). The key benefit of using activations instead of labels is that our proposed method applies equally well to multiclass problems whereas the method of (Tai & Lin, 2012) would yield trivial results in the multiclass setting.

How can the procedure outlined in Algorithm 2 be improved by taking advantage of the fact that activations are low rank? When activations are nominally in $\mathbb{R}^c$ but really only span a smaller subspace of dimension $k$ then the kernel approximation employed in lines 3 and 4 of Algorithm 2 is very wasteful. To illustrate this point we will, for simplicity, focus on kernels that are not only shift invariant, but also rotationally invariant: $K(p, p') = \kappa(||p - p'||_2)$. If $p, p'$ only span a space of dimension $k$ then there exists a $k \times c$ matrix $U$ such that $||p - p'||_2 = ||U^\top p - U^\top p'||_2$. Moreover the matrix $U$ is given by the top $k$ eigenvectors of $\mathbb{E}[pp^\top]$. We can therefore reduce the dimensionality of the activations $p$ with randomized embedding before applying our kernel approximation. This reduces the variance, or, alternatively, requires drawing fewer random vectors to achieve the same level of approximation.

Since each feature function is now computing $\cos(r_i^\top U^\top p + b)$ the random vectors that we use to project the activations are now $Ur_i$ with $r_i \in \mathbb{R}^k$. Furthermore, their covariance is equal to $U\Sigma U^\top$ with $\Sigma \in \mathbb{R}^{k \times k}$ being the covariance of the sampling distribution for $r_i$ (typically a multiple the identity). On the other hand, Bochner’s theorem tells us that there’s a one to one mapping from sampling distributions to positive definite shift invariant kernels. Therefore, projecting the activations is equivalent to tuning the kernel to the observed data.

### 5. Dealing with Computational Issues

There are three computational issues with the algorithm as proposed thus far. First we need to fit individual classifiers for each problem which can be very time consuming if the number of labels $c$ is large. Second, when $c$ is large forming the empirical second moment of the activations and computing the top eigenvectors might be infeasible. Third, the final optimization over the matrix $V$ still requires the solution of a large number of problems. Here we address all of them.

We start with the issue of fitting the $s \times c$ matrix $V$. One possibility is to treat each of the columns of $V$ in parallel as each of them can be learned independently: by this stage we have finished modeling dependencies among labels. For square loss we can alternatively use the recent technique of...
(Vincent, 2014) that shows how to perform stochastic gradient updates for least squares problems when the output is large but sparse. This method only requires \(O(s^2)\) computation instead of \(O(sc)\) where \(s\) is the number of basis functions (i.e., cosines) we use.

We tackle the other two issues together. Our key observation is that in order to run the algorithm we only need to have the projections of the activations. Surprisingly, for the case of linear (and kernel) classifiers it is possible to obtain these without fitting all individual classifiers, via the randomized embedding procedure previously introduced.

Algorithm 3 puts the above ingredients together. Lines 2 through 10 are randomized embedding, which approximates the label projection operator. The additional least squares fit of Line 11 yields the (approximate) feature projection operator. Lines 12 through 14 are algorithm 2, but applied in the low-dimensional space. In particular, each \(r_t \in \mathbb{R}^k\).

A few remarks are in order. For simplicity, we have specified \(k\) as a parameter but randomized embedding can also incorporate a strategy for increasing \(k\) if initial estimates of the captured variance are too low (Halko et al., 2011).

To improve generalization performance, we use a regularized least squares fit for the randomized embedding solves in lines 5 and 11 of Algorithm 3. Regularization is less crucial (and sometimes detrimental) for learning the final \(V\) matrix, but this is not surprising given the regularization inherent in the other aspects of the procedure.

Another (implicit) parameter of the algorithm is the sampling distribution of the vectors \(r_t\). This distribution defines the choice of shift invariant kernel we will be using to measure similarities between activations \(p\) and labels \(y\). Fortunately, we can offer some guidance here using the spectral properties of various shift-invariant kernels (see also (Le et al., 2013) for details). We recommend using Gaussian and Cauchy respectively for low and high dimensional \(y\). These are special cases of the multivariate Student distribution with \(\nu = \infty\) and \(\nu = 1\) degrees of freedom. Intermediate values such as \(\nu = 3\) and \(\nu = 5\) can offer better results for medium dimensional \(y\). The corresponding kernels are from the Matérn family. Some empirical support for their superiority on medium to high dimensional vectors is offered in (Le et al., 2013).

