Online MKL for Structured Prediction

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1 Introduction

Structured prediction (SP) problems are characterized by strong interdependence among the output variables, usually with sequential, graphical, or combinatorial structure [17, 7]. Obtaining good predictors often requires a large effort in feature/kernel design and tuning (usually done via cross-validation). Because discriminative training of structured predictors can be quite slow, especially in large scale settings, it is appealing to learn the kernel function simultaneously.

In multiple kernel learning (MKL, [8]), the kernel is learned as a linear combination of prespecified base kernels. This framework has been made scalable with the advent of wrapper-based methods, in which a standard learning problem (e.g., an SVM) is repeatedly solved in an inner loop up to a prescribed accuracy [14, 11, 6]. Unfortunately, extending such methods to large-scale SP raises practical hurdles: since the output space is large, so are the kernel matrices, and the number of support vectors; moreover, it becomes prohibitive to tackle the inner problem in its batch form, and one usually resorts to online algorithms [12, 3, 13]. The latter are fast learners but slow optimizers [2]; using them in the inner loop with early stopping may misguide the overall MKL optimization.

We propose instead a stand-alone online MKL algorithm which exploits the large-scale tradeoffs directly. The algorithm iterates between subgradient and proximal steps, and has important advantages: (i) it is simple, flexible, and compatible with sparse and non-sparse variants of MKL, (ii) it is adequate for SP, (iii) it offers regret, convergence, and generalization guarantees. Experimentally, the proposed algorithm yields near-optimal solutions faster than wrapper-based approaches (adapted to SP). We use the two following SP experimental testbeds: sequence labeling for handwritten text recognition, and natural language dependency parsing. The potential of our approach is shown in learning combinations of kernels from tens of thousands of training instances, with encouraging results in terms of speed, accuracy, and interpretability.

2 Structured Prediction (SP) and Multiple Kernel Learning (MKL)

In SP, to each input \( x \in \mathcal{X} \) corresponds a set of possible outputs, \( \mathcal{Y}(x) \subseteq \mathcal{Y} \); e.g., in sequence labeling, \( x \in \mathcal{X} \) is an observed sequence and \( y \in \mathcal{Y}(x) \) is a sequence of labels. Let \( \mathcal{U} \triangleq \{(x, y) \mid x \in \mathcal{X}, y \in \mathcal{Y}(x)\} \). Given a dataset \( \mathcal{D} \triangleq \{(x_1, y_1), \ldots, (x_N, y_N)\} \subseteq \mathcal{U} \), the goal is to learn a compatibility function \( f_\theta : \mathcal{U} \rightarrow \mathbb{R} \) whose maximization yields accurate predictions on new inputs, \( \hat{y}(x) = \arg\max_{y \in \mathcal{Y}(x)} f_\theta(x, y) \), according to some cost function \( \ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+ \). In this paper, we bring in the MKL framework [1, 8] and define

\[
\theta(x, y) \triangleq \langle \theta, \phi(x, y) \rangle_{\mathcal{H}} = \sum_{m=1}^{M} \langle \theta_m, \phi_m(x, y) \rangle_{\mathcal{H}_m},
\]

where \( \mathcal{H} = \bigoplus_{m=1}^{M} \mathcal{H}_m \) is a direct sum of RKHS, and \( \theta \) and \( \phi \) are block-structured (parameter and feature) vectors. Learning is carried out by minimizing the regularized empirical risk,

\[
\min_{f_\theta \in \mathcal{H}} \lambda \Omega[f_\theta] + \frac{1}{N} \sum_{i=1}^{N} L(f_\theta; x_i, y_i),
\]

where \( L \) is a convex loss (e.g., the structured SVM hinge loss, \( L(f_\theta; x, y) \triangleq \max_{y' \in \mathcal{Y}(x)} f_\theta(x, y') - f_\theta(x, y) + \ell(y', y) \)), \( \Omega : \mathcal{H} \rightarrow \mathbb{R}_+ \) is a regularizer, and \( \lambda \geq 0 \). Some examples are:
Algorithm 1 Online Proximal MKL

