## Algorithm for bilinear maps

Miaoyan Wang, Aug 21, 2020

#### 1 Notation

- 1.  $\mathbb{O}(d,r) := \{ \boldsymbol{P} \in \mathbb{R}^{d \times r} : \boldsymbol{P}^T \boldsymbol{P} = \boldsymbol{I}_r \}$ , the collection of d-by-r matrices whose columns are orthonormal. When no confusion arises, I use the term "projection matrix" to denote either the matrix  $\boldsymbol{P}\boldsymbol{P}^T \in \mathbb{R}^{d \times d}$  or the matrix  $\boldsymbol{P} \in \mathbb{R}^{d \times r}$ .
- 2.  $\mathcal{K}^{\text{row}}(i, j, \boldsymbol{X}, \boldsymbol{X}') := \langle \Phi(\boldsymbol{X}_{i:}), \Phi(\boldsymbol{X}'_{j:}) \rangle$  denotes the value of row kernel evaluated at the vector pair, (*i*-th row of matrix  $\boldsymbol{X}$ , *j*-th row of matrix  $\boldsymbol{X}'$ ).
- 3. I sometimes use the shorthand  $\mathcal{K}^{\text{row}}(i,j)$  to denote  $\mathcal{K}^{\text{row}}(i,j,\boldsymbol{X},\boldsymbol{X}')$ , when the feature pair  $(\boldsymbol{X},\boldsymbol{X}')$  is clear given the contexts. Note that  $\mathcal{K}^{\text{row}}(i,j)$  can be calcualted without explicit feature mapping. Similar convention for  $\mathcal{K}^{\text{col}}(i,j,\boldsymbol{X},\boldsymbol{X}')$ .
- 4. Let  $\mathbf{W}^{\text{row}} = \mathbf{P}_r \mathbf{P}_r^T = \llbracket w_{ij}^{\text{row}} \rrbracket \in \mathbb{R}^{d_1 \times d_1}$  and  $\mathbf{W}^{\text{col}} = \mathbf{P}_c \mathbf{P}_c^T = \llbracket w_{ij}^{\text{col}} \rrbracket \in \mathbb{R}^{d_2 \times d_2}$  denote the rowand column-wise projection matrices, respectively.

## 2 Algorithm based on bilinear maps

Consider the bilinear mapping,

$$\Phi \colon \mathbb{R}^{d_1 \times d_2} \to (\mathcal{H}_r \times \mathcal{H}_c)^{d_1 \times d_2}$$
$$\boldsymbol{X} \mapsto [\Phi(\boldsymbol{X})_{ij}], \quad \text{where } \Phi(\boldsymbol{X})_{ij} \stackrel{\text{def}}{=} (\phi_c(\boldsymbol{X}_{i:}), \ \phi_r(\boldsymbol{X}_{:j})).$$

Primal problem:

$$\min_{\boldsymbol{P}_r, \boldsymbol{P}_c} \min_{\boldsymbol{C}} \quad \frac{1}{2} \|\boldsymbol{C}\|_F^2 + c \sum_{i=1}^n \xi_i, 
\text{subject to} \quad y_i \langle \boldsymbol{P}_r \boldsymbol{C} \boldsymbol{P}_c^T, \ \Phi(\boldsymbol{X}_i) \rangle \leq 1 - \xi_i \text{ and } \xi_i \geq 0, \ i = 1, \dots, n.$$
(1)

Parameters in the primal problem:  $(P_r, P_c, C)$ , where  $P_r \in \mathbb{O}(d_1, r_1)$ ,  $P_c \in \mathbb{O}(d_2, r_2)$ , and  $C = [(c_i^{\text{row}}, c_j^{\text{col}})] \in (\mathcal{H}_r \times \mathcal{H}_c)^{r_1 \times r_2}$  is the "core matrix" consisting of linear coefficients.

1. Update C, given  $(P_r, P_c)$ .

implicit update 
$$C \leftarrow \sum_i \alpha_i y_i \boldsymbol{P}_r^T \Phi(\boldsymbol{X}_i) \boldsymbol{P}_c$$
.

- Saved quantities: dual variables  $\alpha \in \mathbb{R}^n$ .
- Auxiliary quantities: kernel  $\mathcal{K}(X, X')$  specified below.
- Objective value: objective value for the dual problem.

