

# Fair Kernel K-Means: from Single Kernel to Multiple Kernel

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# Background

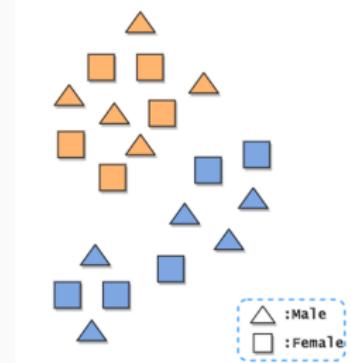
## fairness in clustering (Chierichetti et al.)

For a subset  $\mathbf{Y}$ , the balance of  $\mathbf{Y}$  is defined as

$$\text{balance}(\mathbf{Y}) = \min \left( \frac{\# \text{RED}(\mathbf{Y})}{\# \text{BLUE}(\mathbf{Y})}, \frac{\# \text{BLUE}(\mathbf{Y})}{\# \text{RED}(\mathbf{Y})} \right) \in [0, 1]$$

The balance of a clustering  $\mathcal{C}$  is defined as:

$$\text{balance}(\mathcal{C}) = \min_{C \in \mathcal{C}} \text{balance}(C)$$



**Figure 1:** The effect of fair clustering

## Contribution

- We design a simple yet effective fair regularization term.
- Based on this regularization term, we first propose fair kernel k-means.
- We also provide a generalization analysis for our method and obtain some interesting conclusions about fairness and clustering performance.

# Fair Regularization

- $\mathbf{G} \in \{0, 1\}^{n \times t}$  (protected group indicators)
- $\mathbf{Y} \in \{0, 1\}^{n \times c}$  (cluster indicators)

## Theorem 1

Given  $\mathbf{G}$  and  $\mathbf{Y}$  defined as mentioned before, we can obtain the maximum of fairness by optimizing the following objective function:

$$\min_{\mathbf{Y} \in Ind} \text{Tr} \left( \mathbf{Y}^T \mathbf{G} \mathbf{G}^T \mathbf{Y} (\mathbf{Y}^T \mathbf{Y})^{-1} \right).$$

# Fair Kernel K-means

## fair kernel k-means

$$\begin{aligned} & \min_{\mathbf{Y} \in Ind} \text{Tr}(\mathbf{K}) - \text{Tr}\left(\left(\mathbf{Y}^T \mathbf{Y}\right)^{-\frac{1}{2}} \mathbf{Y}^T \mathbf{K} \mathbf{Y} \left(\mathbf{Y}^T \mathbf{Y}\right)^{-\frac{1}{2}}\right) + \lambda \text{Tr}\left(\mathbf{Y}^T \mathbf{G} \mathbf{G}^T \mathbf{Y} \left(\mathbf{Y}^T \mathbf{Y}\right)^{-1}\right) \\ \iff & \max_{\mathbf{Y} \in Ind} \text{Tr}\left(\mathbf{Y}^T \left(\mathbf{K} - \lambda \mathbf{G} \mathbf{G}^T\right) \mathbf{Y} \left(\mathbf{Y}^T \mathbf{Y}\right)^{-1}\right) \end{aligned}$$

## fair multiple kernel k-means

$$\begin{aligned} & \min_{\mathbf{Y}, \gamma} \text{Tr}\left(\tilde{\mathbf{K}}^* \left(\mathbf{I} - \mathbf{Y} \left(\mathbf{Y}^T \mathbf{Y}\right)^{-1} \mathbf{Y}^T\right)\right) \\ \text{s.t. } & \mathbf{Y} \in Ind, \quad \gamma^T \mathbf{1} = 1, \quad \gamma_p \geq 0, \quad \tilde{\mathbf{K}}^* = \sum_{p=1}^m \gamma_p^2 \tilde{\mathbf{K}}^{(p)} \end{aligned}$$

## p.s.d. guarantee

### Lemma 1

Given two real symmetric matrices  $\mathbf{A}$  and  $\mathbf{B}$  with the same size, where the smallest eigenvalue of  $\mathbf{A}$  is  $\sigma_A$  and the largest eigenvalue of  $\mathbf{B}$  is  $\sigma_B$ . If  $\sigma_A \geq \sigma_B$ , then  $\mathbf{A} - \mathbf{B}$  is p.s.d.

$$\text{Tr} \left( \mathbf{Y}^T \left( \mathbf{K} - \lambda \mathbf{G} \mathbf{G}^T \right) \mathbf{Y} \left( \mathbf{Y}^T \mathbf{Y} \right)^{-1} \right) + \alpha \text{Tr}(\mathbf{I}) = \text{Tr} \left( \mathbf{Y}^T \left( \mathbf{K} + \alpha \mathbf{I} - \lambda \mathbf{G} \mathbf{G}^T \right) \mathbf{Y} \left( \mathbf{Y}^T \mathbf{Y} \right)^{-1} \right)$$

# Pseudo-codes of our method

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## Algorithm 1 Fair Multiple Kernel K-means

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**Input:** Kernel matrices  $\{\mathbf{K}^{(p)}\}_{p=1}^m$ , protected groups  $\mathcal{G}_1, \dots, \mathcal{G}_t$ , fairness hyper-parameter  $\lambda$ .

