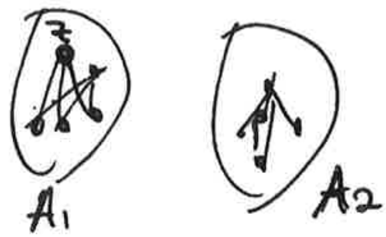
Within Energy Dispersion | 04-12-2017 |

$$W = \sum_{k=1}^{K} \frac{n_k}{2} g(A_k, A_k)$$

$$g(A_k, A_{k'}) = \frac{1}{n_k n_{k'}} \sum_{x \in A_k} \sum_{y \in A_{k'}} \|x - y\|^{\alpha}$$

Two Partitions



$$W = \frac{n_1}{2} g(A_1, A_1) + \frac{n_2}{2} g(A_2, A_2)$$

$$\cancel{= \frac{n_1}{2} \frac{1}{n_1^2} \sum_{x, x'} \|x - x'\| + \frac{n_2}{}}$$

$$= \frac{n_1}{2} \frac{1}{n_1^2} \sum_{x \in A_1} \sum_{x' \in A_1} \|x - x'\| + \frac{n_2}{2} \frac{1}{n_2^2} \sum_{y \in A_2} \sum_{y' \in A_2} \|y - y'\|$$

$$= \frac{1}{2} \frac{1}{n_1} \sum_{x} I(x) + \frac{1}{2} \frac{1}{n_2} \sum_{y} I(y)$$

$$= \frac{1}{2} \frac{1}{n_1} I(z) + \frac{1}{2n_1} \sum_{x \neq z} I(x) + \frac{1}{2n_2} \sum_{y \neq z} I(y)$$

$$\tilde{W} = \frac{\cancel{n_1-1}}{2} \cdot \frac{1}{(n_1-1)^2} \sum_{x \neq z} \sum_{x' \neq z} \|x - x'\|$$

$$+ \frac{\cancel{n_2+1}}{2} \frac{1}{(n_2+1)^2} \sum_{y \in \tilde{A}_2} \sum_{y' \in \tilde{A}_2} \|y - y'\|$$

$$= \frac{1}{2(n_1-1)} \sum_{x \neq z} I(x) +$$

$$+ \frac{1}{2(n_2+1)} \left(\sum_{y' \in \tilde{A}_2} \|z - y'\| + \sum_{y \neq z} \sum_{y' \in \tilde{A}_2} \|y - y'\| \right)$$

$$\downarrow$$

$$\sum_{y \neq z} \|z - y\| + \sum_{y \neq z} \sum_{y' \neq z} \|y - y'\|$$

$$= \frac{1}{2(n_1-1)} \sum_{x \neq z} I(x) + \frac{1}{2(n_2+1)} \left(\sum_{y \neq z} \|z - y\| + \sum_{y \neq z} \sum_{y' \neq z} \|y - y'\| \right)$$

$$= \frac{1}{2(n_1-1)} \sum_{x \neq z} I(x) + \frac{1}{2(n_2+1)} E(z) + \frac{1}{2(n_2+1)} \sum_{y} I(y)$$

③

$$W - \tilde{W} = \frac{1}{2n_1} I(z) + \frac{1}{2n_1}\sum_{x\neq z} I(x) + \frac{1}{2n_2}\sum_{y\neq z} I(y)$$

$$- \frac{1}{2(n_2+1)} E(z) - \frac{1}{2(n_1-1)}\sum_{x\neq z} I(x)$$

$$- \frac{1}{2(n_2+1)}\sum_{y\neq z} I(y)$$

$$= \frac{1}{2n_1} I(z) - \frac{1}{2(n_2+1)} E(z)$$

$$+ \frac{1}{2}\left(\frac{1}{n_1} - \frac{1}{n_1-1}\right)\sum_{x\neq z} I(x) + \frac{1}{2}\left(\frac{1}{n_2} - \frac{1}{n_2+1}\right)\sum_{y\neq z} I(y)$$

