### Robust Multi-view Graph Embedding

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# Graph embedding (GE)

Yan et al. (2007) proposed a method for dimensionality reduction based on graph-embedding with known graph-structured links.



Shimodaira (2016) extended Yan et al. (2007) as CDMCA.





•  $\mathbf{x}_i^{(d)} \in \mathbb{R}^{p_d}$  :data vector,



x<sub>i</sub><sup>(d)</sup> ∈ ℝ<sup>p<sub>d</sub></sup> :data vector,
 w<sub>ij</sub><sup>(de)</sup> ≥ 0 represents the strength of association between x<sub>i</sub><sup>(d)</sup> and x<sub>j</sub><sup>(e)</sup>.



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- $i \in [n_d], j \in [n_e], d \in [D], e \in [D],$ where [n] represents a set  $\{1, 2, \dots, n\}$ .



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 $\mathbf{A}^{(d)} \in \mathbb{R}^{p_d imes K}$  :linear transform matrices to be estimated, so that

$$w_{ij}^{(de)} > 0 \quad \Rightarrow \quad \mathbf{A}^{(d)\top} \mathbf{x}_i^{(d)} pprox \mathbf{A}^{(e)\top} \mathbf{x}_j^{(e)}.$$

CDMCA finds  $\{\hat{A}^{(d)}\}$  that minimizes

$$\phi_0(\mathbf{A}; \mathbf{X}, \mathbf{W}) := \sum_{d=1}^{D} \sum_{e=1}^{D} \sum_{i=1}^{n_d} \sum_{j=1}^{n_e} \tilde{w}_{ij}^{(de)} \|\mathbf{A}^{(d)\top} \mathbf{x}_i^{(d)} - \mathbf{A}^{(e)\top} \mathbf{x}_j^{(e)}\|_2^2,$$

CDMCA finds  $\{\hat{\mathbf{A}}^{(d)}\}$  that minimizes

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with a constraint

$$\sum_{d=1}^{D} \mathsf{A}^{(d) op} \mathsf{C}^{(d)} \mathsf{A}^{(d)} = \mathsf{I}_{\mathcal{K}},$$

where  $\mathbf{C}^{(d)} \succ 0$  and  $\tilde{w}_{ij}^{(de)} := w_{ij}^{de} / \sum_{d=1}^{D} \sum_{e=1}^{D} \sum_{i=1}^{n_d} \sum_{j=1}^{n_e} w_{ij}^{(de)}$ .

It can efficiently be solved by eigendecomposition. For D = 2, CDMCA is equivalent to Cross-view Graph Embedding (Huang et al., 2012; CvGE).

#### CDMCA is an extension of Canonical Correlation Analysis (CCA)



Figure: one-to-one relationship ( $\Leftrightarrow$  CCA)



Figure: many-to-many relationship (⇔ CDMCA)

# Purpose of this study



Figure: A image "Dog" is wrongly tagged with a word "car".

Our purpose is to reduce the adverse effect of improper associations.

### What we do:

#### We **downweight** wrong associations.



# Proposed algorithm

### Iteratively-Reweighted CDMCA (IR-CDMCA)

 $\gamma > {\rm 0}$  is a tuning parameter.

- ▶  $\hat{\mathbf{A}}_{(0)} \leftarrow \mathsf{CDMCA}(\mathbf{X}, \mathbf{W}).$
- ►  $t \leftarrow 0$ .
- Compute a weight  $\mathbf{R}_{(t)} := (r_{ij}^{(de)})$  by

$$r_{ij}^{(de)} := \exp\left(-\gamma \|\hat{\mathbf{A}}_{(t)}^{(d)\top} \mathbf{x}_i^{(d)} - \hat{\mathbf{A}}_{(t)}^{(e)\top} \mathbf{x}_j^{(e)}\|_2^2\right)$$

• update transformation matrix  
$$\hat{\mathbf{A}}_{(t+1)} \leftarrow \text{CDMCA}(\mathbf{X}, \mathbf{W} \circ \mathbf{R}_{(t)}).$$

- ▶  $t \leftarrow t+1$
- Iterate these steps until convergence

$$w_{ij}^{(de)}r_{ij}^{(de)}$$
 is expected to be small if  $w_{ij}^{(de)}$  is false-positive.