1: input: \(D\), kernels \(\{K_m\}_{m=1}^M\), regularizers \(\{\lambda_j \Omega_j\}_{j=1}^J\), number of rounds \(T\), sequence \((\eta_t)_{t=1}^T\)
2: Initialize \(\theta_1 = 0\); set \(N = |D|\)
3: for \(t = 1\) to \(T\) do
4: Take a training pair \((x_t, y_t)\) and obtain a subgradient \(g_{\theta_t} = \partial L(\theta_t; x_t, y_t)\)
5: Subgradient step: \(\tilde{\theta}_t = \theta_t - \eta_t g_{\theta_t}\)
6: for \(j = 1\) to \(J\) do
7: Proximal step: \(\theta_{t+J/j} = \text{prox}_{\eta_t \Omega_j}(\tilde{\theta}_{t+(j-1)/j})\)
8: end for
9: Projection step (optional): \(\theta_{t+1} = \tilde{\theta}_{t+1} : \min \{1, \gamma/\|\tilde{\theta}_{t+1}\|\}\)
10: end for
11: output: the last model \(f_{\sum_{t=1}^T \theta_t/T}\)

- \(\ell_2\)-regularization, \(\Omega[\theta] = \|\theta\|^2/2\), recovers the standard SVM with kernel \(\sum_{m=1}^M K_m\);
- block-norm \(\ell_2,1\) regularization, \(\Omega[\theta] = \frac{1}{2} \|\theta\|_{2,1}^2 = \frac{1}{2} (\sum_{m=1}^M \|\theta_m\|_{\lambda_m})^2\), yields sparse MKL, which is equivalent to learning a kernel of the form \(\sum_{m=1}^M \beta_m K_m\) with \(\beta \geq 0\) and \(\|\beta\|_1 \leq 1\);
- block-norm \(\ell_2,q\) regularization, \(\Omega[\theta] = \frac{1}{2} \|\theta\|_{2,q}^2 = \frac{1}{2} (\sum_{m=1}^M \|\theta_m\|_{\lambda_m}^q)^2/q\), generalizes the two previous cases, and for \(1 < q \leq 2\) yields non-sparse MKL [6], where the kernel coefficients are constrained as \(\beta \geq 0\) and \(\|\beta\|_q \leq 1\) with \(p = q/(2-q)\). The algorithm we propose also tackles the case \(q > 2\), which cannot be handled with the procedure described in [6];
- sums of block-norm regularizers, \(\Omega[\theta] = \frac{1}{2} \sum_{j=1}^J \sigma_j \|\theta\|_{2,q_j}\), with \(\sigma_j \geq 0\), are a further generalization that subsume the elastic MKL of [18]. Our algorithm can also handle these.

Decomposition over parts. As usually in SP [17], features decompose over parts; e.g., if the structure is expressed with a Markov network \((V, E)\), then each part is associated with either a vertex or an edge, and the feature vector is written as \(\phi(x, y) = (\phi_V(x, y), \phi_E(x, y))\), with:

\[
\phi_V(x, y) = \sum_{i \in V} \psi_{X,V}(x, i) \otimes \zeta_{Y,V}(y_i) \quad \text{and} \quad \phi_E(x, y) = \sum_{ij \in E} \psi_{X,E}(x, ij) \otimes \zeta_{Y,E}(y_i, y_j).
\]

We make the common simplifying assumption that \(\zeta_{Y,E}\) is the identity feature mapping, that \(\psi_{X,E} = 1\), and that \(\psi_{Y,E}\) is the identity feature mapping scaled by a positive \(\beta_0\). We then learn the kernel \(K_{X,V}((x, i), (x', i')) = \langle \phi_{X,V}(x, i), \phi_{X,V}(x', i') \rangle\) as a combination of basis kernels \(\{K_{X,V,m}\}_{m=1}^M\). This yields a kernel decomposition of the form

\[
K(u, u') = \sum_{i, i' \in V} \psi_{Y,E}(y_i, y_i') \sum_{m=1}^M \beta_m K_{X,V,m}((x, i), (x', i')) + \beta_0 \cdot \{i, i' : y_i = y_i', y_j = y_j'\}.
\]

In our sequence labeling experiments, vertices and edges correspond to label unigrams and bigrams. We explore two strategies: learning \(\beta_1, \ldots, \beta_M\), with \(\beta_0 = 1\) fixed, or also learning \(\beta_0\).