$$\frac{\cancel{n_1} - 1 - \cancel{n_1}}{n_1(n_1-1)} = \frac{-1}{n_1(n_1-1)} \qquad \frac{\cancel{n_2} + 1 - \cancel{n_2}}{n_2(n_2+1)} = \frac{1}{n_2(n_2+1)}$$

$$= \frac{1}{2n_1} I(z) - \frac{1}{2(n_2+1)} E(z) - \frac{1}{2n_1(n_1-1)}\sum_{x\neq z} I(x)$$

$$+ \frac{1}{2n_2(n_2+1)}\sum_{y\neq z} I(y)$$

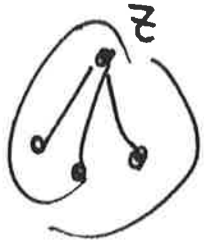
$$\sum_{x\neq z} I(x) = \sum_{x} I(x) - I(z)$$

$$\frac{1}{n_1} + \frac{1}{n_1(n_1-1)} = \frac{1}{n_1}\left(1 + \frac{1}{n_1-1}\right) = \frac{1}{\cancel{n_1}}\,\frac{\cancel{n_1 - 1 + 1}}{n_1-1} = \frac{1}{n_1-1}$$

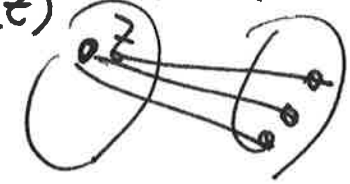
$$W-\tilde{W}=\frac{1}{2}\frac{1}{n_1-1}I(z)-\frac{1}{2}\frac{1}{n_2+1}E(z)$$

$$-\frac{1}{2}\frac{1}{n_1(n_1-1)}\sum_x I(x)+\frac{1}{2}\frac{1}{n_2(n_2+1)}\sum_y I(y)$$

$I(z)=C_{A_1}(z)$



$E(z)=C_{A_2}(z)$



$$\frac{1}{n_1}\sum_{x\in A_1} I(x)=\mathbb{E}_{A_1}[C_{A_1}(x)]$$

$$\frac{1}{n_2}\sum_y I(y)=\mathbb{E}_{A_2}[C_{A_2}(y)]$$

$$2(W-\tilde{W})=\frac{1}{n_1-1}\left(C_{A_1}(z)-\mathbb{E}[C_{A_1}(x)]\right)$$

$$-\frac{1}{n_2+1}\left(C_{A_2}(z)-\mathbb{E}[C_{A_2}(y)]\right)$$

<u>Note</u>

This is exactly the same formula as $2(B-\tilde{B})$ except for the $-$ sign

$$C_{A_1}(z) - \mathbb{E}[C_{A_1}(x)] = \sum_{x \in A_1} \|z - x\| - \frac{1}{n_1} \sum_{x \in A_1} \sum_{x' \in A_1} \|x - x'\|$$

$$= n_1 \left(\frac{1}{n_1} \sum_{x \in A_1} \|z - x\| - \frac{1}{n_1^2} \sum_{x \in A_1} \sum_{x' \in A_1} \|x - x'\| \right)$$

$$= n_1 \, \mathcal{E}(z, A_1)$$

$$C_{A_2}(z) - \mathbb{E}[C_{A_2}(y)] = \sum_{y \in A_2} \|z - x\| - \frac{1}{n_2} \sum_{y \in A_2} \sum_{y' \in A_2} \|y - y'\|$$

$$= n_2 \, \mathcal{E}(z, A_2)$$

$$2(W - \tilde{W}) = \frac{n_1}{n_1 - 1} \mathcal{E}(z, A_1) - \frac{n_2}{n_2 + 1} \mathcal{E}(z, A_2)$$

$W - \tilde{W} > 0 \rightarrow$ move

$\leq 0 \rightarrow$ don't move

Want to minimize W.

