Kernel-Based Machine Learning with Multiple Sources of Information

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Summary  We present a new methodology for fusing information from multiple data sources – or kernels – in machine learning. Previous approaches promoted sparse combinations of kernels, which, however, may discard important information. We present a flexible approach based on \( \ell_p \)-norm regularization, allowing for non-sparse solutions. In a theoretical analysis we show lower and upper generalization bounds of order up to \( O(M/n) \), overcoming the best previously known upper bounds for the problem, which achieved \( O(\sqrt{M/n}) \).

The computational experiments indicate that the novel algorithms are up to two orders of magnitude faster than previous approaches. Applications to computational biology and computer vision show accuracies that go beyond the state-of-the-art.

1 Introduction

In machine learning, we aim at learning the unknown relation between two random variables \( X \) and \( Y \) from data

\[
D = (x_1, y_1), \ldots, (x_n, y_n),
\]

so that, when observing a new \( x \) (called pattern), we may make accurate predictions of the corresponding \( y \) (called label). In the information age, machine learning is becoming an increasingly important tool. For example, consider content-based information retrieval; say \( \{x_1, \ldots, x_n\} \) is a set of images and the label \( y_i \in \{0, 1\} \) indicates whether an image \( x_i \) contains some object, say, for example, a cat. Machine learning then...
computes, from a set of labeled images, a classifier that can predict the presence or absence of a cat in a new, previously unseen image.

A very modern and elegant, yet simple approach consists in the paradigm of kernel-based machine learning, which states that we may convert, in a principled manner, any learning algorithm that is solely based on Euclidean scalar products into a more powerful, non-linear one, by simple substituting the scalar products \( \langle x_i, x_j \rangle \) by the so-called kernel \( k(x_i, x_j) \).\(^1\) A prominent example of a kernel-based learning machine is the support vector machine (SVM), which performs prediction based on the rule

\[
y := \text{sign} \left( \sum_{i=1}^{n} \alpha_i y_i k(x_i, x) \right),
\]

which predicts, for any pattern \( x \), a corresponding label \( y \). The \( \alpha_i \)'s are hereby computed by solving a certain cleverly chosen mathematical program, that is,\(^2\)

\[
\max_{\sum_{i=1}^{n} \alpha_i y_i = 0} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j k(x_i, x_j).
\]

In many modern applications, the data is characterized by multiple sources or representations of information so that multiple views of the data are available. For example, in image retrieval, an image can be represented by its color distribution over spatial tilings, but also by shape and local gradient information. Each view gives rise to a kernel \( k_m \), \( m = 1, \ldots, M \). A sophisticated way to “fuse” the information contained in the various kernels is to form a new, weighted kernel by linear combination of the many kernels, that is,

\[
k = \sum_{i=1}^{M} \theta_m k_m,
\]

where \( \theta_m \geq 0 \) specifies the weight of the \( m \)-th kernel. Previous approaches to this so-called multiple kernel learning (MKL) require the weight vector \( \theta := (\theta_1, \ldots, \theta_M) \) being sparse, that is, many of the weights \( \theta_m \) are put to zero [2; 3].

Sparse kernel combinations can be easily interpreted and analyzed, but, unfortunately, often achieve sub-optimal accuracies [5]. The author believes that much of the enthusiasm of scientists for sparse models in multiple kernel learning stems from a general preference or trend for sparse models in computer science and statistics. But sparse models may discard relevant and possibly complementary information, if the underlying ground truth is dense. In the discussed dissertation [13], we present and analyze a novel methodology for non-sparse information fusion in kernel-based machine learning. The three cornerstones of the thesis can be characterized as follows:

1. **Theoretical foundations:** we prove upper bounds on the statistical generalization performance of multiple kernel learning, achieving rates as fast as \( O(M/n) \), considerably pushing forward the best previously known bounds of [4], who achieved \( O(\sqrt{M/n}) \). We also prove a lower bound, which shows that our result is tight.

2. **Algorithms:** we develop and implement new algorithms for solving the mathematical program associated with multiple kernel learning that are up to two orders of magnitude faster than the best previous algorithms for the problem.