3 An Online Algorithm for MKL

To handle (2), we propose Alg. 1, which can be seen as extending FOBOS [5] by allowing multiple proximal steps to deal with composite regularizers, \(\Omega[\theta] = \sum_{j=1}^J \Omega_j[\theta]\). Like SGD, Alg. 1 is suitable for problems with large \(N\); the proximal steps make it effective for (non-differentiable) sparsity-inducing regularizers. As in PEGASOS [13], if a bound is known on the optimum, \(\|\theta^*\| \leq \gamma\), a projection step (line 9) is used. Naturally, Alg. 1 is entirely (or partially) kernelizable.

Subgradient step (line 4). First, local scores are computed for each part using the current parameters. Then, the highest score output, \(\hat{y}_t = \arg\max_{y_t \in \mathcal{Y}(x_t)} f_{\theta_t}(x_t, y_t) + \ell(y_t, y_t)\), is found (e.g., by dynamic programming). Finally, a subgradient is given as \(g_{\theta_t} = f_{\theta_t}(x_t, \hat{y}_t) - f_{\theta_t}(x_t, y_t)\).

Proximal step (line 7). Given \(\Omega : \mathcal{H} \to \mathbb{R}\), the \(\Omega\)-proximity operator [4] is defined as \(\text{prox}_{\Omega}(\tilde{\theta}) = \arg\min_{\theta} \frac{1}{2} \|\theta - \tilde{\theta}\|^2 + \Omega(\theta)\). The block structure of the parameter vector makes this step particularly efficient, thanks to the following result:

Proposition 1 Let \(\Omega(\theta) = \omega((\|\theta_m\|)_{m=1}^M)\) depend on each block only through its \(\ell_2\)-norm. Then, \(\text{prox}_{\Omega}(\theta)_{m} = \text{prox}_{\lambda_m}(\|\theta_{m}\|)) m(\theta_{m}/\|\theta_m\|)\).
Table 1: Results for handwriting recognition. Averages over 10 runs on the same folds as in [17], training on one and testing on the others. The linear and quadratic kernels are normalized to unit diagonal. In all cases, 20 epochs were used. Results are for the best regularization coefficient $C = 1/(\lambda \mu)$ (chosen from \{0.1, 1, 10, 10^2, 10^3, 10^4\}).

<table>
<thead>
<tr>
<th>Kernel</th>
<th>Training Runtimes</th>
<th>Test Acc. (per char.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear ($L$)</td>
<td>6 sec.</td>
<td>71.8 ± 3.9%</td>
</tr>
<tr>
<td>Quadratic ($Q$)</td>
<td>116 sec.</td>
<td>85.5 ± 0.3%</td>
</tr>
<tr>
<td>Gaussian ($G(\sigma^2 = 5)$)</td>
<td>123 sec.</td>
<td>84.1 ± 0.4%</td>
</tr>
<tr>
<td>Average ($L + Q + G$)</td>
<td>118 sec.</td>
<td>84.3 ± 0.3%</td>
</tr>
<tr>
<td>MKL, $\beta_1 L + \beta_2 Q + \beta_3 G$</td>
<td>279 sec.</td>
<td>87.5 ± 0.3%</td>
</tr>
<tr>
<td>MKL, $\beta_4 L + \beta_2 Q + \beta_3 G$</td>
<td>282 sec.</td>
<td>87.5 ± 0.4%</td>
</tr>
<tr>
<td>$\text{DSE}_{1}$-Spline (15)</td>
<td>8 sec.</td>
<td>75.4 ± 0.9%</td>
</tr>
<tr>
<td>Average ($L + B_1$)/2</td>
<td>15 sec.</td>
<td>83.0 ± 0.3%</td>
</tr>
<tr>
<td>MKL, $\beta_1 L + \beta_2 B_1$</td>
<td>15 sec.</td>
<td>85.2 ± 0.3%</td>
</tr>
<tr>
<td>MKL, $\beta_3 L + \beta_2 B_1$</td>
<td>16 sec.</td>
<td>85.2 ± 0.3%</td>
</tr>
</tbody>
</table>

Hence, any $\ell_{2,q}$-proximity operator can be reduced to an $\ell_q$ one. For sparse MKL ($q = 1, r = 2$) this computation can be carried out in time $\tilde{O}(M)$ [9] ($\tilde{O}$ hides logarithmic terms). For non-sparse MKL, we replace $\ell_{2,q}$ by $\ell_q$ (equivalent up to a change in the regularization constant). The $\ell_q$-proximity operator is separable, hence can be computed coordinatewise.

