Regularization Strategies and Empirical Bayesian Learning for MKL

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Abstract

Multiple kernel learning (MKL), structured sparsity, and multi-task learning have recently received considerable attention. In this paper, we show how different MKL algorithms can be understood as applications of either regularization on the kernel weights or block-norm-based regularization, which is more common in structured sparsity and multi-task learning. We show that these two regularization strategies can be systematically mapped to each other through a concave conjugate operation. When the kernel-weight-based regularizer is separable into components, we can naturally consider a generative probabilistic model behind MKL. Based on this model, we propose learning algorithms for the kernel weights through the maximization of marginal likelihood. We show through numerical experiments that $\ell_2$-norm MKL and Elastic-net MKL achieve comparable accuracy to uniform kernel combination. Although uniform kernel combination might be preferable from its simplicity, $\ell_2$-norm MKL and Elastic-net MKL can learn the usefulness of the information sources represented as kernels. In particular, Elastic-net MKL achieves sparsity in the kernel weights.

1. Introduction

In many learning problems, the choice of feature representation, descriptors, or kernels plays a crucial role. The optimal representation is problem specific. For example, we can represent a web page as a bag-of-words, which might help us in classifying whether the page is discussing politics or economy; we can also represent the same page by the links provided in the page, which could be more useful in classifying whether the page is supporting political party A or B. Similarly in a visual categorization task, a color-based descriptor might be useful in classifying an apple from a lemon but not in discriminating an airplane from a car. Given that there is no single feature representation that works in every learning problem, it is crucial to combine them in a problem dependent manner for a successful data analysis.

In this paper, we consider the problem of combining multiple data sources in a kernel-based learning framework. More specifically, we assume that a data point $x \in \mathcal{X}$ lies in a space $\mathcal{X}$ and we are given $M$ candidate kernel functions $k_m : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ ($m = 1, \ldots, M$). Each kernel function corresponds to one data source. A conical combination of $k_m$ ($m = 1, \ldots, M$) gives the combined kernel function $\bar{k} = \sum_{m=1}^{M} d_m k_m$, where $d_m$ is a nonnegative weight. Our goal is to find a good set of kernel weights based on some training examples.

Various approaches have been proposed for the above problem under the name multiple kernel learning (MKL) (Lanckriet et al., 2004; Bach et al., 2004; Zien and Ong, 2007; Varma and Ray, 2007; Aflalo et al., 2009; Gehler and Nowozin, 2009; Kloft et al., 2009; Longworth and Gales, 2009;
Recently, Kloft et al. (2009, 2010) have shown that many MKL approaches can be understood as application of the penalty-based regularization (Tikhonov regularization) or constraint-based regularization (Ivanov regularization) on the kernel weights $d_m$. Meanwhile, there is a growing interest in learning under structured sparsity assumption (Yuan and Lin, 2006; Argyriou et al., 2008; Huang et al., 2009; Jacob et al., 2009; Jenatton et al., 2009), which employs another regularization based on the so-called block-norm.

Therefore, a natural question to ask is how these two regularization strategies are related to each other. For simple cases the correspondence is well known (see Bach et al. (2004, 2005); Kloft et al. (2009)). Moreover, in the context of structured sparsity, Micchelli et al. (2010) have proposed a more sophisticated class of penalty functions that employ both Tikhonov and Ivanov regularizations on the kernel weights and have shown the corresponding block-norm regularization. The first contribution of this paper is to show that under some mild assumptions the kernel-weight-based regularization and the block-norm-based regularization can be mapped to each other in a systematic manner through a concave conjugate operation.

All the regularization strategies we discussed so far is formulated as convex optimization problems. The second contribution of this paper is to propose a nonconvex regularizer based on the marginal likelihood. Although the overall minimization problem is nonconvex, we propose a iterative algorithm that alternately minimize two convex objectives. Although Bayesian approaches have been applied to MKL earlier in a transductive nonparametric setting by Zhang et al. (2004), and a setting similar to the relevance vector machine (Tipping, 2001) by Girolami and Rogers (2005); Damoulas and Girolami (2008), our formulation is more coherent with the correspondence between Gaussian process classification/regression and kernel methods (Rasmussen and Williams, 2006). Note that very recently Archambeau and Bach (2010); Urtasun (2010) also studied similar models.

This paper is structured as follows. In Section 2, we start from analyzing learning with fixed kernel combination. Then we discuss the two regularization strategies (kernel-weight-based regularization and block-norm-based regularization). Finally, we present our main result on the correspondence between the two formulations. In Section 3, we start from viewing the separable kernel-weight-based model as a hierarchical maximum a posteriori(MAP) estimation problem, and propose an empirical Bayesian approach for the same model. Furthermore, we show a connection to the general framework we discuss in Section 2. We numerically compare the proposed empirical Bayesian MKL and various MKL models on visual categorization tasks from the Caltech 101 dataset (Fei-Fei et al., 2004) using 1,760 kernel functions. Finally, we summarize our contributions in Section 5.

2. Multiple kernel learning frameworks and their connections

In this section, we first consider the problem of learning a classifier with a fixed kernel combination. Then we extend this framework to jointly optimize the kernel weights together with the classifier. Second, we consider the block-norm based regularization, which have been discussed in structured sparsity literature (including group lasso) (Yuan and Lin, 2006; Argyriou et al., 2008; Huang et al., 2009; Jacob et al., 2009; Jenatton et al., 2009). Our main concern is in how these two formulations are related to each other. We show two theorems (Theorem 1 and 7) that map the two formulations. Using these theorems, we show that previously proposed regularized MKL models can be systematically transformed from one formulation to another.
2.1 Learning with fixed kernel combination

We assume that we are given $N$ training examples $(x_i, y_i)_{i=1}^N$ where $x_i$ belongs to an input space $\mathcal{X}$ and $y_i$ belongs to an output space $\mathcal{Y}$ (usual settings are $\mathcal{Y} = \{\pm 1\}$ for classification and $\mathcal{Y} = \mathbb{R}$ for regression).