Algorithm 3 describes training but not inference. In practice we find Algorithm 3 can be used with multiple inference procedures if we use a proper scoring rule for equation (3), such as squared loss\(^1\), logistic loss (for multiclass), or sum over classes of per-class logistic loss (for multilabel). Inference can be per-example for example-averaged metrics such as Hamming loss or precision-at-\(k\), whereas \(^1\)This is a poor choice for data sets where some labels are rare.

### Algorithm 3: Multilabel via Smooth and Low-Rank Link

1. **Input:** \(X, Y, k, \lambda\)
2. \((\ell, q) \leftarrow (20, 1)\)
3. \(Q \leftarrow \text{randn}(c, k + \ell)\)
4. for \(i \in \{1, \ldots, q\} \) do
5. \(Z \leftarrow \arg\min_{Z \in \mathbb{R}^d \times (k + \ell)} ||YQ - XZ||^2_F + \lambda||Z||_F^2\)
6. \(Q \leftarrow \text{orthogonalize}(Y^T X Z)\)
7. end for
8. \(F \leftarrow (Y^T XQ)^\top (Y^T X Q)\)
9. \((U, \Sigma^2) \leftarrow \text{eig}(F, k)\)
10. \(U \leftarrow Q\Sigma^2\)
11. \(W = \arg\min_{W \in \mathbb{R}^d \times k} ||YU - XW||^2_F + \lambda||W||_F^2\)
12. Draw random vectors \(r_t\) and biases \(b_t\) \(t = 1, \ldots, s\)
13. Featurize projected predictions
   \[
   \phi_t(x_i) = \cos(r^\top_t W x_i + b_t)
   \]
14. Learn weight matrix
   \[
   V = \arg\min_{V \in \mathbb{R}^{c \times c}} \text{loss}(Y, \Phi(X)V) + \lambda||V||^2_F \quad \text{(3)}
   \]

### 6. Related Work

The algorithms presented here are examples of a stacking architecture (Wolpert, 1992), in which the predictions of (simpler) classifiers are used as input to another model which produces a (hopefully improved) joint prediction. In particular, the idea of combining independent predictions using stacking in the multilabel setting was proposed by (Godbole & Sarawagi, 2004), and has been thoroughly explored, e.g., (Montañoés et al., 2011; Nam et al., 2014; Read & Hollmén, 2015). Our contributions to this line of research are twofold. First, we empirically demonstrate that kernel machines, with shift invariant kernels approximated in the primal, provide an effective and computation-ally convenient choice for the final classifier. Second, we train our pipeline without fitting \(c\) independent classifiers as a first step.

Our technique can also be viewed as a calibration procedure, as the second stage is nothing but a link function mapping independent predictions to joint predictions. Many calibration procedures (Platt et al., 1999; Zadrozny & Elkan, 2001; Kakade et al., 2011) have focused on binary classification and they are now widely used in applications together with diagnostic tools such as calibration plots. Calibration for multiclass and multilabel classification has received little empirical attention. A notable exception for multiclass is (Zadrozny & Elkan, 2002).
which first produces calibrated probability estimates for induced binary problems and then combines these estimates to a final estimate of the posterior probability of each class. However, it is not clear how well calibrated the final multiclass estimates are. In high dimensions, given hardness results (Hazan & Kakade, 2012) and a lack of diagnostic tools, our approach follows a more pragmatic route: select a family of flexible link functions via a kernel machine parameterization, then learn an efficient approximation to a good link function in that family using random features.

The use of embeddings is pervasive in the multilabel literature, as it provides both computational and statistical benefits. (Weston et al., 2002) embed both features and labels into a common vector space, and use pre-image search for inference. Our procedure can be considered a more efficient analog of this where the search is approximated by inference. (Hsu et al., 2009), motivated by advances in compressed sensing, utilized a random embedding of the labels along with a sparse decoding strategy. Our embedding is not oblivious and takes into account both inputs and outputs, and in our experimental section we demonstrate a resulting improvement. (Bengio et al., 2010) combined a tree based decomposition with a low-dimensional label embedding, jointly learning both. End-to-end fine-tuning of our architecture is conceptually straightforward and plausibly useful, but this is outside the scope of this paper. The principal label space transform (PLST) (Tai & Lin, 2012) constructs a low-dimensional embedding using principal components on the empirical label covariance, which is then utilized along with a greedy sparse decoding strategy. Because it uses the empirical label covariance, PLST is not applicable to the multiclass setting.