Algo

1. Initialize $\{A_1, \ldots, A_K\}$
2. For z in $\{x_1, \ldots, x_N\}$:

   pick partition z belongs to $A_i^{(z)}$.

   Compute $f = \frac{n_i}{n_i - 1} \mathcal{E}(z, A_i^{(z)})$

   compute $g = \min_j \frac{n_j}{n_j + 1} \mathcal{E}(z, A_j)$

3. If $g < f \rightarrow$ move z to A_j

repeat

Equivalently

$$2(W - \tilde{W}) = \frac{1}{n_1 - 1}\left(C_{A_1}(z) - \mathbb{E}[C_{A_1}(x)]\right) - \frac{1}{n_2+1}\left(C_{A_2}(z) - \mathbb{E}[C_{A_2}(y)]\right)$$

Algo.

1. Initialize $\{A_1, \ldots, A_K\}$
2. For z in data
   $A_j^{(z)} \to$ partition z belongs.
   compute $f = \frac{1}{n_i - 1}\left(C_{A_i}(z) - \mathbb{E}[C_{A_i}(x)]\right)$
   compute $g = \min_j \frac{1}{n_j+1}\left(C_{A_j}(z) - \mathbb{E}[C_{A_j}(y)]\right)$
3. If $g < f$ move z to A_j

repeat

Ideas for Approximation

1) Is $C_{A_1}(z)$ dominant over $\mathbb{E}[C_{A_1}(x)]$, etc.? Maybe can just use the first term.
2) Introduce a threshold such That Terms where $\|x-y\|$ are small do not contribute (same idea in spectral clustering).

Between Energy Stats $\quad |04-12-2017| \quad$ 1

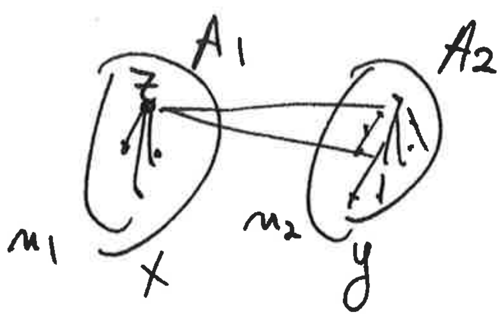
$$B = \sum_{1 < k, k' \le K} \frac{n_k n_{k'}}{2N} \mathcal{E}(A_k, A_{k'})$$

$$\mathcal{E}(A_k, A_{k'}) = 2g(A_k, A_{k'}) - g(A_{k'}, A_{k'}) - g(A_k, A_k)$$

$$= \frac{2}{n_k n_{k'}} \sum_{x \in A_k} \sum_{y \in A_{k'}} \|x - y\|^\alpha - \frac{1}{n_{k'}^2} \sum_{y \in A_{k'}} \sum_{y'} \|y - y'\|$$

$$- \frac{1}{n_k^2} \sum_{x} \sum_{x'} \|x - x'\|$$

Two Partitions



$$I(z) = \sum_{x \in A_1} \|z - x\| \quad \text{internal cost}$$

$$E(z) = \sum_{y \in A_2} \|z - y\| \quad \text{External cost}$$

$$D(z) = E(z) - I(z) \quad \text{Net cost.}$$

$$\mathcal{E} = \frac{2}{n_1 n_2} \sum_x \sum_y \|x - y\| - \frac{1}{n_1^2} \sum_x \sum_{x'} \|x - x'\| - \frac{1}{n_2^2} \sum_y \sum_{y'} \|y - y'\|$$

$$= \frac{1}{n_1} \sum_x \left(\frac{1}{n_2} \sum_y \|x - y\| - \frac{1}{n_1} \sum_{x'} \|x - x'\| \right)$$

$$+ \frac{1}{n_2} \sum_y \left(\frac{1}{n_1} \sum_x \|y - x\| - \frac{1}{n_2} \sum_{y'} \|y - y'\| \right)$$