**Kernelization.** The computation of local scores, which precedes the gradient step, only involves inner products. Hence, the whole algorithm can be kernelized. We only need to keep track of the $\ell_2$-norm of each block, which can be updated after each gradient step via

$$
\|\theta_{t,m}\|^2 = \|\theta_{t,m}\|^2 - 2\eta t \theta_{t,m} \langle \phi_m(x_t, y_t) \rangle + \eta_t^2 \|\phi_m(x_t, y_t)\|^2
$$

and rescaled after each proximal and projection steps.

**Regret, Convergence and Generalization Bounds.** Let the loss $L$ be convex and $G$-Lipschitz on the $\gamma$-radius $\ell_2$-ball (e.g., hinge or logistic), the regularizers $\Omega_j$ be convex and satisfy additional mild conditions (satisfied, e.g., by $\Omega_j = \lambda_j \|\theta\|_{p_j}^q$, for $p_j, q_j \geq 1$). We show [9] that Alg. 1 converges to $\epsilon$ precision, with high confidence, in $O(1/\epsilon^2)$ iterations (as the best batch MKL algorithms). If $L$ or $\Omega$ are strongly convex (e.g., if at least one regularizer $\Omega_j$ is a squared $\ell_{2,q}$-norm, for $q > 1$), the bound improves to $O(1/\epsilon)$. The generalization bounds are of the same order. This follows from the fact, shown in [9], that using rate $\eta_t = \eta_0/\sqrt{t}$ yields cumulative regret (w.r.t. the best fixed hypothesis) $\text{Reg}_T \leq (2\gamma^2)/\eta_0 + G^2 \eta_0 \sqrt{T}$; in the presence of $\sigma$-strong convexity, a rate $\eta_t = 1/(\sigma t)$ yields $\text{Reg}_T \leq G^2 (1 + \log T)/(2\sigma)$.

4 Experiments

**Handwriting recognition.** We use an OCR dataset [17] with 6,877 words written by 150 people (52,152 characters). Each character is a 16 x 8 binary image with one of 26 labels (a–z). Our first experiment (upper part of Tab. 1) compares linear, quadratic, and Gaussian kernels, used individually, combined via a simple average, or with MKL via Alg. 1. The results show that MKL outperforms the others, and that learning the bigram weight $\beta_0$ did not make any difference.

The second experiment shows that Alg. 1 handles both feature and kernel sparsity by learning a combination of a linear (explicit features) with a generalized $B_1$-spline kernel ($K(x, x') = \max\{0, 1 - \|x - x'\|/h\}$, with $h$ such that the kernel matrix has $\sim 95\%$ zeros). The idea is to combine a simple feature-based kernel with one depending only on a few nearest neighbors. The results (Tab. 1, bottom part) show that MKL outperforms the individual kernels and the averaged kernel. The runtime is much shorter than in the previous experiment, with a mild accuracy decrease.

The third experiment compares Alg. 1 with two wrapper-based schemes: a Gauss-Seidel method alternating between optimizing the SVM and the kernel weights, and a gradient method (SimpleMKL [11]). In both cases, the SVMs were tackled with structured PEGASOS. As shown in Fig. 1, Alg. 1 converges in a small number of epochs to a near-optimal region, suggesting its usefulness in settings where each epoch is costly.

**Dependency parsing.** We train non-projective dependency parsers on the dataset of the CoNLL-2008 shared task [15] (39,278 training, 2,399 test sentences). The output to be predicted from each input sentence is the set of dependency arcs, which must define a directed spanning tree (example in Fig. 2). We use arc-factored models, and define a total of 507 feature groups (our linear kernels to be combined) conjoining words, lemmas, parts-of-speech, distance and direction of attachment. This
Non-projective Dependency Parsing using Spanning Tree Algorithms
Ryan McDonald Fernando Pereira
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Czech, non-projective dependencies are more frequent. Rich inflection systems reduce reliance on word order to express

yields a problem with > 50 million instantiated features. The feature vectors associated with each candidate arc, however, are very sparse and this is exploited in the implementation. We run Alg. 1 with explicit features. Although MKL did not outperform an SVM, it showed a good performance at pruning irrelevant feature templates (Fig. 2, bottom right). Besides interpretability, this pruning is also appealing in a two-stage architecture, where a standard learner at a second stage will only need to handle a small fraction of the groups initially hypothesized, perhaps giving speedups in inference.

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References
