Algorithmic perspectives of kernel method

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1 A choice of feature mapping Φ

To derive an algorithm, I choose to use Mapping 1 in the previous note for convenience.

$$\Phi \colon \mathbb{R}^{d_1 \times d_2} \to \mathcal{H}_r^{d_1} \times \mathcal{H}_c^{d_2}$$

$$\boldsymbol{X} \mapsto (\Phi_r(\boldsymbol{X}) \Phi_c(\boldsymbol{X})) \stackrel{\text{def}}{=} (\phi_r([\boldsymbol{X}]_{1:}), \dots, \phi_r([\boldsymbol{X}]_{d_1:}), \phi_c([\boldsymbol{X}]_{:1}) \dots, \phi([\boldsymbol{X}]_{:d_2})).$$

We define decision function,

$$f(\boldsymbol{X}) = \langle \boldsymbol{B}, \Phi(\boldsymbol{X}) \rangle, \text{ where } \boldsymbol{B} = (\boldsymbol{B}_r, \boldsymbol{B}_c) \in \mathcal{H}_r^{d_1} \times \mathcal{H}_c^{d_2}$$

$$= \langle \boldsymbol{B}_r, \Phi_r(\boldsymbol{X}) \rangle + \langle \boldsymbol{B}_c, \Phi_c(\boldsymbol{X}) \rangle$$

$$= \sum_{k=1}^n \alpha_k^r \sum_{i,j \in [d_2]} w_{ij}^{row} K([\boldsymbol{X}_k]_{i\cdot}, [\boldsymbol{X}]_{j\cdot}) + \sum_{k=1}^n \alpha_k^c \sum_{i,j \in [d_2]} w_{ij}^{col} K([\boldsymbol{X}_k]_{\cdot i}, [\boldsymbol{X}]_{\cdot j}),$$

$$(1)$$

where $X^1, ... X^n$ are sampled matrix features and $W^{\text{col}}, W^{\text{row}}$ are some positive semi definite matrices with low rank. We estimate $\boldsymbol{\alpha}^r = (\alpha_1^r, ..., \alpha_n^r), \boldsymbol{\alpha}^c = (\alpha_1^c, ..., \alpha_n^c), W^{\text{col}}, \text{ and } W^{\text{row}}$ from the training data set.

Could you provide the correspondence between (alpha, W) and the outputs in our Algorithm?

We will use W (or P) for visualization/interpretation in data applications —> similar to loading matrices in PCA.

2 Algorithm derivation

We solve an optimization problem

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

where $\|\boldsymbol{B}\|_F^2 = \|\boldsymbol{B}_r\|_F^2 + \|\boldsymbol{B}_c\|_F^2$. From the low rank assumption on \boldsymbol{B} such that

$$B = (B_r, B_c) = CP^T = (C_r, C_c)(P_r, P_c)^T,$$

where $C = (C_r, C_c) \in \mathcal{H}_r^r \times \mathcal{H}_c^r$ and $P = (P_r, P_c) \in \mathbb{R}^{d_1 \times r} \times \mathbb{R}^{d_2 \times r}$. We assume that P_r, P_c are orthonormal matrices.

1. First we update C holding P fixed. The dual problem of Equation (2) is

$$\min_{\boldsymbol{\alpha}=(\alpha_1,\dots,\alpha_n)} - \sum_{i=1}^n \alpha_i + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \langle \Phi(\boldsymbol{X}_i) \boldsymbol{P} \boldsymbol{P}^T, \Phi(\boldsymbol{X}_j) \boldsymbol{P} \boldsymbol{P}^T \rangle$$
subject to
$$\sum_{i=1}^n y_i \alpha_i = 0, \text{ and } 0 \le \alpha_i \le C, i = 1, \dots, n.$$

Define $\mathbf{K}(i,j) \in \mathbb{R}^{d_1 \times d_1} \times \mathbb{R}^{d_2 \times d_2}$ as

$$\boldsymbol{K}(i,j) = (\boldsymbol{K}_r(i,j), \boldsymbol{K}_c(i,j)) \stackrel{\text{def}}{=} \Phi(\boldsymbol{X}_i)^T \Phi(\boldsymbol{X}_j)$$

where
$$[\boldsymbol{K}_r(i,j)]_{pq} = K_r([\boldsymbol{X}_i]_{p:}, [\boldsymbol{X}_i]_{q:}), \stackrel{\text{def}}{=} \langle \phi_r([\boldsymbol{X}_i]_{p:}), \phi_r([\boldsymbol{X}_j]_{q:}) \rangle,$$

