rls_dual_mkl: A PFBS-based Implementation for Multiple Kernel Learning

(Jeremiah) Zhe Liu zhl112@mail.harvard.edu
Department of Biostatistics
Harvard School of Public Health
Boston, MA, 02115

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1. Introduction

1.1. Multiple Kernel Learning Problem

Multiple kernel learning (MKL) (Bach et al. (2004)) is the process of finding an optimal kernel from a prescribed (convex) set $\mathcal{K}$ of basis kernels, for learning a real-valued function by regularization. In this work, we consider a RKHS $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \cdots \oplus \mathcal{H}_M$ with reproducting kernel $\mathbf{k} \in \mathcal{K} = \{\sum_{i=1}^M c_i \mathbf{k}_i | (c_i \geq 0 \forall i) \wedge \sum_{i=1} c_i = 1\}$ such that $f = \sum_{i=1}^M f_i, f_i \in \mathcal{H}_i$. By Micchelli and Pontil (2005), the problem of multiple kernel learning corresponds to find f^* such that:

$$\arg\min_{f \in \mathcal{H}} \Big\{ \frac{1}{n} \sum_{i=1}^n Q(\sum_{j=1}^M f_j(\mathbf{x}), \mathbf{y}) + \tau g\big((\sum_{j=1}^M ||f_j||_{\mathcal{H}})^2 \big) \Big\}$$

Rosasco et al. (2009) generalized above problem by taking Q to be square loss, $g(.) = \sqrt{.}$ and also impose L1 regularization, leading to the elastic-net-regulated problem:

$$\arg\min_{f \in \mathcal{H}} \Big\{ \frac{1}{n} \sum_{i=1}^n (\sum_{j=1}^M f_j(x_i) - y_i)^2 + \mu \sum_{j=1}^M ||f_j||_{\mathcal{H}}^2 + 2\tau \sum_{j=1}^M ||f_j||_{\mathcal{H}} \Big\} \tag{1}$$

1.2. Iterative PFBS Algorithm

By Theorem 1 of Rosasco et al. (2009), since the penalty function is lower semicontinuous, coercive, convex and one-homogenous, solution to problem 1 f^* is the unique fixed point of the the contractive mapping with step size σ:

$$\mathcal{T}_\sigma(f) = (\mathbf{I} - \pi_{\frac{\tau}{\sigma}K})\big(f - \frac{1}{2\sigma} \nabla_f [\frac{1}{n} ||f - y||^2]\big)$$

where $\pi_{\frac{\tau}{\sigma}K}(g)$ is a project operator which project g to $\mathcal{H}' = \{f \in \mathcal{H} \big| \ ||f_j||_{\mathcal{H}_j} \leq \frac{1}{\tau/\sigma} \ \forall j\}$, or more rigorously:

$$\pi_{\frac{\tau}{\sigma}K}(g) = \frac{\tau}{\sigma} v, \qquad \text{where } v = \arg \min_{v \in \mathcal{H}, ||v_j|| \leq 1} ||\frac{\tau}{\sigma} v - g||_{\mathcal{H}}^2$$

Above mapping can also be written in terms of Kernel matrices by generalizing representer theorem and write $f_j^*(x) = \sum_{i=1}^n \alpha_{ji}^T k_j(x_i, x) = \boldsymbol{\alpha}_j^T \mathbf{k}_j(x)$, where $\boldsymbol{\alpha}_j$ and $\mathbf{k}_j(x)$ are $n \times 1$ vectors. Further, if denote:

$$\begin{aligned}
\boldsymbol{\alpha}_{Mn\times 1} &= (\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_M)^T \\
\mathbf{k}(x)_{Mn\times 1} &= (\mathbf{k}_1(x)^T, \ldots, \mathbf{k}_M(x)^T)^T \\
\mathbf{K}_{Mn\times Mn} &= \begin{bmatrix} \mathbf{K}_1 & \ldots & \mathbf{K}_M \\ \vdots & \ddots & \vdots \\ \mathbf{K}_1 & \ldots & \mathbf{K}_M \end{bmatrix}, \text{where } \mathbf{K}_i = \mathbf{k}_i(.)\mathbf{k}_i(.)^T \\
\mathbf{y}_{Mn\times 1} &= (y_{n\times 1}^T, \ldots, y_{n\times 1}^T)^T
\end{aligned}$$