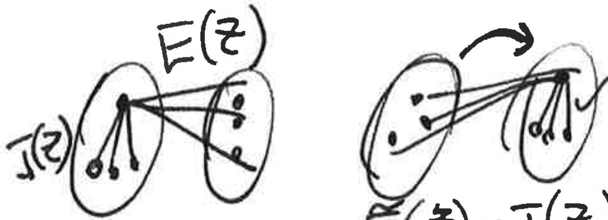
$$\mathcal{E} = \frac{1}{n_1} \sum_x \left\{ \frac{1}{n_2} E(x) - \frac{1}{n_1} I(x) \right\} + \frac{1}{n_2} \sum_y \left\{ \frac{1}{n_1} E(y) - \frac{1}{n_2} I(y) \right\}$$

1. Suppose $z \in A_1$, $z \notin A_2$

$$\mathcal{E}(A_1, A_2) = \frac{1}{n_1}\left(\frac{1}{n_2}E(z) - \frac{1}{n_1}I(z)\right) + \frac{1}{n_1}\sum_{x \neq z}\left\{\frac{1}{n_2}E(x) - \frac{1}{n_1}I(x)\right\}$$
$$+ \frac{1}{n_2}\sum_{y}\left\{\frac{1}{n_1}E(y) - \frac{1}{n_2}I(y)\right\}$$

2. Suppose $z \in \tilde{A}_2$, $z \notin \tilde{A}_1$. We put z into A_2

$$\mathcal{E}(\tilde{A}_1, \tilde{A}_2) = \frac{1}{n_1-1}\sum_{x}\left\{\frac{1}{n_2+1}E(x) - \frac{1}{n_1-1}I(x)\right\}$$
$$+ \frac{1}{n_2+1}\sum_{y}\left\{\frac{1}{n_1-1}E(y) - \frac{1}{n_2+1}I(y)\right\}$$
$$= \frac{1}{n_1-1}\sum_{x \neq z}\left\{\frac{1}{n_2+1}E(x) - \frac{1}{n_1-1}I(x)\right\}$$
$$+ \frac{1}{n_2+1}\left(\frac{1}{n_1-1}\tilde{E}(z) - \frac{1}{n_2+1}\tilde{I}(z)\right) + \frac{1}{n_2+1}\sum_{y \neq z}\left\{\frac{1}{n_1-1}E(y) - \frac{1}{n_2+1}I(y)\right\}$$



$\tilde{I}(z) = E(z)$

$\tilde{E}(z) = I(z)$

$$\mathcal{E}(\tilde{A}_1, \tilde{A}_2) = \frac{1}{n_1-1}\sum_{x \neq z}\left(\frac{1}{n_2+1}E(x) - \frac{1}{n_1-1}I(x)\right) + \frac{1}{n_2+1}\left(\frac{1}{n_1-1}I(z) - \frac{1}{n_2+1}E(z)\right)$$
$$+ \frac{1}{n_2+1}\sum_{y \neq z}\left\{\frac{1}{n_1-1}E(y) - \frac{1}{n_2+1}I(y)\right\}$$

$$B = \frac{n_1 n_2}{2N} \mathcal{E}(A_1, A_2)$$

$$\tilde{B} = \frac{(n_1 - 1)(n_2 + 1)}{2N} \mathcal{E}(\tilde{A}_1, \tilde{A}_2)$$

$$2N\,B = n_2\left(\frac{1}{n_2}E(z) - \frac{1}{n_1}I(z)\right) + n_2 \sum_{x \neq z} \left\{ \frac{1}{n_2}E(x) - \frac{1}{n_1}I(x) \right\}$$
$$+ \; n_1 \sum_{y \neq z} \left\{ \frac{1}{n_1}E(y) - \frac{1}{n_2}I(y) \right\}$$