 $[\boldsymbol{K}_c(i,j)]_{pq} = K_c([\boldsymbol{X}_i]_{:p}, [\boldsymbol{X}_i]_{:q}) \stackrel{\text{def}}{=} \langle \phi_c([\boldsymbol{X}_i]_{:p}), \phi_c([\boldsymbol{X}_j]_{:q}) \rangle.$

Therefore, we can successfully estimate α with quadratic programming based on K without description of feature mapping ϕ_r, ϕ_c . We update C as

$$C = \sum_{i=1}^{n} \alpha_i y_i \Phi(\mathbf{X}_i) \mathbf{P} \in \mathcal{H}_r^r \times \mathcal{H}_c^r.$$
(3)

2. Second, we update P holding C fixed. The dual problem of Equation (2) is

$$\min_{\boldsymbol{\beta} = (\beta_1, \dots, \beta_n)} - \sum_{i=1}^n \beta_i + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \beta_i \beta_j y_i y_j \langle \boldsymbol{C} \left((\boldsymbol{C}^T \boldsymbol{C})^{-1} \boldsymbol{C}^T \boldsymbol{\Phi}(\boldsymbol{X}_i) \right), \boldsymbol{C} \left((\boldsymbol{C}^T \boldsymbol{C})^{-1} \boldsymbol{C}^T \boldsymbol{\Phi}(\boldsymbol{X}_j) \right) \rangle, \tag{4}$$

subject to
$$\sum_{i=1}^{n} y_i \beta_i = 0$$
, and $0 \le \beta_i \le C, i = 1, \dots, n$,

Notice $C\left((C^TC)^{-1}C^T\Phi(X_i)\right) \in \mathcal{H}^{d_1} \times \mathcal{H}^{d_2}$ is well defined by matrix product: for $A_1 \in \mathcal{H}^r$ and $A_2 \in \mathcal{H}^d$, $A_1^TA_2 = \llbracket a_{ij} \rrbracket \in \mathbb{R}^{r \times d}$, where $a_{ij} = \langle [A_1]_i, [A_2]_j \rangle$. We can find an optimizer of (4) without the feature mapping. To show this, notice that by plugging (3) into (4), we have

$$C^{T}C = \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} \mathbf{P}^{T} \mathbf{K}(i, j) \mathbf{P} \in \mathbb{R}^{r \times r} \times \mathbb{R}^{r \times r},$$

$$C^{T}\Phi(\mathbf{X}_{i}) = \sum_{i=1}^{n} \alpha_{i} y_{i} \mathbf{P}^{T} \mathbf{K}(i, j) \in \mathbb{R}^{r \times d_{1}} \times \mathbb{R}^{r \times d_{2}}.$$
(5)

(5) makes inner product in (4) expressed in terms of only P and $\{K(i,j): i, j \in [n]\}$ by the following equation.

$$\langle C\left((C^TC)^{-1}C^T\Phi(X_i)\right), C\left((C^TC)^{-1}C^T\Phi(X_j)\right)\rangle = \operatorname{tr}\left(\left(C^T\Phi(X_i)\right)^T(C^TC)^{-1}\left(C^T\Phi(X_i)\right)\right).$$
Good.

3 Relation with the previous algorithm symmetric trick

Define symmetric feature matrix $\tilde{\boldsymbol{X}} = \begin{pmatrix} 0_{d_1 \times d_2} & \boldsymbol{X} \\ \boldsymbol{X}^t & 0_{d_2 \times d_1} \end{pmatrix} \in \mathbb{R}^{(d_1 + d_2) \times (d_1 + d_2)}$. Feature mapping 3 is defined as

$$\tilde{\Phi} \colon \mathbb{R}^{d_1 \times d_2} \to \mathcal{H}^{d_1 + d_2}$$
$$\boldsymbol{X} \mapsto \left(\phi([\tilde{\boldsymbol{X}}]_{1:}), \dots, \phi([\tilde{\boldsymbol{X}}]_{d_1 + d_2:}) \right)$$

where ϕ is induced by kernel $K: \mathbb{R}^{(d_1+d_2)\times(d_1+d_2)} \times \mathbb{R}^{(d_1+d_2)\times(d_1+d_2)} \to \mathbb{R}$. Since all entries of $\Phi_r(\boldsymbol{X})$ are corresponding to $[\tilde{\Phi}(\boldsymbol{X})]_{1:d_1}$ and $\Phi_c(\boldsymbol{X})$ to $[\tilde{\Phi}(\tilde{\boldsymbol{X}})]_{d_1+1:d_1+d_2}$, we have an equivalent representation of (1)

$$f(X) = \langle B, \Phi(X) \rangle$$

$$= \langle \boldsymbol{B}_r, \Phi_r(\boldsymbol{X}) \rangle + \langle \boldsymbol{B}_c, \Phi_c(\boldsymbol{X}) \rangle$$