The contraction mapping can be written as:

$$\mathcal{T}_\sigma(f) = (\mathbf{I} - \pi_{\frac{\tau}{\sigma}K})\big(\big[(1-\frac{\mu}{\sigma})\boldsymbol{\alpha} - \frac{1}{\sigma n}(\mathbf{K}\boldsymbol{\alpha} - \mathbf{y})\big]^T\mathbf{k}\big) \qquad \text{where} \tag{2}$$

$$\pi_{\frac{\tau}{\sigma}K}(g)_j = min\{1, \frac{||g_j||_{\mathcal{H}_j}}{\tau/\sigma}\} * \frac{g_j}{||g_j||_{\mathcal{H}_j}} = min\{1, \frac{\sqrt{\boldsymbol{\alpha}_j^T\mathbf{K}_j\boldsymbol{\alpha}_j}}{\tau/\sigma}\} * \frac{\boldsymbol{\alpha}_j^T\mathbf{k}_j}{\sqrt{\boldsymbol{\alpha}_j^T\mathbf{K}_j\boldsymbol{\alpha}_j}}$$

Thus the projection $\mathbf{I} - \pi_{\frac{\tau}{\sigma}K}$ corresponds to the soft-thresholding operator for $\boldsymbol{\alpha}_j$:

$$\mathbf{S}_{\frac{\tau}{\sigma}}(K, \boldsymbol{\alpha})_j = \frac{\boldsymbol{\alpha}_j^T}{\sqrt{\boldsymbol{\alpha}_j^T\mathbf{K}_j\boldsymbol{\alpha}_j}}(\sqrt{\boldsymbol{\alpha}_j^T\mathbf{K}_j\boldsymbol{\alpha}_j} - \frac{\tau}{\sigma})_+$$

Above discussions lead to below algorithm:

Algorithm 1: MKL Algorithm

set $\boldsymbol{\alpha}^0 = \mathbf{0}$

for $p = 1$ to `MAX_ITER` **do**

$\boldsymbol{\alpha}_0^p = (1 - \frac{\mu}{\sigma})\boldsymbol{\alpha}^{p-1} - \frac{1}{\sigma n}(\mathbf{K}\boldsymbol{\alpha}^{p-1} - \mathbf{y})$
$\boldsymbol{\alpha}^p = \mathbf{S}_{\frac{\tau}{\sigma}}(K, \boldsymbol{\alpha}_0^p)$

end for

return $f^{\texttt{MAX\_ITER}} = (\boldsymbol{\alpha}^{\texttt{MAX\_ITER}})^T\mathbf{k}$

1.3. Implementation Detail

1.3.1. Block-wise Update

Notice that in (2), $\mathcal{T}_\sigma$ updates $\boldsymbol{\alpha}$ by group, it is thus possible to write $\mathcal{T}$ at p^{th} step as:

$$\mathcal{T}_\sigma^p = [\mathcal{T}_{\sigma,1}^p, \mathcal{T}_{\sigma,2}^p, \ldots, \mathcal{T}_{\sigma,M}^p] \qquad \text{with} \qquad \mathcal{T}_{\sigma,j}^p = \mathbf{S}_{\frac{\tau}{\sigma}}\Big(K, \boldsymbol{\alpha}_0\Big)_j$$

$$\boldsymbol{\alpha}_0 = (1 - \frac{\mu}{\sigma})\boldsymbol{\alpha}_j^{p-1} - \frac{1}{n\sigma} * \boldsymbol{\epsilon}^{p-1} \qquad \text{where } \boldsymbol{\epsilon}^{p-1} = (\sum_{j=1}^{M}\mathbf{K}_j\boldsymbol{\alpha}_j^{p-1} - y)$$

by using above method we are able to avoid working directly with the $Mn \times Mn$ matrix $\mathbf{K}$ (as defined earlier in section 1.2), which led to reduced memory cost [1] and reduced difficulty in selecting stepsize and regularization parameters.

1. $O(Mn^2)$ instead of $O(M^2n^2)$

1.3.2. Choice of Stepsize

Based on Bach et al. (2004), it can be shown that a suitable choice of σ is $\sigma = \frac{1}{4}(a * L_{min} + b * L_{max}) + \mu$, where (b, a) denotes the lower/upper bound on the eigenvalue of $\mathbf{K}$, and (L_{min}, L_{max}) denotes the lower/upper bound of $\nabla^2 Q(\mathbf{f}, \mathbf{y})$.