Details: We use kernel trick to solve for  $\alpha$  without explicit feature mapping. Given the projections  $(P_r, P_c)$ , the optimization (1) is a standard SVM with kernel

$$\mathcal{K}(\boldsymbol{X}, \boldsymbol{X}') = \langle \boldsymbol{P}_r^T \Phi(\boldsymbol{X}) \boldsymbol{P}_c, \ \boldsymbol{P}_r^T \Phi(\boldsymbol{X}') \boldsymbol{P}_c \rangle 
= (\sum_{i,j} w_{ij}^{\text{col}}) (\sum_{i,j} w_{ij}^{\text{row}} K^{\text{row}}(i,j)) + (\sum_{i,j} w_{ij}^{\text{row}}) (\sum_{i,j} w_{ij}^{\text{col}} K^{\text{col}}(i,j)).$$
(2)

for all feature pairs (X, X'). Here I have used the shorthand  $K^{\text{row}}(i, j)$  to denote the value of row kernel evaluated on the *i*-th row of X and *j*-th row of X'.

Remark 1 (Computational consideration). We can compute the summations in (2) without explicit loop. In particular, both identities hold:  $\sum_{i,j} w_{ij}^{\text{col}} = \|\mathbf{1}^T \mathbf{P}_c\|_2^2$  and  $\sum_{i,j} w_{ij}^{\text{row}} K^{\text{row}}(i,j) = \text{trace}(\mathbf{W}^T \mathbf{K})$ , where  $\mathbf{K} \leftarrow [\![K^{\text{row}}(i,j,\mathbf{X},\mathbf{X}')]\!]$  is a pre-stored matrix (or array, if we go through all possible feature pairs  $(\mathbf{X},\mathbf{X}')$ ).

2. Update  $P_r^{\text{new}}$ , given  $(C, P_c)$ .

explicit update 
$$\tilde{\boldsymbol{P}}_r^{\text{new}} \leftarrow \sum_i \beta_i y_i \Phi(\boldsymbol{X}_i) \boldsymbol{P}_c \boldsymbol{C}^T = \sum_{i,j} \beta_i \alpha_j y_i y_j \underbrace{\Phi(\boldsymbol{X}_i) \boldsymbol{P}_c \boldsymbol{P}_c^T \Phi^T(\boldsymbol{X}_j)}_{d_1\text{-by-}d_1 \text{ matrix over } \mathbb{R}} \boldsymbol{P}_r$$
normalize  $\boldsymbol{P}_r^{\text{new}} \leftarrow \text{QR}$  decomposition of  $\tilde{\boldsymbol{P}}_r^{\text{new}}$ .

- Saved quantities:  $\mathbf{P}^{\text{new}} \in \mathbb{O}(d_1, r_1)$ .
- Auxiliary quantities: matrix  $\Phi(\boldsymbol{X}_i)\boldsymbol{P}_c\boldsymbol{P}_c^T\Phi^T(\boldsymbol{X}_j)$ , dual variables  $\boldsymbol{\beta}\in\mathbb{R}^n$ .
- Objective value: objective value for the dual problem.

Details: for each feature pair  $(i, j) \in [n]^2$ , we compute the matrix  $\Phi(\mathbf{X}_i) \mathbf{P}_c \mathbf{P}_c^T \Phi^T(\mathbf{X}_j)$  without explicit feature mapping,

$$\underbrace{\Phi(\boldsymbol{X}_{i})\boldsymbol{P}_{c}\boldsymbol{P}_{c}^{T}\Phi^{T}(\boldsymbol{X}_{j})}_{=:\boldsymbol{M}} = \left(\sum_{s,s'}w_{ss'}^{\operatorname{col}}\right)\begin{bmatrix}K^{\operatorname{row}}(1,1,\boldsymbol{X}_{i},\boldsymbol{X}_{j}) & \cdots & K^{\operatorname{row}}(1,d_{1},\boldsymbol{X}_{i},\boldsymbol{X}_{j})\\ \vdots & \vdots & \vdots\\ K^{\operatorname{row}}(d_{1},1,\boldsymbol{X}_{i},\boldsymbol{X}_{j}) & \cdots & K^{\operatorname{row}}(d_{1},d_{1},\boldsymbol{X}_{i},\boldsymbol{X}_{j})\end{bmatrix} + \\
\left(\sum_{s,s'}w_{ss'}^{\operatorname{col}}K^{\operatorname{col}}(s,s',\boldsymbol{X}_{i},\boldsymbol{X}_{j})\right)\begin{bmatrix}1 & 1 & \cdots & 1\\ \vdots & \vdots & \vdots & \vdots\\ 1 & 1 & \cdots & 1\end{bmatrix}, \quad (3)$$