The conditional principal label space transformation (CPLST), another dimensionality reduction approach to multilabel classification, has strong connections to our technique. In particular (Chen & Lin, 2012) initially SVD the same matrix as in algorithm 3, denoted here as $Y^T X Z^*$, albeit without leveraging randomized techniques. The similarities are intriguing given that CPLST is motivated by a bound on Hamming loss. However, CPLST solves an optimization problem which is designed to make an independent decode strategy effective, and apply kernelization to the feature space; whereas we learn a decoder and apply kernelization to the decoding problem, i.e., predictions. We attribute the broad applicability of shift-invariant kernels on the output to the shared statistical structure of multilabel problems encountered in practice, as opposed to the diverse statistical structure of features, e.g., sparse high-cardinality text vs. dense low-cardinality images. In other words, the choice of kernel in our procedure is greatly simplified.

Tree-based approaches are another major category of multilabel learning algorithms. Due to the richness of the literature, we refer the reader to a survey paper (Cerri et al., 2014). Here we discuss FastXML (Prabhu & Varma, 2014), a multilabel tree ensemble method for which we have direct experimental comparisons. FastXML makes several design choices to mitigate the computational expense of applying decision trees to high label cardinality (aka extreme) multilabel problems. In particular, FastXML partitions the feature space, in contrast to some approaches that partition the label space. Furthermore, FastXML also avoids solving an expensive label assignment problem at each node by using the union of the labels encountered in the training set (ordered by empirical frequency). This yields state of the art performance on multiple datasets when using a precision-at-$k$ metric.

### 7. Experiments

Unless otherwise indicated, confidence intervals on test set metrics are 90% confidence intervals and are estimated using the bootstrap (Efron & Tibshirani, 1994).

#### 7.1. Small Benchmark Datasets

We begin by demonstrating the effectiveness of the technique on several multilabel data sets from mulan.sourceforge.net (Tsoumakas et al., 2010), utilizing their train-test splits. Table 1 lists the details of these datasets, which span several application domains. All datasets are used as-is without preprocessing.

| DATASET   | DOMAIN | EXAMPLES | INPUTS | OUTPUTS |
|-----------|--------|----------|--------|---------|
| BIBTEX    | TEXT   | 7395     | 1836   | 159     |
| COREL5K   | IMAGE  | 5000     | 499    | 374     |
| MEDIAMILL | VIDEO  | 43K      | 120    | 101     |
| YEAST     | BIOLOGY| 2417     | 103    | 14      |
| INDUSTRIES| TEXT   | 23K      | 47K    | 354     |
| ODP       | TEXT   | 1.5M     | 0.5M   | 100K    |
| LSHTC     | TEXT   | 2.4M     | 1.6M   | 325K    |

We compare our approach with the best reported results from the multilabel survey paper of (Metz et al., 2015), which considered 1543 publications using the mulan datasets, disqualifying all but 64 for reasons such as duplicate papers with different titles, or using preprocessing which is not publicly available. We further confirmed that the best reported result from (Metz et al., 2015) was at least as good as the results reported for PLST and CPLST. The metrics we used are example-based Hamming Loss (HL) and label-based macro-averaged $F_1$ ($F_1^M$), defined in the standard way (Metz et al., 2015).
we compare against Lomtree (LT), which has 93.46 2014, 0.04 0.30 0.87 0.32 LT 0.01 2014 0.01 0.19 3 we conclude our T rather than the increased flexibility. Optimization for equation (3) was attained by Algorithm 3. In Table 3, ODP results. k = 300 for both embedding strategies.

Table 3. ODP results. k = 300 for both embedding strategies.

| METHOD          | ALG 3 | CS + LR | LT |
|-----------------|-------|---------|----|
| TEST ERROR (%)  | [83.21, 83.39] | [85.39, 85.56] | 93.46 |

be the case that we could have just obtained the same results by a much simpler method? Here we illustrate that simple methods such as blindly using a kernel (approximation) directly to the inputs and predicting the labels independently produce very different results than our judicious use of flexibility to model inter-label dependencies.