We first consider a learning problem with fixed kernel weights. More specifically, we fix non-negative kernel weights $d_1, d_2, \ldots, d_M$ and consider the RKHS $\mathcal{H}$ corresponding to the combined kernel function $k = \sum_{m=1}^M d_m k_m$. The squared RKHS norm of a function $f$ in the combined RKHS $\mathcal{H}$ can be represented as follows:

$$\|f\|_{\mathcal{H}}^2 := \min_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M} \sum_{m=1}^M \frac{\|f_m\|_{\mathcal{H}_m}^2}{d_m} \quad \text{s.t.} \quad \bar{f} = \sum_{m=1}^M f_m,$$

where $\mathcal{H}_m$ is the RKHS that corresponds to the kernel function $k_m$. If $d_m = 0$, the ratio $\|f_m\|_{\mathcal{H}_m}^2/d_m$ is defined to be zero if $\|f_m\|_{\mathcal{H}_m} = 0$ and infinity otherwise. See Sec 6 in Aronszajn (1950), and also Lemma 25 in Micchelli and Pontil (2005) for the proof. We also provide some intuition for a finite dimensional case in Appendix A.

Using the above representation, a supervised learning problem with a fixed kernel combination can be written as follows:

$$\min_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M} \sum_{i=1}^N \ell \left(y_i, \sum_{m=1}^M f_m(x_i) + b\right) + \frac{C}{2} \sum_{m=1}^M \frac{\|f_m\|_{\mathcal{H}_m}^2}{d_m},$$

where $\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is a loss function and we assume that $\ell$ is convex in the second argument; for example, the loss function can be the hinge loss $\ell_H(y_i, z_i) = \max(0, 1 - y_i z_i)$, or the quadratic loss $\ell_Q(y_i, z_i) = (y_i - z_i)^2/(2\sigma_y^2)$.

It might seem that we are making the problem unnecessarily complex by introducing $M$ functions $f_m$ to optimize instead of simply optimizing over $\bar{f}$. However, explicitly handling the kernel weights enables us to consider various regularization strategies on the weights as we see in the next subsection.

2.2 Kernel-weight-based regularization

Now we are ready to also optimize the kernel weights $d_m$ in the above formulation. Clearly there is a need for regularization, because the objective (2) is a monotone decreasing function of the kernel weights $d_m$. Intuitively speaking, $d_m$ corresponds to the complexity allowed for the $m$th regression function $f_m$; the more complexity we allow, the better the fit to the training examples becomes. Thus without any constraint on $d_m$, we can get a severe overfitting problem.

Let $h : \mathbb{R}_+^M \to \mathbb{R} \cup \{+\infty\}$ be a function from a non-negative real vector $d \in \mathbb{R}_+^M$ to a real number. One way to penalize the complexity is to minimize the objective (2) together with the regularizer $h(d)$ as follows:

$$\min_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M, \quad b \in \mathbb{R}, \quad d \in \mathbb{R}_+^M} \sum_{i=1}^N \ell \left(y_i, \sum_{m=1}^M f_m(x_i) + b\right) + \frac{C}{2} \left(\sum_{m=1}^M \frac{\|f_m\|_{\mathcal{H}_m}^2}{d_m} + h(d)\right).$$
Note that if $h$ is a convex function, the above optimization problem is jointly convex in $f_m$ and $d_m$ (see Boyd and Vandenberghe (2004, Example 3.18)).

**Example 1 ($\ell_p$-norm MKL via Tikhonov regularization)** Let $h(d) = \sum_{m=1}^{M} d_m^p/p$. Then we have

$$
\min_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M} \sum_{i=1}^{N} \ell(y_i, \sum_{m=1}^{M} f_m(x_i) + b) + C \sum_{m=1}^{M} \left( \frac{\|f_m\|_{\mathcal{H}_m}^2}{d_m} + \frac{d_m^p}{p} \right)
$$

The special case $p = 1$ was considered earlier in Varma and Ray (2007).

**Example 2 ($\ell_p$-norm MKL via Ivanov regularization)** Let $h(d) = 0$ if $\sum_{m=1}^{M} d_m^p \leq 1$ and $h(d) = +\infty$ otherwise. Then we have

$$
\min_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M} \sum_{i=1}^{N} \ell(y_i, \sum_{m=1}^{M} f_m(x_i) + b) + C \sum_{m=1}^{M} \frac{\|f_m\|_{\mathcal{H}_m}^2}{d_m} \quad \text{s.t.} \quad \sum_{m=1}^{M} d_m^p \leq 1.
$$

This formulation was considered by Kloft et al. (2008, 2009). The special case $p = 2$ was considered by Cortes et al. (2009).

**Example 3 (Multi-task learning)** In this example, the linear combination inside the loss term is defined in a sample-dependent manner. More precisely, we assume that there are $n$ tasks, and each sample is associated with the $l(i)$th task. Let $\mathcal{H}$ be an RKHS over the input space $X$. We consider $M = n + 1$ functions $f_1, \ldots, f_M \in \mathcal{H}$ to model the task dependent component and the task independent component. The first $n$ functions $f_1, \ldots, f_n \in \mathcal{H}$ represent the task dependent components of the classifiers, and the last function $f_M \in \mathcal{H}$ represents the component that is common to all tasks. Accordingly, the optimization problem can be expressed as follows:

$$
\min_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M} \sum_{i=1}^{N} \ell(y_i, f_{l(i)}(x_i) + f_M(x_i) + b) + C \sum_{m=1}^{M} \frac{\|f_m\|_{\mathcal{H}_m}^2}{d_m} \quad \text{s.t.} \quad \sum_{m=1}^{M} d_m \leq 1.
$$

Evgeniou and Pontil (2004); Evgeniou et al. (2005) proposed a related model that only has one parameter; they used $d_m = n\lambda$ for $m = 1, \ldots, n$ and $\sum_{m=1}^{n} d_m/n^2 + d_M \leq 1$ instead of the constraint in the above formulation. However they did not discuss joint optimization of the hyperparameter $\lambda$ and the classifier.