where  $K^{\text{row}}(s, s', \boldsymbol{X}_i, \boldsymbol{X}_j)$  denotes the value of row kernel value evaluated on the s-th row of  $\boldsymbol{X}_i$  and s'-th row of  $\boldsymbol{X}_j$ , and likewise for  $K^{\text{col}}(s, s', \boldsymbol{X}_i, \boldsymbol{X}_j)$ .

The coefficient  $\beta$  is obtained from a standard SVM with kernel

$$\mathcal{K}(\boldsymbol{X}, \boldsymbol{X}') = \text{trace}(\underbrace{\Phi(\boldsymbol{X})\boldsymbol{P}_{c}\boldsymbol{C}^{T}}_{=:\boldsymbol{A}}(\underbrace{\boldsymbol{C}\boldsymbol{C}^{T}}_{=:\boldsymbol{B}})^{-1}\underbrace{\boldsymbol{C}\boldsymbol{P}_{c}^{T}\boldsymbol{\Phi}^{T}(\boldsymbol{X}')}_{=:\boldsymbol{A}^{T}}),$$

for feature pair (X, X'), where

$$B = CC^{T} = \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} P_{r}^{T} \Phi(\mathbf{X}_{i}) P_{c} P_{c}^{T} \Phi^{T}(\mathbf{X}_{j}) P_{r},$$

$$A = \Phi(\mathbf{X}) P_{c} C^{T} = \sum_{i} \alpha_{i} y_{i} \Phi(\mathbf{X}) P_{c} P_{c}^{T} \Phi^{T}(\mathbf{X}_{i}) P_{r}.$$

are calculated using (3).

- 3. Update  $C^{\text{new}}$ , given  $(P_r^{\text{new}}, P_c)$ .
- 4. Update  $P_c$ , given  $(C^{\text{new}}, P_r^{\text{new}})$ ; denoted by  $(C, P_r)$  in the following formula.

explicitle update 
$$P_c^{\text{new}} \leftarrow \sum_i \gamma_i y_i \Phi^T(\boldsymbol{X}_i) P_r \boldsymbol{C} = \sum_{i,j} \gamma_i \alpha_j y_i y_j \underbrace{\Phi^T(\boldsymbol{X}_i) P_r P_r^T \Phi(\boldsymbol{X}_j)}_{d_2\text{-by-}d_2 \text{ matrix over } \mathbb{R}} P_c$$
normalize  $P_c^{\text{new}} \leftarrow \text{QR}$  decomposition of  $\tilde{P}_c^{\text{new}}$ .

The auxiliary quantities,  $\Phi^T(X_i)P_rP_r^T\Phi(X_j)$  and  $\gamma$ , are calculated similarly as in step 2.

# 3 Outputs

- 1. Convergence criterum? Objective value in the dual problem.
- 2. How to read off the decision function from the algorithm?

$$f(\boldsymbol{X}_{\text{new}}) = \langle \boldsymbol{P}_r^T \Phi(\boldsymbol{X}_{\text{new}}) \boldsymbol{P}_c, \sum_i \alpha_i y_i \boldsymbol{P}_r^T \Phi(\boldsymbol{X}_i) \boldsymbol{P}_c \rangle$$

$$= \sum_i \alpha_i y_i \left\{ \left( \sum_{s,s'} w_{ss'}^{\text{col}} \right) \left( \sum_{s,s'} w_{ss'}^{\text{row}} K^{\text{row}}(s,s',\boldsymbol{X}_i,\boldsymbol{X}_{\text{new}}) \right) + \left( \sum_{s,s'} w_{ss'}^{\text{row}} \right) \left( \sum_{s,s'} w_{ss'}^{\text{col}} K^{\text{col}}(s,s',\boldsymbol{X}_i,\boldsymbol{X}_{\text{new}}) \right) \right\}.$$