In the context where Q is square loss (i.e. $\nabla^2_{\mathbf{f}} Q(\mathbf{f}, \mathbf{y}) = 2$), we have:

$$\sigma = \frac{1}{2}(a + b) + \mu$$

A naive choice of a would be the largest eigenvalue of $\mathbf{K}_{nM\times nM}$, which not only is computationally expensive but also leads to overly slow convergence. In pactice, if denote the maximum eigenvalue of each kernel matrix K_j to be a_j, it is found that setting a to be $\max\limits_{j\in\{1,..,M\}}(a_j)$ is suffice to guarantee convergence. This is because the mapping $\boldsymbol{\alpha}^{p-1} \mapsto \boldsymbol{\alpha}_0^p$ can be written as:

$$\boldsymbol{\alpha}_0 = (1 - \frac{\mu}{\sigma})\boldsymbol{\alpha}_j^{p-1} - \frac{1}{n} * \sum_{j=1}^{M} \frac{1}{\sigma}(\mathbf{K}_j \boldsymbol{\alpha}_j^{p-1} - \frac{y}{n})$$

As shown, in $\boldsymbol{\alpha}^{p-1} \mapsto \boldsymbol{\alpha}_0^p$ we actually updated $\boldsymbol{\alpha}^{p-1}$ M times, with step size $\frac{1}{\sigma}(\mathbf{K}_j\boldsymbol{\alpha}_j^{p-1} - \frac{y}{n})$ in each step. It is thus sufficient to find a a that properly scale the magnitude of all $||\mathbf{K}||$, leading natually to the choice $a = \max\limits_{j\in\{1,..,M\}}(a_j)$.

1.3.3. Effect of μ and τ

The convergence of the aforementioned procedure is guaranteed by Banach Fixed Point theorem, given proper choice of σ.

Zou and Hastie (2005)

Rosasco et al. (2009)

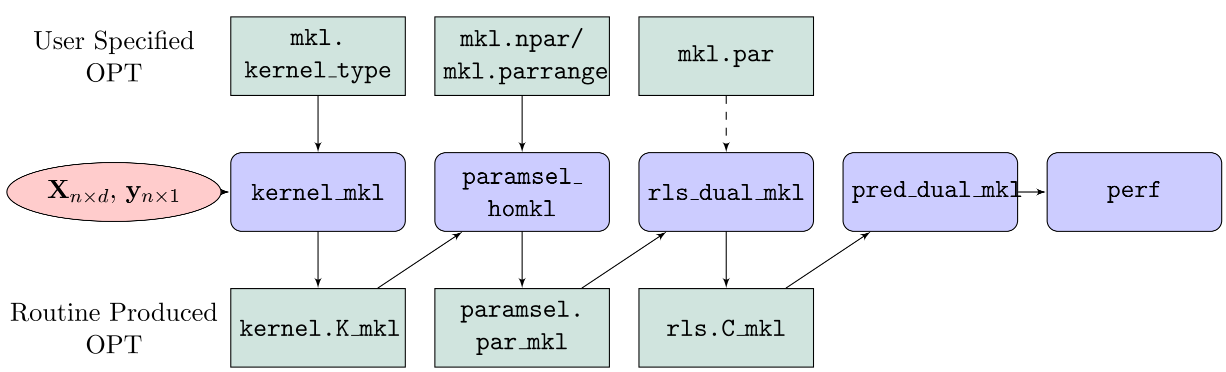
Contraction mapping

$||(1 - \frac{\mu}{\sigma})\mathbf{I} - \frac{1}{\sigma n}\mathbf{K}||$

Continuation strategy.

$\frac{\tau}{\sigma}_{max} = \frac{||y||^2}{||\mathbf{K}||}$

2. Software Structure and Usage



1. Parameter Specification
   - util/gurls_defopt_mkl
2. Kernel Generation
   - kernel/kernel_mkl
3. Parameter Selection
   - kernel/paramsel_homkl
   - util/paramsel_L1ratioguesses
4. Optimization
   - optimizers/rls_dual_mkl
   - optimizers/rls_dual_mkl_pfbs
   - util/ConsoleProgressBar
   - summary/plot_mkl_L1path
5. Prediction
   - kernel/predkernel_traintest
   - optimizers/pred_dual_mkl
6. Performance assessment
   - perf/perf_rmsestd

3. Example

[2]

2. LIBSVM Data Repository: 'https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary.html'

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