**Example 4 (Wedge penalty)** Let $h(d) = \sum_{m=1}^{M} d_m$ if $d_m \geq d_{m+1}$ for all $m = 1, \ldots, M - 1$, and $h(d) = +\infty$ otherwise. Then we have

$$
\min_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M} \sum_{i=1}^{N} \ell(y_i, \sum_{m=1}^{M} f_m(x_i) + b) + C \sum_{m=1}^{M} \left( \frac{\|f_m\|_{\mathcal{H}_m}^2}{d_m} + d_m \right) \quad \text{s.t.} \quad d \in W,
$$

where

$$
W = \{d : d \in \mathbb{R}_+^M, d_m \geq d_{m+1}, m = 1, \ldots, M - 1\}.
$$

This penalty function was considered by Micchelli et al. (2010).
2.3 Block-norm-based regularization

Historically Bach et al. (2004, 2005) and Micchelli and Pontil (2005) pointed out that the problem of learning kernel weights and classifier simultaneously can be reduced to the problem of learning the classifier under some special regularizer, which we call block norm based regularizer in this paper. Generalizing the presentation in the earlier papers, we define the block-norm-based regularization as follows:

\[
\min_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M, b \in \mathbb{R}} \sum_{i=1}^N \ell \left( y_i, \sum_{m=1}^M f_m(x_i) + b \right) + C \frac{g(\|f_1\|_{\mathcal{H}_1}^2, \ldots, \|f_M\|_{\mathcal{H}_M}^2)}{\|f_m\|_{\mathcal{H}_m}},
\]

where \( g : \mathbb{R}^M_+ \to \mathbb{R} \) is called the block-norm-based regularizer.

Example 5 (Block 1-norm MKL) Let \( g(x) = \sum_{m=1}^M \sqrt{x_m} \). Then we have

\[
\min_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M, b \in \mathbb{R}} \sum_{i=1}^N \ell \left( y_i, \sum_{m=1}^M f_m(x_i) + b \right) + C \sum_{m=1}^M \|f_m\|_{\mathcal{H}_m}.
\]

This formulation was discussed earlier in Bach et al. (2005). When all the kernels are linear kernels defined on non-overlapping subset of input variables, this is equivalent to the group lasso Yuan and Lin (2006).

Example 6 (Overlapped group lasso) Suppose that we have \( D \) input variables \( x = (x^{(1)}, \ldots, x^{(D)})^\top \) and kernel functions \( k_m \) are defined as overlapped linear kernels as follows:

\[
k_m(x, y) = \sum_{l \in \mathcal{G}_m} x^{(l)} y^{(l)} \quad (m = 1, \ldots, M),
\]

where \( \mathcal{G}_m \) is a subset of (overlapped) indices from \( \{1, \ldots, D\} \). Introducing weight vectors \( w_m \in \mathbb{R}^{\|\mathcal{G}_m\|} \), we can rewrite \( f_m(x) = w_m^\top x^{(\mathcal{G}_m)} \), where \( x^{(\mathcal{G}_m)} = (x^{(l)})_{l \in \mathcal{G}_m} \). In addition, \( \|f_m\|_{\mathcal{H}_m}^2 = \|w_m\|^2 \). Then employing the same regularizer as in Example 5, we have

\[
\min_{w_1 \in \mathbb{R}^{\|\mathcal{G}_1\|}, \ldots, w_M \in \mathbb{R}^{\|\mathcal{G}_M\|}, b \in \mathbb{R}} \sum_{i=1}^N \ell \left( y_i, \sum_{m=1}^M w_m^\top x^{(\mathcal{G}_m)}_i + b \right) + C \sum_{m=1}^M \|w_m\|.
\]

This formulation was considered by Jacob et al. (2009). Except for the particular choice of the kernel function (6), this is a special case of the block 1-norm MKL in Example 5.

Example 7 (Elastic-net MKL) Let \( g(x) = \sum_{m=1}^M \left( (1 - \lambda) \sqrt{x_m} + \frac{\lambda}{2} x_m \right) \). Then we have

\[
\min_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M, b \in \mathbb{R}} \sum_{i=1}^N \ell \left( y_i, \sum_{m=1}^M f_m(x_i) + b \right) + C \sum_{m=1}^M \left( (1 - \lambda) \|f_m\|_{\mathcal{H}_m} + \frac{\lambda}{2} \|f_m\|_{\mathcal{H}_m}^2 \right).
\]

This formulation was discussed earlier in Shawe-Taylor (2008); Longworth and Gales (2009); Tomioka and Suzuki (2010). Note that the elastic-net MKL (8) reduces to the block 1-norm MKL (5) for \( \lambda = 0 \) and the uniform-weight combination (\( d_m = 1 \) in Equation (2)) for \( \lambda = 1 \).
2.4 Connection between the two formulations

In this subsection, we present two theorems that connect the kernel-weight-based regularization (Section 2.2) and the block-norm-based regularization (Section 2.3).

The following theorem states that under some assumptions about the regularizer $h$, we can analytically eliminate the kernel weights $d$ from the optimization problem (3).

**Theorem 1** We assume that the kernel weight based regularizer $h$ is convex, zero at the origin, and satisfies the generalized monotonicity in the following sense: for $x, y \in \mathbb{R}^M_+$ satisfying $x_m \leq y_m$ ($m = 1, \ldots, M$), $h$ satisfies

$$h(x) \leq h(y).$$

Moreover, let $\tilde{h}(y) := -h(1/y_1, \ldots, 1/y_M)$. Then $\tilde{h}$ is a concave function and the optimization problem (3) can be reduced to the following one:

$$\min_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M} \sum_{i=1}^N \ell \left( y_i, \sum_{m=1}^M f_m(x_i) + b \right) + C g(\|f_1\|_{\mathcal{H}_1}^2, \ldots, \|f_M\|_{\mathcal{H}_M}^2),$$

(10)

where

$$g(x) = \frac{1}{2} \inf_{y \in \mathbb{R}^M_+} \left( x^\top y - \tilde{h}(y) \right)$$

(11)

is the concave conjugate function of $\tilde{h}$ (divided by two). Moreover, if $g$ is differentiable, the optimal kernel weight $d_m$ is obtained as follows:

$$d_m = \left( 2 \frac{\partial g(\|f_1\|_{\mathcal{H}_1}^2, \ldots, \|f_M\|_{\mathcal{H}_M}^2)}{\partial x_m} \right)^{-1}.$$