$$2N\,\tilde{B} = (n_2+1) \sum_{x \neq z} \left(\frac{1}{n_2+1}E(x) - \frac{1}{n_1-1}I(x) \right) + (n_1 - 1)\left(\frac{1}{n_1-1}I(z) - \frac{1}{n_2+1}E(z)\right)$$
$$+ \; (n_1 - 1) \sum_{y \neq z} \left(\frac{1}{n_1-1}E(y) - \frac{1}{n_2+1}I(y) \right)$$

$$2N(B - \tilde{B}) = E(z) - \frac{n_2}{n_1}I(z) - I(z) + \frac{n_1-1}{n_2+1}E(z)$$
$$+ \; n_2 \sum_{x \neq z} \left\{ \frac{1}{n_2}E(x) - \frac{1}{n_1}I(x) \right\}$$
$$- \; (n_2+1) \sum_{x \neq z} \left\{ \frac{1}{n_2+1}E(x) - \frac{1}{n_1-1}I(x) \right\}$$
$$+ \; n_1 \sum_{y \neq z} \left\{ \frac{1}{n_1}E(y) - \frac{1}{n_2}I(y) \right\}$$
$$- \; (n_1-1) \sum_{y \neq z} \left(\frac{1}{n_1-1}E(y) - \frac{1}{n_2+1}I(y) \right)$$

$$2N(B-\tilde{B}) = \left(1 + \frac{n_1 - 1}{n_2+1}\right)E(z) - \left(1 + \frac{n_2}{n_1}\right)I(z)$$

$$+ \sum_{x\neq z}\left\{\cancel{E(x)} - \frac{n_2}{n_1}I(x)\right\} - \sum_{x\neq z}\left\{\cancel{E(x)} - \frac{n_2+1}{n_1-1}I(x)\right\}$$

$$+ \sum_{y\neq z}\left\{\cancel{E(y)} - \frac{n_1}{n_2}I(y)\right\} - \sum_{y\neq z}\left\{\cancel{E(y)} - \frac{n_1-1}{n_2+1}I(y)\right\}$$

$$= \frac{N}{n_2+1}E(z) - \frac{N}{n_1}I(z)$$

$$- \sum_{x\neq z}\left(\frac{n_2}{n_1}I(x) - \frac{n_2+1}{n_1-1}I(x)\right) - \sum_{y\neq z}\left(\frac{n_1}{n_2}I(y) - \frac{n_1-1}{n_2+1}I(y)\right)$$

$$= N\left(\frac{1}{n_2+1}E(z) - \frac{1}{n_1}I(z)\right)$$

$$- \sum_{x\neq z}\frac{n_2(n_1-1) - n_1(n_2+1)}{n_1(n_1-1)}I(x) - \sum_{y\neq z}\frac{n_1(n_2+1) - n_2(n_1-1)}{n_2(n_2+1)}I(y)$$

$$\cancel{n_2 n_1} - n_2 - \cancel{n_1 n_2} - n_1 = -N \qquad \cancel{n_1 n_2} + n_1 - \cancel{n_2 n_1} + n_2 = N$$

$$= N\left(\frac{1}{n_2+1}E(z) - \frac{1}{n_1}I(z)\right) + \frac{N}{n_1(n_1-1)}\sum_{x\neq z}I(x) - \frac{N}{n_2(n_2+1)}\sum_{y\neq z}I(y)$$

Therefore

$$2(B-\tilde{B}) = \frac{1}{n_2+1}E(z) - \frac{1}{n_1}I(z)$$
$$+ \frac{1}{n_1(n_1-1)}\sum_{x\neq z} I(x) - \frac{1}{n_2(n_2+1)}\sum_{y\neq z} I(y)$$

! For Balanced clusters I would guess the last two terms do not matter much.

so maybe $B-\tilde{B} \cong \frac{1}{2}\frac{1}{n_2+1}E(z) - \frac{1}{2}\frac{1}{n_1}I(z)$

is already a good approximation!