- 1: Construct protected group indicator matrix  $\mathbf{G}$  and calculate  $\alpha$  as  $\alpha = |\mathcal{G}_{max}| * \lambda$ .
- 2: Construct the corresponding fair kernel by  $\tilde{\mathbf{K}}^{(p)} = \mathbf{K}^{(p)} + \alpha \mathbf{I} - \lambda \mathbf{G} \mathbf{G}^T$  for each base kernel matrix  $\mathbf{K}^{(p)}$ .
- 3: Initialize  $\gamma = \frac{1}{m}$  and  $\mathbf{Y}$  by running standard kernel k-means on  $\sum_{p=1}^m \gamma_p^2 \mathbf{K}^{(p)}$ .
- 4: **repeat**
- 5:   Update  $\mathbf{Y}$  row by row by solving  $\max_{\mathbf{Y} \in Ind} \text{Tr} \left( \mathbf{Y}^T \tilde{\mathbf{K}}^* \mathbf{Y} (\mathbf{Y}^T \mathbf{Y})^{-1} \right)$ .
- 6:   Update  $\gamma$  by  $\gamma_p = \frac{h_p^{-1}}{\sum_{j=1}^m h_j^{-1}}$ .
- 7: **until** Converges

**Output:** The final partition matrix  $\mathbf{Y}$ .

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# Assumption

## Assumption 1

Each  $\tilde{\mathbf{K}}^{(p)} = \mathbf{K}^{(p)} + \alpha \mathbf{I} - \lambda \mathbf{G}\mathbf{G}^T$  is a valid kernel matrix, i.e.,  $\tilde{\mathbf{K}}^{(p)}$  is symmetric and p.s.d.

## Assumption 2

All  $\mathbf{K}^{(p)}$  are upper bounded. We denote  $b$  as the maximum of elements in all  $\mathbf{K}^{(p)}$ .

# Generalization Analysis

- function class of our method:

$$\mathcal{F} = \left\{ f : \mathbf{x} \mapsto \min_{y \in \{\mathbf{e}_1, \dots, \mathbf{e}_c\}} \|\Phi_\gamma(\mathbf{x}) - \mathbf{M}y\|_{\mathcal{H}}^2 \mid \gamma^\top \mathbf{1} = 1, \gamma_p \geq 0, \mathbf{m}_k \in \mathcal{H} \right\}.$$

## Theorem 2

any  $\delta \geq 0$ , with probability at least  $1 - \delta$ , the following inequality holds:

$$\begin{aligned} \mathbb{E}[f(\mathbf{x})] &\leq \frac{1}{n} \sum_{i=1}^n f(\mathbf{x}_i) + \frac{2\sqrt{2\pi}}{\sqrt{n}} \left[ (1 + c^2)(b + \alpha) - \left(1 + \frac{c^2}{t}\right)\lambda + c\sqrt{2(b + \alpha - \lambda)\left(b + \alpha - \frac{\lambda}{t}\right)} \right] \\ &\quad + \left(4(b + \alpha) - 2\left(1 + \frac{1}{t}\right)\lambda\right) \sqrt{\frac{\log(1/\delta)}{2n}} \end{aligned}$$

# Generalization Analysis

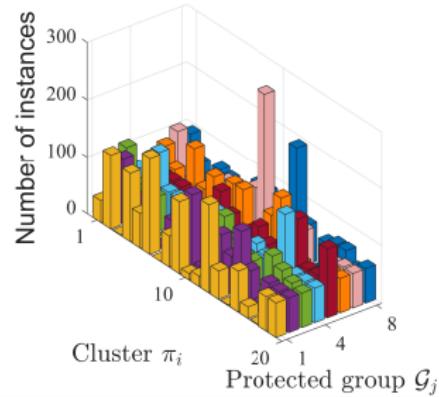
$$\begin{aligned} & \frac{2\sqrt{2\pi}}{\sqrt{n}} \left[ (1 + c^2)(b + \alpha) - (1 + \frac{c^2}{t})\lambda + c\sqrt{2(b + \alpha - \lambda)\left(b + \alpha - \frac{\lambda}{t}\right)} \right] \\ & + \left(4(b + \alpha) - 2\left(1 + \frac{1}{t}\right)\lambda\right) \sqrt{\frac{\log(1/\delta)}{2n}} \\ & \geq \frac{2\sqrt{2\pi}}{\sqrt{n}} \left[ (1 + c^2)b + \left(|\mathcal{G}_{max}| - 1 + \frac{c^2(|\mathcal{G}_{max}|t - 1)}{t}\right)\lambda + c\sqrt{2(b + (|\mathcal{G}_{max}| - 1)\lambda)\left(b + \frac{|\mathcal{G}_{max}|t - 1}{t}\lambda\right)} \right] \\ & + (4b + 4(|\mathcal{G}_{max}| - 1)\lambda) \sqrt{\frac{\log(1/\delta)}{2n}} \end{aligned}$$