**Proof** In order to show the concavity of $\tilde{h}$, we show the convexity of $h(1/y_1, \ldots, 1/y_M)$. This is a straightforward generalization of the scalar composition rule in (Boyd and Vandenberghe, 2004, p84). Let $\phi$ be any scalar convex function. Then

$$h(\phi(\theta x_1 + (1-\theta)y_1), \ldots, \phi(\theta x_M + (1-\theta)y_M))$$

$$\leq h(\theta \phi(x_1) + (1-\theta)\phi(y_1), \ldots, \theta \phi(x_M) + (1-\theta)\phi(y_M))$$

$$\leq \theta h(\phi(x_1), \ldots, \phi(x_M)) + (1-\theta)h(\phi(y_1), \ldots, \phi(y_M)),$$

In the second line, we used the convexity of $\phi$ and the monotonicity of $h$ in Equation (9). Therefore, letting $\phi(x) = 1/x$, we have the convexity of $h(1/y_1, \ldots, 1/y_M)$ and the concavity of $\tilde{h}$. Now if the infimum in the minimization (11) exists in $\mathbb{R}^M_+$, we have the block-norm formulation (10) by substituting $x_m = \|f_m\|_{\mathcal{H}_m}$ and $y_m = 1/d_m$ for $m = 1, \ldots, M$. The case $y_m = +\infty$ for some $m$ happens only if $x_m = \|f_m\|_{\mathcal{H}_m} = 0$ because $\tilde{h}(y) \leq 0$, and this corresponds to $d_m = 0$ in the original formulation (3). The last part of the theorem follows from fact that

$$\tilde{h}(y) = \inf_{x \in \mathbb{R}^M_+} \left( x^\top y - 2g(x) \right)$$

and the optimality condition

$$\frac{1}{d_m} - 2 \frac{\partial g(\|f_1\|_{\mathcal{H}_1}^2, \ldots, \|f_M\|_{\mathcal{H}_M}^2)}{\partial x_m} = 0.$$
Note that the monotonicity assumption (9) and the convexity of $h$ form a strong sufficient condition for the above correspondence to hold. What we need is the concavity of $\tilde{h}$. In the context of variational Bayesian inference, such condition has been intensively studied. See Section 3 and Wipf and Nagarajan (2009); Seeger and Nickisch (2008).

In the particularly simple cases where the kernel-weight-based regularizer $h$ is separable, the block-norm-based regularizer $g$ is also separable as in the following corollary.

**Corollary 2 (Separable regularizer)** Suppose that the kernel-weight-based regularizer is defined as a separable function (with a slight abuse of notation) as follows:

$$h_{\text{sep}}(d) = \sum_{m=1}^{M} h(d_m),$$

and $h$ is convex and nondecreasing. Then, the corresponding block-norm-based regularizer is also separable and can be expressed as follows:

$$g_{\text{sep}}(x) = \frac{1}{2} \sum_{m=1}^{M} \inf_{y_m \geq 0} \left( x_m y_m - \tilde{h}(y_m) \right),$$

where $\tilde{h}(y) = -h(1/y)$.

**Proof** The proof is straightforward and is omitted (see e.g., Boyd and Vandenberghe (2004, p95)).

Separable regularizers proposed earlier in literature are summarized in Table 1.

The monotonicity assumption (9) holds for the regularizers defined in Examples 1–4. Therefore, we have the following corollaries.

**Corollary 3 (Block q-norm formulation via Tikhonov regularization)** Applying Theorem 1 to the $\ell_p$-norm MKL in Example 1, we have

$$\minimize_{f_1 \in H_1, \ldots, f_M \in H_M, b \in \mathbb{R}} \sum_{i=1}^{N} \ell \left( y_i, \sum_{m=1}^{M} f_m(x_i) + b \right) + \frac{C}{q} \sum_{m=1}^{M} \|f_m\|_{H_m}^q, \quad (12)$$

where $q = 2p/(1 + p)$.

**Proof** Note that the regularizer $h(d) = \sum_{m=1}^{M} d_m^p / p$ in Example 1 is separable as in Corollary 2. Therefore, we define $\tilde{h}(y_m) = -y_m^p / p$, and accordingly we have $g(x_m) = \frac{1+p}{2p} x_m^{p/(1+p)}$, from which we obtain Equation (12).

**Corollary 4 (Block q-norm formulation via Ivanov regularization)** Applying Theorem 1 to the $\ell_p$-norm MKL in Example 2, we have

$$\minimize_{f_1 \in H_1, \ldots, f_M \in H_M, b \in \mathbb{R}} \sum_{i=1}^{N} \ell \left( y_i, \sum_{m=1}^{M} f_m(x_i) + b \right) + \frac{C}{2} \left( \sum_{m=1}^{M} \|f_m\|_{H_m}^q \right)^{2/q}, \quad (13)$$

where $q = 2p/(1 + p)$.

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Proof For the regularizer defined in Example 2, we have
\[
\tilde{h}(y) = \begin{cases} 
0 & \text{if } \sum_{m=1}^{M} y_m^{-p} \leq 1, \\
-\infty & \text{otherwise}.
\end{cases}
\]

Then the block-norm-based regularizer \( g \) (11) is defined as the minimum of the following constrained minimization problem
\[
g(x) = \frac{1}{2} \min_{y \in \mathbb{R}^M_+} x^\top y \quad \text{s.t.} \quad \sum_{m=1}^{M} y_m^{-p} \leq 1.
\]

We define the Lagrangian \( L = \frac{1}{2} x^\top y + \frac{\eta}{2p} (\sum_{m=1}^{M} y_m^{-p} - 1) \). Taking the derivative of the Lagrangian and setting it to zero, we have
\[
y_m = \left( \frac{\eta}{x_m} \right)^{1/(1+p)}.
\]

In addition, the multiplier \( \eta \) is obtained as \( \eta = \left( \sum_{m=1}^{M} x_m^{p/(1+p)} \right)^{(1+p)/p} \). Combining the above two expressions, we have
\[
g(x) = \frac{1}{2} \left( \sum_{m=1}^{M} x_m^{p/(1+p)} \right)^{(1+p)/p},
\]
from which we obtain Equation (13).

Except for the special structure inside the loss term, the multi-task learning problem is a special case of the \( \ell_p \)-norm MKL with \( p = 1 \). Therefore, we have the following corollary.