3. How to estimate the intercept in the primal problem?

$$\hat{b}_0 = \underset{b_0 \in \mathbb{R}}{\operatorname{arg min}} \left\{ \sum_{i=1}^n (1 - y_i f(\mathbf{X}_i) - y_i b_0)_+ \right\}.$$

4. Penalty in the primal problem?

$$\|\boldsymbol{C}\|_F^2 = \sum_{i,j} \alpha_i \alpha_j y_i y_j \operatorname{trace}(\Phi(\boldsymbol{X}_i) \boldsymbol{P}_c \boldsymbol{P}_c^T \Phi^T(\boldsymbol{X}_j) \boldsymbol{P}_r \boldsymbol{P}_r^T) = (\boldsymbol{\alpha} \circ \boldsymbol{y})^T [\![ \mathcal{K}(\boldsymbol{X}_i, \boldsymbol{X}_j) ]\!] (\boldsymbol{\alpha} \circ \boldsymbol{y}),$$

where  $[\![\mathcal{K}(\boldsymbol{X}_i, \boldsymbol{X}_j)]\!] \in \mathbb{R}^{n \times n}$  is defined in (2) and  $\boldsymbol{\alpha} \in \mathbb{R}^n$  is the dual parameter in step 1 or 3. We omit the explicit expression of  $\|\boldsymbol{C}\|_F^2$  because it is not needed in our algorithm.

#### 4 Sanity check

- 1. Monotonic decreasing in objective value? Yes.
- 2. Consistent with earlier linear kernel algorithm, smmk(....)? Yes.
- 3. Consistent with one-way linear mapping? Yes.

```
## generate data with linear kernel
source("SMMfunctions.R")
set.seed (1818)
m = 3; n = 3; r = 1; N = 100; b0 = 0.1
result = gendat(m,n,r,N,b0)
X = result$X; y = result$y; dat = result$dat;B = result$B
X_t=X ## transform
y_true=rep(0,N)
for(i in 1:N){
X_t[[i]]=t(X[[i]])
y_true[i]=sum(B*X[[i]])
svd(B)$v[,1] ## true col projection
svd(B)$u[,1] ## true row projection
## Algorithm 1: earlier algorithm
source("SMMKfunctions.R")
old= smmk(X,y,r=1,kernel = "linear");
old$V ## est col projection
old_t= smmk(X_t,y,r=1,kernel = "linear");
old_t$V ## est row projection
## Algorithm 2: one-way map. Separate row/column projection.
source("SMMKfunctions_bilinear.R")
new = smmk_new(X,y,kernel_row="const",kernel_col="linear",
r=c(1,1),cost=10/3);
new$P_col ## est col projection; similar to earlier old$V
new = smmk_new(X,y,kernel_row="linear",kernel_col="const",
```

```
r=c(1,1),cost=10/3);
new$P_row ## est row projection; similar to earlier old_t$V

### Algorithm 2: two-way map. Simultaneous row/column projections.
new_double = smmk_new(X,y,kernel_row="linear",kernel_col="linear",
r=c(1,1),cost=10,rep=1);
plot(new_double$obj)
new_double$P_col ## est col projection
new_double$P_row ## est row projection
plot(new_double$fitted,y_true)

### Algorithm 2: two-way map + transform. Results should be consistent.
new_double = smmk_new(X_t,y,kernel_row="linear",kernel_col="linear",
r=c(1,1),cost=10,rep=1);
new_double$P_row ## est col projection
new_double$P_row ## est row projection
new_double$P_col ## est row projection
plot(new_double$fitted,y_true)
```

Sanity check under linear kernel, d = 3, r = 1, N = 100.

Parameters	Truth	Symmetric trick (SMMK)	Bilinear map
col projection	(0.63, 0.33, 0.70)	(0.66, 0.33, 0.67)	(0.70, 0.39, 0.58)
			(0.64, 0.53, 0.55)
row projection	(-0.54, 0.83, 0.08)	(-0.55, 0.83, 0.06)	(-0.48, 0.87, 0.09)
			(-0.53, 0.84, 0.07)