3. **Applications:** we apply the novel methodology to challenging problems from computer vision and bioinformatics, significantly advancing the state-of-the-art.

\[\text{References:}\]

\[\text{[1] Gaussian kernel:}\]

\[\text{[2] Excellent introduction to kernel-based learning}\]

\[\text{[3] Proven choice of a kernel:}\]

\[\text{[5] Sparse models in computer science and statistics.}\]
3 Algorithms

In the dissertation [13], we present three efficient algorithms for solving the optimization problem (5):

- a block coordinate descend method [5]
- a cutting plane algorithm with sequential quadratically constrained programming [6]
- a Newton descend method [7].

The most simple of the three algorithms is the block coordinate descend one, which works as follows:

Algorithm 1:
1: initialization:
   - initialize \( \theta_m = \sqrt{1/M} \) for all \( m = 1, \ldots, M \)
2: repeat
3: \( \alpha \)-step: solve (5) with respect to variables \( \alpha_1, \ldots, \alpha_m \), keeping the \( \theta_m \)s fixed.
4: \( \theta \)-step: solve the primal of (5) with respect to \( \theta_1, \ldots, \theta_M \), keeping the \( \alpha \)s fixed.
5: until converged.

An advantage of the proposed algorithm is that it provably converges, as established by the following theorem:

Theorem 1. If the kernels \( k_1, \ldots, k_M \) are strictly positive definite, Algorithm 1 converges to a globally optimal point.

All algorithms are implemented in C++ into the SHOGUN machine learning toolbox [8] and equipped with interfaces to MATLAB, Octave, Python und R. From the empirical analysis shown in Fig. 1, we observe that our algorithms – for the first time – facilitate to effectively employ thousands of kernels and ten thousands of data points at the same time. We observe them to be up to two orders of magnitude faster than the state-of-the-art, namely, SimpleMKL [3] and HessianMKL [9]. While the latter went out of memory for some 10 000 data points and 1000 kernels, our algorithms can deal with large-scale data by an efficient on-the-fly implementation.

4 Theoretical Analysis

The proposed methodology enjoys favorable theoretical guarantees: we show the following upper bound on the local Rademacher complexity of \( \ell_p \)-norm multiple kernel learning [10; 11].

Theorem 2 (Rademacher bound). The local Rademacher complexity of \( \ell_p \)-norm multiple kernel learning is bounded by

\[
R(H_p) \leq \min_{r \in \{1,2\}} \sqrt{\frac{16}{\eta_m} \frac{1}{n} + \frac{\sqrt{BDM} \tau^*}{n}},
\]

where \( \eta_m = \sum_{j=1}^{\infty} \min_{r} \left( \mathcal{M}^{1-t^*} \eta \mathcal{C} \right)^{2} \), \( \eta = (\eta_1, \ldots, \eta_M) \), and \( \lambda^{(m)}_{j} \) denotes the \( j \)th eigenvalue of the \( m \)th kernel (sorted in descending order). Furthermore, we denote \( B^2 := \sup_{x,y} k(x,y) \), \( q = 2p/(p+1) \), and \( t^* := \frac{1}{m} \) for the conjugated exponent of \( t \).

We also prove a matching upper bound,

\[
R(H_p) \geq \frac{1}{n} \sum_{j=1}^{\infty} \min_{r} \left( \mathcal{M}^{1-t^*} \eta \mathcal{C} \right)^{2} \mathcal{F} \mathcal{F} \mathcal{M}^{1-t^*} \mathcal{F} \mathcal{F} = \frac{1}{n} \sum_{j=1}^{\infty} \lambda^{(m)}_{j} \frac{1}{m},
\]

so that we may conclude that our result is tight. It follows the following generalization bound for learning with multiple kernels:

Theorem 3 (Generalization bound). Suppose \( \|k\|_{\infty} \leq B \) and \( \exists \alpha > 0, \alpha > 1 \), so that \( \forall m : \lambda^{(m)}_{j} \leq d_{\text{max}}^{-\alpha} \). Then the following holds: The loss of \( \ell_p \)-norm multiple kernel learning is, for any \( p \in [1, \ldots, 2] \) and \( z > 0 \), with probability greater than \( 1 - e^{-z} \), bounded by

\[
P(l^* - l_{\text{opt}}^*) \leq \min_{r \in \{1,2\}} 186 \cdot \left( \frac{3 - \alpha_m}{1 - \alpha_m} \right) \mathcal{D} M^{1/2} \mathcal{F} \mathcal{F} \mathcal{M}^{1/2} \mathcal{F} \mathcal{F} + \frac{47 \sqrt{BDLM} \sqrt{\tau^*}}{n} + \frac{(2BDLM \tau^* + 27F)z}{n}
\]

We observe that the above bound leads to convergence rates of order up to \( O(M/n) \), which considerably improves the tightest previous result, that is, the bound of order \( O(\sqrt{M/n}) \) proved by [4]. Note that, typically, the number of kernels, \( M \), is much smaller than the number of data points, \( n \). For instance, when \( M = 10 \) and \( n = 100 000 \), the bound of [4] contains a factor of \( \sqrt{M/n} = 1/100 \), while our bound achieves a factor of \( M/n = 1/10 000 \) – an improvement of two orders of magnitude.

5 Applications

In the application domains of computational biology and computer vision, we often encounter a multitude of complementary information sources/kernels, which renders the use of multiple kernel learning very attractive. Previous analyses – with the notable exception of the analysis of [12] on subcellular localization of proteins – failed to prove the effectiveness of multiple kernel learning. In
5.1 Visual Object Recognition

This area of computer vision concerns the recognition of objects in images—a difficult task because objects can be rotated, displaced, illuminated, and partially obstructed from view. Furthermore, some features may be crucial for the detection of certain object classes, but almost unnecessary for another class. For instance, color information can be very helpful to detect stop signs, but is ineffective to detect cars or balloons. Although this cries for the use of methods that incorporate multiple information sources or kernels, previous analyses did not show any advantage to those methods over a plain SVM.

We experiment on the official dataset of the PASCAL VOC Challenge 2008, which consists of 8780 images associated with up to 20 object classes. We employ multiple kernels based on color histograms of oriented gradients, visual words, and pixel colors over two color channels. In total this results in 12 kernels. We evaluate the algorithms based on the official error measure of the challenge, that is, the average prediction precision of an image averaged over all recall values. The results are shown in Fig. 2; vertical bars indicate the difference in average precision with respect to a plain SVM (using a simple kernel average).

![Figure 2](image)

Figure 2: Accuracy of proposed methodology in an object recognition experiment.

In contrast, we show that the proposed methodology can significantly raise the bar; we focus on computer vision in this presentation and refer the interested reader to the dissertation [13] for further details on applications in computational biology.

6 Conclusion

We have developed a methodology to non-sparse information fusion in kernel-based machine learning, which enjoys favorable theoretical guarantees. Our empirical analysis on challenging problems from the domains of computer vision and computation biology showed that accuracies can be achieved that go beyond the state-of-the-art. The proposed optimization algorithms were shown to be up to two orders of magnitude faster than existing ones. The method is undermined by deep foundations of statistical learning theory: we show upper and lower bounds on the generalization error of order $O(M/n)$, while previous bounds achieved $O(\sqrt{M/n})$.

Finally, we would like to remark that it might be worthwhile to rethink the current strong preference for sparse methods in machine learning—or in the scientific community in general. The present work clearly demonstrates that sparse models may improve over dense ones quite impressively. In fact such rethinking seems to already taking place: for instance in the social sciences, Gelman [15] claims that even in causal models “There are (almost) no true zeros”; in contrast, Gelman suggests that already weak connectivity in a causal graphical model may be sufficient for all variables to be required for optimal predictions (i.e., to have non-zero coefficients).

The present work serves as a foundation for non-sparse information fusion in machine learning and may serve as a good starting point for further applications in science and technology.

References


Distinguished Dissertations


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