Corollary 5 (Multi-task learning) Applying Theorem 1 to the multi-task learning problem in Example 3, we have
\[
\minimize_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M, b \in \mathbb{R}, d \in \mathbb{R}_+^M} \sum_{i=1}^{N} \ell(y_i, f_{l(i)}(x_i) + f_M(x_i) + b) + \frac{C}{2} \left( \sum_{m=1}^{M} \|f_m\|_{\mathcal{H}_m} \right)^2. \tag{14}
\]

Moreover, the one-parameter case considered in Evgeniou and Pontil (2004); Evgeniou et al. (2005), we have
\[
\minimize_{f_1 \in \mathcal{H}_1, \ldots, f_M \in \mathcal{H}_M, b \in \mathbb{R}, d \in \mathbb{R}_+^M} \sum_{i=1}^{N} \ell(y_i, f_{l(i)}(x_i) + f_M(x_i) + b) + \frac{C}{2} \left( \sqrt{\frac{1}{n} \sum_{m=1}^{M} \|f_m\|_{\mathcal{H}_m}^2 + \|f_M\|_{\mathcal{H}_M}} \right)^2.
\]
Proof The first part is a special case of Corollary 4. The one-parameter case can be derived using Jensen’s inequality as follows. Let \( d_m = n \lambda \) \((m = 1, \ldots, n)\) and \( d_M = 1 - \lambda \). Using Jensen’s inequality, we have

\[
\frac{1}{n} \sum_{m=1}^{n} \frac{f_m^2}{\| H_m \|} + \frac{f_M^2}{1 - \lambda} = \lambda \left( \frac{\sqrt{1/n} \sum_{m=1}^{n} f_m^2}{\lambda} \right)^2 + (1 - \lambda) \left( \frac{f_M^2}{1 - \lambda} \right)^2 \geq \left( \sqrt{1/n} \sum_{m=1}^{n} f_m^2 + \| f_M \|_{H_M} \right)^2.
\]

The equality holds when \((1 - \lambda)/\lambda = \| f_m \|_{H_M} / \sqrt{1/n} \sum_{m=1}^{n} f_m^2 \).

Note that in the one-parameter case discussed in Evgeniou and Pontil (2004); Evgeniou et al. (2005), the solution of the joint optimization of task similarity \( d_m \) and the classifier results in either \( \sqrt{1/n} \sum_{m=1}^{n} f_m^2 = 0 \) (all the tasks are the same) or \( \| f_M \|_{H_M} = 0 \) (all the tasks are different). For the general problem (14), some \( \| f_m \|_{H_m} \) may become zero but not necessarily all tasks.

Corollary 6 (Wedge penalty) Applying Theorem 1 to the Wedge regularization in Example 4, we have

\[
\min \left\{ f_1, \ldots, f_M, b \in \mathbb{R} \right\} \sum_{i=1}^{N} \ell \left( y_i, \sum_{m=1}^{M} f_m(x_i) + b \right) + C g \left( \| f_1 \|_{H_1}^2, \ldots, \| f_M \|_{H_M}^2 \right). \tag{15}
\]

where

\[
g(x_1, \ldots, x_M) = \sup_{\eta_0, \ldots, \eta_{M-1} \geq 0} \sum_{m=1}^{M} \sqrt{(1 + \eta_{m-1} - \eta_m)x_m}, \tag{16}
\]

with \( \eta_0 = \eta_M = 0 \).

Proof For the regularizer defined in Example 4, we have

\[
g(x) = \frac{1}{2} \min_{y \in \mathbb{R}} \sum_{m=1}^{M} \left( x_m y_m + y_m^{-1} \right) \quad \text{s.t.} \quad y_m^{-1} \leq y_{m+1}^{-1} \quad (m = 1, \ldots, M - 1).
\]

We define the Lagrangian \( \mathcal{L} \) as follows:

\[
\mathcal{L} = \frac{1}{2} \left( \sum_{m=1}^{M} \left( x_m y_m + y_m^{-1} \right) + \sum_{m=1}^{M-1} \eta_m (y_m^{-1} - y_{m+1}^{-1}) \right).
\]

Minimizing the Lagrangian with respect to \( y \), we have

\[
y_m = \sqrt{\frac{1 + \eta_{m-1} - \eta_m}{x_m}},
\]

where we define \( \eta_0 = \eta_M = 0 \) for convenience. Substituting the above expression back into the Lagrangian and forming the dual problem we obtain Equation (16).
Theorem 7 (Converse of Theorem 1) If the block-norm-based regularizer $g$ in formulation (4) is a concave function, we can derive the corresponding kernel-weight based regularizer $h$ as follows:

$$h(d_1, \ldots, d_M) = -2g^*(1/(2d_1), \ldots, 1/(2d_M)),$$

where $g^*$ denotes the concave conjugate of $g$ defined as follows:

$$g^*(y) = \inf_{x \in \mathbb{R}^M_+} (x^\top y - g(x)).$$

Proof The converse statement holds because

$$h(d_1, \ldots, d_M) = -\tilde{h}(1/d_1, \ldots, 1/d_M) = -(2g)^*(1/d_1, \ldots, 1/d_M) = -2g^*(1/(2d_1), \ldots, 1/(2d_M)),$$

where $g^*$ is the concave conjugate of $g$.

Theorem 7 can be used to derive the kernel-weight-based regularizer $h$ corresponding to the elastic-net MKL in Example 7 as in the following corollary.

Corollary 8 (Kernel-weight-based formulation for Elastic-net MKL) The block-norm-based regularizer $g$ defined in Example 7 is a concave function, and the corresponding kernel-weight-based regularizer can be obtained as follows:

$$h(d) = \sum_{m=1}^M \frac{(1-\lambda)^2d_m}{1-\lambda d_m}.$$

Proof Since the regularizer $g$ defined in Example 7 is a convex combination of two concave functions (square-root and linear functions), it is clearly a concave function. Next, noticing that the regularizer $g$ is separable into each component, we obtain its concave conjugate as follows:

$$\tilde{h}(y_m) = \inf_{x_m \geq 0} \left( x_my_m - 2 \left( (1-\lambda)\sqrt{x_m} + \frac{\lambda}{2}x_m \right) \right).$$

Taking the derivative with respect to $x_m$, we have

$$y_m - \frac{1-\lambda}{\sqrt{x_m}} - \lambda = 0.$$

Substituting the above expression back into Equation (17), we have

$$\tilde{h}(y_m) = -\frac{(1-\lambda)^2}{y_m - \lambda}.$$

Therefore

$$h(d_1, \ldots, d_M) = -\sum_{m=1}^M \tilde{h}(1/d_m) = \sum_{m=1}^M \frac{(1-\lambda)^2d_m}{1-\lambda d_m}.$$