(*) Check this more carefully. Also notice that we need $O(n)$ only to compute this approx, contrary to $O(n^2)$.

$$\sum_{x\neq z} I(x) = \sum_{x} I(x) - I(z).$$

$$\frac{1}{n_1(n_1-1)} + \frac{1}{n_1} = \frac{1}{n_1}\left(1+\frac{1}{n_1-1}\right) = \frac{1}{\cancel{n_1}}\frac{\cancel{n_1}}{n_1-1}$$

So

$$2(B-\tilde{B}) = \frac{1}{n_2+1}E(z) - \frac{1}{n_1-1}I(z)$$
$$+ \frac{1}{n_1(n_1-1)}\sum_{x} I(x) - \frac{1}{n_2(n_2+1)}\sum_{y} I(y)$$

we want to maximize B.

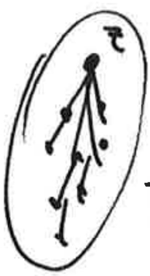
Thus $\begin{cases} \text{if } B - \tilde{B} \geq 0 & \text{we keep } z \text{ in } A_1 \\ \text{if } B - \tilde{B} < 0 & \text{we move } z \text{ to } A_2 \end{cases}$

$$2(B-\tilde{B}) = \underbrace{\left(-\frac{1}{n_1-1} I(z) + \frac{1}{n_1(n_1-1)} \sum_x I(x)\right)}_{\text{depends on } A_1 \text{ only}}$$

$$+ \underbrace{\left(\frac{1}{n_2+1} E(z) - \frac{1}{n_2(n_2+1)} \sum_y I(y)\right)}_{\text{depends on } A_2 \text{ only}}$$

$$\frac{1}{n_1(n_1-1)} \sum_x I(x) - \frac{1}{n_1-1} I(z)$$

$$\frac{1}{n_2(n_2+1)} \sum_y I(y) - \frac{1}{n_2+1} E(z)$$

A_1 

$I(z)$ cost of z with its current partition

$\sum_x I(x)$ is the total cost of the partition. $\frac{1}{n_1} \sum_x I(x) = \mathbb{E}_{A_1} I(x)$ is the average cost of a typical point in A_1 with its partition.

Thus $f(z) = \frac{1}{n_1-1} \mathbb{E}_{A_1} I(x) - \frac{1}{n_1-1} I(z)$

on the opposite:

$$f(z) = \frac{1}{n_1 - 1}\left(I(z) - \mathbb{E}_{A_1}(I(x)) \right)$$

$$g(z) = \frac{1}{n_2 + 1}\left(E(z) - \mathbb{E}_{A_2}(I(y)) \right)$$

$$\boxed{2(B - \tilde{B})} = -f(z) + g(z) = \underline{g(z) - f(z)}$$

$$= -\left(f(z) - g(z) \right)$$

Let $C_A(z)$ be the cost of point z to partition A, i.e.

$$C_A(z) = \sum_{x \in A} \| z - x \|^{\alpha}$$

Let $\mathbb{E}[C_A] = \frac{1}{n_A} \sum_{x \in A} C_A(x) = \frac{1}{n_A} \sum_{x \in A} \sum_{x' \in A} \| x - x' \|^{\alpha}$

be the average cost of each point in A with its partition.

The function
$$f_A = \frac{1}{n_A - 1}\left(C_A(z) - \mathbb{E}[C_A] \right)$$

$$g_B = \frac{1}{n_B + 1}\left(C_B(z) - \mathbb{E}[C_B] \right)$$

$B - \tilde{B} \sim g_B - f_A$

If $g_B \geq f_A$ keep z in A
$g_B < g_A$ move z to B

<u>Algorithm</u>

1. Initialize $\{A_1, A_2, \ldots A_K\}$
   $\quad\quad\quad\quad n_1 \quad n_2 \quad \ldots n_K$

2. For each $z \in \{x_1, x_2, \ldots, x_N\}$
   - Pick the partition that z belongs to and compute f_A
   - Compute $g_j^* = \min_j \frac{1}{n_j+1}\left(C_{A_j}(z) - \mathbb{E}[C_{A_j}]\right)$
   - If $g_j^* < f_A$ move z to A_j