# Experiments

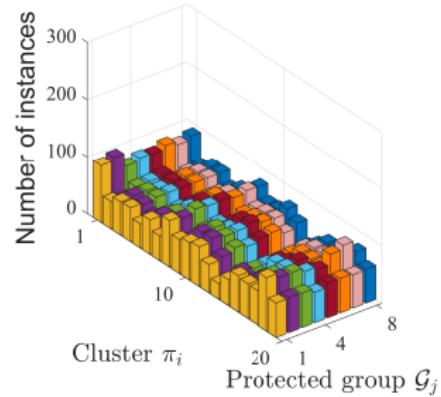
**Table 1:** Comparison results on the single kernel setting. The best and second best results are denoted in **bold** and underlined, respectively.

Data sets		K-means	KKM	SC	FairSC	VFC	FFC	FKKM-f	FKKM
D&S	ACC	0.555	0.552	0.558	0.433	0.539	0.521	<b>0.648</b>	<u>0.636</u>
	NMI	0.650	0.602	0.652	0.575	0.617	0.583	<b>0.724</b>	<u>0.683</u>
	Bal	0	0	0	0	<u>0.186</u>	0.100	0	<b>0.559</b>
	MNCE	0.156	0.531	0.023	0	<u>0.923</u>	0.712	0.477	<b>0.991</b>
HAR	ACC	0.524	0.620	0.680	<u>0.742</u>	0.600	0.602	0.689	<b>0.771</b>
	NMI	0.596	0.609	0.618	<u>0.703</u>	0.654	0.490	0.625	<b>0.710</b>
	Bal	0	0	0	0	<u>0.200</u>	0.007	0	<b>0.250</b>
	MNCE	0.933	0.930	0.914	0	<u>0.983</u>	0.953	0.920	<b>0.989</b>
MNIST-USPS	ACC	0.363	0.396	0.406	<b>0.458</b>	0.360	<u>0.437</u>	0.403	0.432
	NMI	0.423	0.421	<b>0.435</b>	<u>0.429</u>	0.306	0.412	0.426	0.380
	Bal	0	0	0	0	0.142	<u>0.217</u>	0	<b>0.847</b>
	MNCE	0	0.003	0	0	0.544	<u>0.684</u>	0	<b>0.997</b>
Jaffe	ACC	0.927	0.948	0.901	0.957	<u>0.981</u>	0.901	0.954	1
	NMI	0.914	0.922	0.889	0.943	<u>0.969</u>	0.918	0.930	1
	Bal	0	0	0	0	<u>0.400</u>	0.250	0	<b>0.500</b>
	MNCE	0.808	0.900	0.765	0.827	<u>0.983</u>	0.924	0.897	<b>0.989</b>
Credit Card	ACC	0.362	0.381	0.311	0.351	0.381	0.364	<u>0.400</u>	<b>0.404</b>
	NMI	0.139	0.140	0.126	0.123	0.142	0.139	<u>0.145</u>	<b>0.148</b>
	Bal	0.510	0.550	0.567	<u>0.603</u>	0.586	0.550	0.536	<b>0.624</b>
	MNCE	0.953	0.961	0.967	<u>0.973</u>	0.970	0.969	0.956	<b>0.985</b>
K1b	ACC	0.742	0.669	0.667	<b>0.853</b>	0.778	0.663	<u>0.826</u>	0.809
	NMI	0.589	0.537	0.536	<b>0.666</b>	0.553	0.503	<u>0.628</u>	0.591
	Bal	0.666	0.775	0.763	0.667	<u>0.794</u>	0.773	0.703	<b>0.800</b>
	MNCE	0.971	0.989	0.987	0.971	<u>0.990</u>	0.989	0.978	<b>0.991</b>

# Visualization



**Figure 2:** standard kernel



**Figure 3:** our fair kernel

Last

**Thank you!**