Note that in the special case $\lambda = 0$ (corresponding to Example 5), the kernel-weight-based regularizer (17) reduces to the $\ell_p$-norm MKL with $p = 1$ in Example 1. See also Table 1.
Table 1: Correspondence between the regularizer $h$ in the kernel-weight-based regularization (3) and the concave function $g$ in the block-norm formulation (4). $I_{[0,1]}$ denotes the indicator function of the interval $[0,1]$; i.e., $I_{[0,1]}(x) = 0$ (if $x \in [0,1]$), and $I_{[0,1]}(x) = \infty$ (otherwise).

| MKL model         | $g(x)$ | $h(d_m)$ | Optimal kernel weight |
|-------------------|--------|----------|-----------------------|
| block 1-norm MKL  | $\sqrt{x}$ | $d_m$ | $d_m = \|f_m\|_m$       |
| $\ell_p$-norm MKL | $\frac{1}{2p}x^{p/(1+p)}$ | $d_m^p/p$ | $d_m = \|f_m\|_m^{2/(1+p)}$ |
| Uniform-weight MKL (block 2-norm MKL) | $x/2$ | $I_{[0,1]}(d_m)$ | $d_m = 1$ |
| block $q$-norm MKL ($q > 2$) | $\frac{1-q}{q}x^{q/2}$ | $\frac{2-2^q}{q}d_m^{-q/(q-2)}$ | $d_m = \|f_m\|_m^{2-q}$ |
| Elastic-net MKL    | $(1-\lambda)\sqrt{x} + \lambda x$ | $(1-\lambda)^2d_m/(1-\lambda d_m)$ | $d_m = \|f_m\|_m/(1-\lambda + \lambda \|f_m\|_m)$ |

3. Empirical Bayesian multiple kernel learning

For a separable regularizer (see Corollary 2), the kernel-weight-based formulation (3) allows a probabilistic interpretation as a hierarchical maximum a posteriori (MAP) estimation problem as follows:

$$\min_{f_i \in H_1, \ldots, f_M \in H_M, \mathbf{d} \in \mathbb{R}_+^M} \sum_{i=1}^N \ell(y_i; \sum_{m=1}^M f_m(x_i) + \mathbf{b}) + M \sum_{m=1}^C \left( \frac{\|f_m\|_m^2}{d_m} + h(d_m) \right). \quad (18)$$

The loss term can be considered as a negative log-likelihood. The first regularization term $\|f_m\|_m^2/d_m$ can be considered as the negative log of a Gaussian process prior with variance scaled by the hyper-parameter $d_m$. The last regularization term $h(d_m)$ corresponds to the negative log of a hyper-prior distribution $p(d_m) \propto \exp(-h(d_m))$. In this section, instead of a MAP estimation, we propose to maximize the marginal likelihood (evidence) to obtain the kernel weights; we call this approach empirical Bayesian MKL.

We rewrite the (separable) kernel-weight regularization problem (18) as a probabilistic generative model as follows:

$$d_m \sim \frac{1}{Z_1} \exp(-h(d_m)) \quad (m = 1, \ldots, M),$$
$$f_m \sim GP(f_m; 0, d_m k_m) \quad (m = 1, \ldots, M),$$
$$y_i \sim \frac{1}{Z_2} \exp(-\ell(y_i; f_1(x_i) + f_2(x_i) + \cdots + f_M(x_i))),$$

where $Z_1$ and $Z_2$ are normalization constants; $GP(f; 0, k)$ denotes the Gaussian process (Rasmussen and Williams, 2006) with mean zero and covariance function $k$. We omit the bias term for simplicity.

When the loss function is quadratic $\ell(y_i, z_i) = (y_i - z_i)^2/(2\sigma_i^2)$, we can analytically integrate out the Gaussian process random variable $(f_m)_{m=1}^M$ and compute the negative log of the marginal likelihood as follows:

$$-\log p(y| \mathbf{d}) = \frac{1}{2} \mathbf{y}^\top \mathbf{K}(\mathbf{d})^{-1} \mathbf{y} + \frac{1}{2} \log |\mathbf{K}(\mathbf{d})| \quad (19)$$
where \( \mathbf{d} = (d_1, \ldots, d_M)\top \), \( \mathbf{K}_m = (k_m(x_i, x_j))_{i,j=1}^N \) is the Gram matrix, and

\[
\mathbf{K}(\mathbf{d}) := \sigma_y^2 \mathbf{I}_N + \sum_{m=1}^M d_m \mathbf{K}_m.
\]

Using the quadratic upper-bounding technique in Wipf and Nagarajan (2008), we can rewrite the marginal likelihood (19) in a more meaningful expression as follows:

\[
-\log p(\mathbf{y}|\mathbf{d}) = \min_{f_1 \in \mathbb{R}^N, \ldots, f_M \in \mathbb{R}^N} \left( \frac{1}{2\sigma_y^2} \left\| \mathbf{y} - \sum_{m=1}^M f_m \right\|^2 + \frac{1}{2} \sum_{m=1}^M \frac{\|f_m\|^2}{d_m} \right) + \frac{1}{2} \log \left\| \sigma_y^2 \mathbf{I}_N + \sum_{m=1}^M d_m \mathbf{K}_m \right\|
\]

where \( f_m := (f_m(x_1), \ldots, f_m(x_N))\top \), and \( \|f_m\|_\mathbf{K}_m := f_m\top \mathbf{K}_m^{-1} f_m \). See Wipf and Nagarajan (2008, 2009) for more details. Now we can see that the minimization of marginal likelihood (20) is a special case of kernel-weight-based regularization (3) with a \emph{concave, nonseparable} regularizer defined as

\[
h(\mathbf{d}) = \log \left\| \sigma_y^2 \mathbf{I}_N + \sum_{m=1}^M d_m \mathbf{K}_m \right\|.
\]

We ask whether we can derive the block-norm formulation (see Section 2.3) for the marginal likelihood based MKL. Unfortunately Theorem 1 is not applicable because \( h \) is not convex. The result in Wipf and Nagarajan (2009, Appendix B) suggests that reparameterizing \( d_m = \exp(\eta_m) \), we have the following expression for the block-norm-based regularizer:

\[
g(\mathbf{x}) = \frac{1}{2} \inf_{\eta \in \mathbb{R}^M} \left( \sum_{m=1}^M x_m e^{-\eta_m} + \log \left\| \sigma_y^2 \mathbf{I}_N + \sum_{m=1}^M e^{\eta_m} \mathbf{K}_m \right\| \right).
\]

Importantly, the above minimization is a convex minimization problem. However, this does not change the fact that the original minimization problem (20) is a non-convex one. In fact, the term \( \|f_m\|_\mathbf{K}_m^{-1} e^{-\eta_m} \) is convex for \( \eta_m \) but not jointly convex for \( f_m \) and \( \eta_m \).