$$= \langle \tilde{\boldsymbol{B}}_r, [\tilde{\Phi}(\boldsymbol{X})]_{1:d_1} \rangle + \langle \tilde{\boldsymbol{B}}_c, [\tilde{\Phi}(\boldsymbol{X})]_{d_1+1:d_1+d_2} \rangle, \text{ where } \tilde{\boldsymbol{B}}_r \in \mathcal{H}^{d_1}, \tilde{\boldsymbol{B}}_c \in \mathcal{H}^{d_2}$$

$$= \langle \tilde{\boldsymbol{B}}, \tilde{\Phi}(\boldsymbol{X}) \rangle, \text{ where } \tilde{\boldsymbol{B}} = (\tilde{\boldsymbol{B}}_r, \tilde{\boldsymbol{B}}_c) \in \mathcal{H}^{d_1+d_2}.$$

Assume that $\tilde{\boldsymbol{B}} = \tilde{\boldsymbol{C}}\tilde{\boldsymbol{P}}^T$ where $\tilde{\boldsymbol{C}} \in \mathcal{H}^r$, $\tilde{\boldsymbol{P}} = (\tilde{\boldsymbol{P}}_r, \tilde{\boldsymbol{P}}_c) \in \mathbb{R}^{(d_1+d_2)\times r}$ and $\tilde{\boldsymbol{P}}_r \in \mathbb{R}^{d_1\times r}, \tilde{\boldsymbol{P}}_c \in \mathbb{R}^{d_2\times r}$. Let Π_r, Π_c are permutation operators such that

$$\operatorname{Proj}_{\mathcal{H}_r} \left(\Pi_r [\tilde{\Phi}(\boldsymbol{X})]_{1:d_1} \right) = \Phi_r(\boldsymbol{X})$$
$$\operatorname{Proj}_{\mathcal{H}_c} \left(\Pi_c [\tilde{\Phi}(\boldsymbol{X})]_{d_1+1:d_1+d_2} \right) = \Phi_c(\boldsymbol{X}).$$

Here, we denote $\operatorname{Proj}_{\mathcal{H}_c} \colon \mathcal{H} \to \mathcal{H}_r$ and $\operatorname{Proj}_{\mathcal{H}_r} \colon \mathcal{H} \to \mathcal{H}_c$ as entry-wise projection mappings. Then the following holds

$$\begin{split} \langle \tilde{\boldsymbol{B}}, \tilde{\boldsymbol{\Phi}}(\boldsymbol{X}) \rangle &= \langle \tilde{\boldsymbol{C}}(\tilde{\boldsymbol{P}}_r, \tilde{\boldsymbol{P}}_c)^T, \tilde{\boldsymbol{\Phi}}(\boldsymbol{X}) \rangle \\ &= \langle \tilde{\boldsymbol{C}}\tilde{\boldsymbol{P}}_r^T, [\tilde{\boldsymbol{\Phi}}(\boldsymbol{X})]_{1:d_1} \rangle + \langle \tilde{\boldsymbol{C}}\tilde{\boldsymbol{P}}_C^T, [\tilde{\boldsymbol{\Phi}}(\boldsymbol{X})]_{d_1+1:d_1+d_2} \rangle \\ &= \langle \Pi_r \tilde{\boldsymbol{C}}\tilde{\boldsymbol{P}}_r^T, \Pi_r [\tilde{\boldsymbol{\Phi}}(\boldsymbol{X})]_{1:d_1} \rangle + \langle \Pi_c \tilde{\boldsymbol{C}}\tilde{\boldsymbol{P}}_c^T, \Pi_c [\tilde{\boldsymbol{\Phi}}(\boldsymbol{X})]_{d_1+1:d_1+d_2} \rangle \\ &= \langle \tilde{\boldsymbol{C}}_r \tilde{\boldsymbol{P}}_r^T, \boldsymbol{\Phi}_r(\boldsymbol{X}) \rangle + \langle \tilde{\boldsymbol{C}}_c \tilde{\boldsymbol{P}}_c^T, \boldsymbol{\Phi}_c(\boldsymbol{X}) \rangle, \end{split}$$

where $\tilde{C}_r = \operatorname{Proj}_{\mathcal{H}_r}(\Pi_r \tilde{C})$ and $\tilde{C}_c = \operatorname{Proj}_{\mathcal{H}_c}(\Pi_c \tilde{C})$. Therefore, we can conclude that the low rankness of the coefficient on the feature image of $\tilde{\Phi}(X)$ implies the same low rankness of the coefficient of the feature image of $\Phi(X)$. The other direction is also true.

Good. Updating schemes in both algorithms are also equivalent.