3. Repeat 2 until nothing changes.

Relatio To kernel

04-12-2017

(1)

$$\gamma_k^2(P,Q) = \mathbb{E}k(X,X') + \mathbb{E}k(Y,Y') - 2\mathbb{E}k(X,Y)$$
$$= \frac{1}{2}\mathcal{E}(P,Q)$$

$$W = \sum_{k=1}^{k} \frac{n_k}{2} g(A_k, A_k)$$

$$\partial_k^2(A_k, A_k) = \mathbb{E}k(X,X') + \mathbb{E}k(X,X') - 2\mathbb{E}k(X,X')$$
$$= 0.$$

$$W = \sum_{k=1}^{k} \frac{n_k}{2} \mathbb{E}K(X,X')$$
$$= \sum_{k=1}^{k} \frac{n_k}{2} \frac{1}{n_k^2} \sum_{X\in A_k} \sum_{X'\in A_k} k(X,X')$$
$$= \sum_{k=1}^{k} \frac{1}{2n_k} \sum_{X,X'\in A_k} K(X,X')$$

two class problem:

$$W = \frac{1}{2n_1}\sum_{X,X'} k(X,X') + \frac{1}{2n_2}\sum_{y,y'} k(y,y')$$

(2)

$$K = \begin{pmatrix} k(x_1, x_1) & k(x_1, x_2) & \cdots & k(x_1, x_N) \\ k(x_2, x_1) & k(x_2, x_2) & \cdots & k(x_2, x_N) \\ & \vdots & & \end{pmatrix}$$

$$k = \left(\begin{array}{c|c} k(x, x') & k(x, y') \\ \hline k(x, y) & k(y, y') \end{array}\right)$$

$$\begin{pmatrix} k_{11} & k_{12} & \cdots \\ & & \end{pmatrix} \begin{array}{c} x \\ \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ \vdots & \vdots \\ 0 & \end{pmatrix} \end{array}$$

$$\begin{pmatrix} k_{x_1x_1} & k_{x_1x_2} & k_{x_1y_1} & k_{x_1y_2} \\ k_{x_2x_1} & k_{x_2x_2} & k_{x_2y_1} & k_{x_2y_2} \\ k_{y_1x_1} & k_{y_1x_2} & k_{y_1y_1} & k_{y_1y_2} \\ k_{y_2x_1} & k_{y_2x_2} & k_{y_2y_1} & k_{y_2y_2} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} k_{x_1x_1} + k_{x_1x_2} & k_{x_1y_1} + k_{x_1y_2} \\ k_{x_2x_1} + k_{x_2x_2} & k_{x_2y_1} + k_{x_2y_2} \\ k_{y_1x_1} + k_{y_1x_2} & k_{y_1y_1} + k_{y_1y_2} \\ k_{y_2x_1} + k_{y_2x_2} & k_{y_2y_1} + k_{y_2y_2} \end{pmatrix}$$

$$\mathrm{tr} \left(\begin{array}{c|c} k_{x_1x_1} + k_{x_1x_2} + k_{x_2x_1} + k_{x_2x_2} & k_{x_1y_1} + k_{x_1y_2} + k_{x_2y_1} + k_{x_2y_2} \\ \hline k_{y_1x_1} + k_{y_1x_2} + k_{y_2x_1} + k_{y_2x_2} & k_{y_1y_1} + k_{y_1y_2} + k_{y_2y_1} + k_{y_2y_2} \end{array}\right)$$

③

$$\mathrm{Tr}\left(D Z^T K Z \right)$$

$$\mathrm{Tr}\left(D^{1/2} Z^T K Z D^{1/2} \right)$$

$$\boxed{\mathrm{Tr}\left((Z D^{1/2})^T K (Z D^{1/2}) \right)}$$