Instead of directly minimizing (e.g., by gradient descent) the marginal likelihood (19) to obtain a hyperparameter maximum likelihood estimation, we employ an alternative approach known as the MacKay update (MacKay, 1992; Wipf and Nagarajan, 2009). The MacKay update alternates between the minimization of right-hand-side of Equation (20) with respect to \( f_m \) and an (approximate) minimization of Equation (21) with respect to \( \eta_m \). The minimization in Equation (20) is a fixed kernel-weight learning problem (see Section 2.1) and for the special case of quadratic loss, it is simply a least-squares problem. For the approximate minimization of Equation (21) with respect to \( \eta_m \), we simply take the derivative of Equation (21) and set it to zero as follows:

\[
-x_m e^{-\eta_m} + \text{Tr} \left( \sigma^2 \mathbf{I}_N + \sum_{m=1}^M e^{\eta_m} \mathbf{K}_m \right)^{-1} e^{\eta_m} \mathbf{K}_m = 0,
\]

from which we have the following update equation:

\[
e^{\eta_m} \leftarrow \frac{x_m}{\text{Tr} \left( \sigma^2 \mathbf{I}_N + \sum_{m=1}^M e^{\eta_m} \mathbf{K}_m \right)^{-1} e^{\eta_m} \mathbf{K}_m}.
\]
Therefore, substituting $d_m = e^{nm}$ and $x_m = \| f_m \|^2_{K_m}$, we obtain the following iteration:

$$ (f_m)_{m=1}^M \leftarrow \arg\min_{(f_m)_{m=1}^M} \left( \frac{1}{2\sigma^2} \| y - \sum_{m=1}^M f_m \|^2 + \frac{1}{2} \sum_{m=1}^M \frac{\| f_m \|^2_{K_m}}{d_m} \right) $$

(22)

$$ d_m \leftarrow \frac{\| f_m \|^2_{K_m}}{\text{Tr} \left( (\sigma^2 I_N + \sum_{m=1}^M d_m K_m)^{-1} d_m K_m \right)} (m = 1, \ldots, M). $$

(23)

The convergence of this procedure is not established theoretically, but it is known to converge rapidly in many practical situations (Tipping, 2001).

4. Numerical experiments

In this section, we numerically compare MKL algorithms we discussed in this paper on three binary classification problems we have taken from Caltech 101 dataset (Fei-Fei et al., 2004). We have generate 1,760 kernel functions by combining four SIFT features, 22 spacial decompositions (including the spatial pyramid kernel), two kernel functions, and 10 kernel parameters\(^1\). More precisely, the kernel functions were constructed as combinations of the following four factors in the preprocessing pipeline:

- Four types of SIFT features, namely hsvsift (adaptive scale), sift (adaptive scale), sift (scale fixed to 4px), sift (scale fixed to 8px). We used the implementation by van de Sande et al. (2010). The local features were sampled uniformly (grid) from each input image. We randomly chose 200 local features and assigned visual words to every local features using these 200 points as cluster centers.

- Local histograms obtained by partitioning the image into rectangular cells of the same size in a hierarchical manner; i.e., level-0 partitioning has 1 cell (whole image) level-1 partitioning has 4 cells and level-2 partitioning has 16 cells. From each cell we computed a kernel function by measuring the similarity of the two local feature histograms computed in the same cell from two images. In addition, the spatial-pyramid kernel (Grauman and Darrell, 2007; Lazebnik et al., 2006), which combines these kernels by exponentially decaying weights, was computed. In total, we used 22 kernels (=one level-0 kernel + four level-1 kernels + 16 level-2 kernels + one spatial-pyramid kernel). See also Gehler and Nowozin (2009) for a similar approach.

- Two kernel functions (similarity measures). We used the Gaussian kernel:

$$ k(q(x), q(x')) = \exp \left( -\sum_{j=1}^n \frac{(q_j(x) - q_j(x'))^2}{2\gamma^2} \right), $$

for 10 band-width parameters ($\gamma$'s) linearly spaced between 0.1 and 5 and the $\chi^2$-kernel:

$$ k(q(x), q(x')) = \exp \left( -\gamma^2 \sum_{j=1}^n \frac{(q_j(x) - q_j(x'))^2}{(q_j(x) + q_j(x'))} \right). $$

\(^1\) Preprocessed data is available from \url{http://www.ibis.t.u-tokyo.ac.jp/ryotat/prmu09/data/}.  

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The combination of 4 sift features, 22 spatial regions, 2 kernel functions, and 10 parameters resulted in 1,760 kernel functions in total.

We compare uniform kernel combination, block 1-norm MKL, Elastic-net MKL with $\lambda = 0.5$, Elastic-net MKL with $\lambda$ chosen by cross validation on the training-set, $\ell_2$-norm MKL Cortes et al. (2009); Kloft et al. (2009) and empirical Bayesian MKL. $\ell_2$-norm MKL uses the hinge loss, and the other MKL models (except empirical Bayesian MKL) use the logit loss. We also include uniform kernel combination with the squared loss to make the comparison between the empirical Bayesian MKL and the rest possible. Since the difference between Uniform (logit) and Uniform (square) is small, we expect that the discussion here is not specific to the choice of loss functions. For the Elastic-net MKL (8), we either fix the constant $\lambda$ as $\lambda = 0.5$ (Elastic (0.5)) or we choose the value of $\lambda$ from $\{0, 0.0001, 0.001, 0.01, 0.1, 1, 10\}$. MKL models with the logit loss are implemented in SpicyMKL toolbox (Suzuki and Tomioka, 2009). For the empirical Bayesian MKL, we use the MacKay update (22)-(23). We used the implementation of $\ell_2$-norm MKL in Shogun toolbox Sonnenburg et al. (2010). The regularization constant $C$ was chosen by 2×4-fold cross validation on the training-set for each method. We used the candidate $\{0, 0.0001, 0.001, 0.01, 0.1, 1, 10\}$ for all methods except $\ell_2$-norm MKL and $\{0.0001, 0.001, 0.01, 0.1, 1, 10, 100, 1000\}$ for the $\ell_2$-norm MKL.