We focus on the RCV1 industries dataset that has a small training set, compared to its number of features. Based on this, we should expect that naive application of flexible modeling can lead to decreased generalization performance. Indeed, we performed three experiments: learn individual logistic regressions to predict each of the 354 categories, learn individual kernel logistic regressions with a Gaussian kernel approximation (the bandwidth was selected as in the previous experiments), and Algorithm 3 with squared loss for equation (3). The best test Hamming loss of 0.00159 was attained by Algorithm 3. Second was the independent logistic regression with a loss of 0.00163. Finally, learning independent kernel logistic regressions had a loss of 0.00193. Using the bootstrap, we obtained confidence intervals at most \( \pm 7 \cdot 10^{-6} \) so none of the confidence intervals overlap.

7.3. ODP

The Open Directory Project (DMOZ, 2014) is a public human-edited directory of the web which was processed by (Bennett & Nguyen, 2009) into a multiclass data set. Here we compare with (Choromanska & Langford, 2014), utilizing the same train-test split, features, and labels. Specifically there is a fixed train-test split of 2:1 for all experiments, the representation of document is a bag of words, and the unique class assignment for each document is the most specific category associated with the document.

Training was via Algorithm 3, with logistic loss used for equation (3). We used a linear kernel, i.e., in lieu of lines 12 and 13 we merely use the embedding directly for equation (3). Essentially this is rank-constrained logistic regression, i.e., we are only exploiting the regularization of Algorithm 3 rather than the increased flexibility. Optimization of equation (3) was via preconditioned SGD with momentum, introducing four additional optimization-related hyperparameters (learning rate, learning rate decay, momentum, and number of data set passes). The embedding dimension \( k \) was chosen to capture 90% of the empirical label covariance. All other hyperparameters were determined by extracting a 10% holdout set from the original training set and optimizing via random search (Bergstra & Bengio, 2012); once hyperparameters were determined a final assessment was done using the original train-test split. Note hyperparameters were tuned separately for each metric.

Inference is done per-example for Hamming Loss, and per-class for \( F_1^M \). Per-example inference merely thresholds the predicted probability of each class at 1/2. Per-class \( F_1 \) inference is described in Algorithm 4, which is a simplified version of the \( F_1 \) inference procedure in (Dembczynski et al., 2013). From Table 2 we conclude our approach is typically competitive with the best reported results and sometimes superior.

7.2. Is it Just About Flexibility?

Our approach seems to be working well in practice but a reasonable question at this point is where is the better performance stemming from? Since we have a two stage procedure with non-linear features at the second step, could it training was via Algorithm 3, with sum over classes of per-class logistic loss used for equation (3). We used a random feature approximation to a Gaussian kernel, introducing two additional hyperparameters (bandwidth and number of basis functions). Optimization of equation (3) was via preconditioned SGD with momentum, introducing four additional optimization-related hyperparameters (learning rate, learning rate decay, momentum, and number of data set passes). The embedding dimension \( k \) was chosen to capture 90% of the empirical label covariance. All other hyperparameters were determined by extracting a 10% holdout set from the original training set and optimizing via random search (Bergstra & Bengio, 2012); once hyperparameters were determined a final assessment was done using the original train-test split. Note hyperparameters were tuned separately for each metric.

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Algorithm 4 \( F_1 \) inference for a single class. \( \hat{Z} \) are the predicted label probabilities for the test set, and \( p \) is the empirical frequency of the label on the training set.

1. **Input:** \( \hat{Z}, p \)
2. Estimate number of positives: \( n_+ \leftarrow p|\hat{Z}| \)
3. Sort probabilities: \( \hat{Z}_{\text{sorted}} \leftarrow \text{sort}(\hat{Z}, \text{descend'}) \)
4. Estimate denom: \( r \leftarrow \{n_++1, \ldots, n_++|\hat{Z}_{\text{sorted}}|\} \)
5. Estimate \( f \): \( f \leftarrow 2 \text{cumsum}(\hat{Z}_{\text{sorted}})/r \)
6. Maximize estimate: \( m^* = \text{argmax} f \)
7. Threshold at \( m^* \): \( \hat{Y} \leftarrow (\hat{Z} \geq \hat{Z}_{\text{sorted}}(m^*)) \)
8. Return \( \hat{Y} \)