Figures 1–3 show the results of applying different MKL algorithms. We can see that overall $\ell_2$-norm MKL, Elastic-net MKL, and uniformly-weighted MKL perform favorable compared to other MKL methods. Empirical Bayesian MKL and block 1-norm MKL tend to perform worse than the above three methods, especially when the number of samples per class is smaller than 20. However, 2. Available from http://www.simplex.t.u-tokyo.ac.jp/~s-taiji/software/SpicyMKL/.
in Figure 3, they do perform comparably for the number of samples per class above 30. Although Elastic-net MKL and $\ell_2$-norm MKL perform almost the same as uniform MKL in terms of accuracy, the right panels show that these methods can find important kernel components automatically. More specifically, on the “Cannon vs Cup” dataset (Figure 1), Elastic-net MKL chose 88 Gaussian RBF kernel functions and 792 $\chi^2$ kernel functions. Thus it prefers $\chi^2$ kernels to Gaussian RBF kernels.
This agrees with the common choice in computer vision literature. In addition, Elastic-net MKL consistently chose the band width parameter $\gamma = 0.1$ for the Gaussian RBF kernels but it never chose $\gamma = 0.1$ for the $\chi^2$ kernels; instead it averaged all $\chi^2$ kernels from $\gamma = 1.2$ to $\gamma = 10$.

5. Conclusion

We have shown that various MKL and structured sparsity models including $\ell_p$-norm MKL, Elastic-net MKL, multi-task learning, Wedge penalty, and overlapped group lasso can be seen as applications of different regularization strategies. These models have been conventionally presented in either kernel-weight-based regularization or block-norm-based regularization. We have shown that these two formulations can be systematically mapped to each other under some conditions through a concave conjugate transformation; see Table 1.

Furthermore, we have proposed a marginal-likelihood-based kernel learning algorithm. We have shown that the propose empirical Bayesian MKL can be considered to be employing a nonconvex nonseparable regularizer on the kernel weights. Furthermore, we have derived the expression for the block-norm regularizer corresponding to the proposed empirical Bayesian MKL.

We have tested the classification performance as well as the resulting kernel weights of various regularized MKL models we have discussed on visual categorization task from Caltech 101 dataset using 1,760 kernels. We have shown that Elastic-net MKL can achieve comparable classification accuracy to uniform kernel combination with roughly half of the candidate kernels and provide information about the usefulness of the candidate kernels. $\ell_2$-norm MKL also achieves similar classification performance and qualitatively similar kernel weights. However $\ell_2$-norm MKL does not achieve sparsity in the kernel weights in contrast to Elastic-net MKL. Empirical Bayesian MKL tends to perform worse than the above two methods probably because the kernel weights it obtains becomes extremely sparse. One way to avoid such solution is to introduce hyper-priors for the kernel weights as in Urtasun (2010).

We are currently aiming to relax the sufficient condition in Theorem 1 to guarantee mapping from the kernel-weight-based formulation to block-norm-based formulation. We would also like to have a finer characterization of the block-norm regularizer corresponding to the empirical Bayesian MKL (see also Wipf and Nagarajan (2008)). Theoretical argument concerning when to use sparse MKL models (e.g., $\ell_1$-norm MKL or empirical Bayesian MKL) and when to use non-sparse MKL models ($\ell_p$-norm MKL) is also necessary.

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Appendix A. Proof of Equation (1) in a finite dimensional case

In this section, we provide a proof of Equation (1) when $\mathcal{H}_1, \ldots, \mathcal{H}_m$ are all finite dimensional. We assume that the input space $\mathcal{X}$ consists of $N$ points $x_1, \ldots, x_N$, for example the training points. The function $f_m \in \mathcal{H}_m$ is completely specified by the function values at the $N$-points $f_m = (f_m(x_1), \ldots, f_m(x_N))^\top$. The kernel function $k_m$ is also specified by the Gram matrix $K_m = (k_m(x_i, x_j))_{i,j=1}^N$. The inner product $\langle f_m, g_m \rangle_{\mathcal{H}_m}$ is written as $\langle f_m, g_m \rangle_{\mathcal{H}_m} = f_m^\top K_m^{-1} g_m$, where $g_m$ is the $N$-dimensional vector representation of $g_m \in \mathcal{H}_m$, assuming that the Gram matrix $K_m$ is positive definite. It is easy to check the reproducibility; in fact, $\langle f_m, k_m(\cdot, x_i) \rangle = f_m^\top K_m^{-1} K_m(:, i) = f(x_i)$, where $K_m(:, i)$ is a column vector of the Gram matrix $K_m$ that corresponds to the $i$th sample point $x_i$.

The right-hand side of Equation (1) is written as follows:

$$\min_{f_1, \ldots, f_M \in \mathbb{R}^N} \sum_{m=1}^M \frac{f_m^\top K_m^{-1} f_m}{d_m} \quad \text{s.t.} \quad \sum_{m=1}^M f_m = \bar{f}. $$

Forming the Lagrangian, we have

$$\sum_{m=1}^M \frac{f_m^\top K_m^{-1} f_m}{d_m} = \sum_{m=1}^M \frac{f_m^\top K_m^{-1} f_m}{d_m} + 2\alpha^\top \left( \bar{f} - \sum_{m=1}^M f_m \right) \geq -\alpha^\top \left( \sum_{m=1}^M d_m K_m \right) \alpha + 2\alpha^\top \bar{f} \geq \max_{\alpha} \bar{f}^\top \left( \sum_{m=1}^M d_m K_m \right)^{-1} \bar{f},$$

where the equality is obtained for $f_m = d_m K_m \left( \sum_{m=1}^M d_m K_m \right)^{-1} \bar{f}$. 

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