Table 2. Mulan Test Set Metrics

| METRIC | DATASET | SURVEY | THIS PAPER |
|--------|---------|--------|------------|
| HL (↓) | BIBTEX  | 0.01   | [0.0138, 0.0145] |
|        | COREL5K | 0.01   | [0.0102, 0.0106] |
|        | MEDIAMILL | 0.03   | [0.0310, 0.0316] |
|        | YEAST   | 0.30   | [0.212, 0.226] |
| \( F_1^M \) (↑) | BIBTEX  | 0.32   | [0.301, 0.333] |
|        | COREL5K | 0.04   | [0.0511, 0.0583] |
|        | MEDIAMILL | 0.19   | [0.238, 0.258] |
|        | YEAST   | 0.87   | [0.428, 0.450] |

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7.2. Is it Just About Flexibility?

Our approach seems to be working well in practice but a reasonable question at this point is where is the better performance stemming from? Since we have a two stage procedure with non-linear features at the second step, could it
training and test time complexity logarithmic in the number of classes (Choromanska & Langford, 2014). LT is provided by the Vowpal Wabbit (Langford, 2007) machine learning tool. We also compare against a compressed sensing analog of Algorithm 3 (CS + LR), where the matrix \( U \) computed in lines 2 through 10 is replaced by a Gaussian random matrix. Both variants of Algorithm 3 outperform Lomtree, which is unsurprising given Lomtree’s emphasis on computational complexity. Furthermore, there is a lift from using a tuned embedding instead of a random one.

To the best of our knowledge, this is the best published result on this dataset.

On a standard desktop\(^3\) it takes approximately 6000 seconds to compute the embedding (lines 2-11 of Algorithm 3), of which 3000 seconds is due to line 11 (which is also necessary with compressed sensing). Each data pass for optimizing equation (3) takes 1200 seconds, and validation error starts to turn up after 30 iterations.

7.4. LSHTC

The Large Scale Hierarchical Text Classification Challenge (version 4) was a public competition involving multilabel classification of documents into approximately 350,000 categories (Kaggle, 2014). The training examples and labels and the test examples are available from the Kaggle platform. The features are bag of words representations of each document.

Training was via Algorithm 3, with sum over classes of per-class logistic loss used for equation (3). We found Cauchy distributed random vectors, corresponding to the Laplacian kernel, gave good results. Optimization of equation (3) was via preconditioned SGD with momentum, introducing four additional optimization-related hyperparameters (learning rate, learning rate decay, momentum, and number of data set passes). The embedding dimension and other hyperparameters were tuned by hand, although we were ultimately limited by available memory on our standard desktop\(^2\), i.e., it appears a larger (than 800) embedding dimension and more (than 4000) basis functions would further improve results.

We used per-example inference, thresholding each classes predicted probability at 1/2. This produces poor results on macro-averaged F1, which is what the Kaggle oracle uses to evaluate submissions. However it does well on example-based metrics. We compare with published results of (Prabhu & Varma, 2014), who report example-averaged precision-at-\( k \) on the label ordering induced for each example. To facilitate comparison we do a 75:25 train-test split of the public training set, which is the same proportions as in their experiments (albeit a different split).

\[ \text{Table 4. LSHTC results.} \]

| METHOD | ALG 3 | FASTXML | LPSR-NB |
|--------|-------|----------|---------|
| TEST   | 53.39 | 49.78    | 27.91   |

Table 4 contains the results. LPSR-NB is the Label Partitioning by Sub-linear Ranking algorithm of (Weston et al., 2013) composed with a Naive Bayes base learner, as reported in (Prabhu & Varma, 2014), where they also introduce and report precision for the multilabel tree learning algorithm FastXML.

8. Conclusions

In this paper we have proposed a procedure for learning a flexible regularized link function for multilabel (as well as multiclass) problems. Our procedure empirically works better than many strong baselines and scales to large output spaces. Thus, similar to (Read & Hollmén, 2015), we conclude that simple label dependency models lead to state of the art computational and statistical performance.

In the future we plan to investigate the applicability and effectiveness of analogous procedures in more complex output spaces where the dependency structure of the output variables is specified by a graphical model.

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