#### Theorem

#### IR-CDMCA monotonically reduces a loss function

$$\begin{split} \phi_{\gamma}(\mathbf{A};\mathbf{X},\mathbf{W}) &:= -\frac{1}{\gamma} \log \sum_{d=1}^{D} \sum_{e=1}^{D} \sum_{i=1}^{n_{d}} \sum_{j=1}^{n_{e}} \tilde{w}_{ij}^{(de)} \\ &\times \exp\left(-\gamma \|\mathbf{A}^{(d)\top}\mathbf{x}_{i}^{(d)} - \mathbf{A}^{(e)\top}\mathbf{x}_{j}^{(e)}\|_{2}^{2}\right) \end{split}$$

as 
$$\phi_{\gamma}(\hat{\mathbf{A}}_{(t)}; \mathbf{X}, \mathbf{W}) \geq \phi_{\gamma}(\hat{\mathbf{A}}_{(t+1)}; \mathbf{X}, \mathbf{W}).$$

This function  $\phi_{\gamma}(\mathbf{A}; \mathbf{X}, \mathbf{W})$  is analogous to  $\gamma$ -divergence (Fujisawa and Eguchi, 2008).

#### Theorem

$$\phi_{\gamma}(\hat{\mathbf{A}}_{(t)}; \mathbf{X}, \mathbf{W}), (t = 1, 2, ...)$$
 converges.

These theorems indicate the termination of our algorithm.

Due to the following theorem, IR-CDMCA can be regarded as a generalization of CDMCA.

#### Theorem

$$\phi_{\gamma}(\mathbf{A}; \mathbf{X}, \mathbf{W}) \rightarrow \phi_{0}(\mathbf{A}; \mathbf{X}, \mathbf{W}), \text{ as } \gamma \downarrow 0.$$

#### Recall that

- ▶ CDMCA minimizes  $\phi_0(\mathbf{A}; \mathbf{X}, \mathbf{W})$  s.t.  $\mathbf{A} \in \mathcal{S}(\mathbf{C})$ ,
- ▶ IR-CDMCA minimizes  $\phi_{\gamma}(\mathbf{A}; \mathbf{X}, \mathbf{W})$  s.t.  $\mathbf{A} \in \mathcal{S}(\mathbf{C})$ ,

where

$$\mathcal{S}(\mathbf{C}) := \left\{ \mathbf{A} = (\mathbf{A}^{(1)\top}, \cdots, \mathbf{A}^{(D)\top})^\top \middle| \sum_{d=1}^D \mathbf{A}^{(d)\top} \mathbf{C}^{(d)} \mathbf{A}^{(d)} = \mathbf{I} \right\}.$$

## Simulation settings



(1) Underlying common data structure in  $\mathbb{R}^{p_0} = \mathbb{R}^2$ :

$$\mathbf{x}_i^{(0)} := (\cos 2\pi i/10, \sin 2\pi i/10) \in \mathbb{R}^2.$$

(2) Generate vectors sharing the structure by

$$\mathbf{x}_{ij}^{(d)} \sim N[\mathbf{B}^{(d)\top}\mathbf{x}_i^{(0)}, \sigma^2 \mathbf{I}_{p_d}],$$
  
 $(j = 1, 2, \dots, 10; i = 1, 2, \dots, 10).$ 

(3) Associate all vectors in the same class across views (=**W**<sub>0</sub>).
(4) Resample these links at rate α ∈ (0,1) (=**W**<sub>0</sub>).
(5) Associate vectors in the different class at rate ξ ≥ 0 (=**W**<sub>ξ</sub>).

Illustrative example ( $\alpha = 0.5, \sigma = 0.2$ )



Figure: CDMCA (existing method)



Figure: IR-CDMCA with  $\gamma = 1$  (proposed method)

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### Experiment 1: Verification of robustness

Setting: 
$$D = 3$$
,  $p_1 = p_2 = p_3 = 10$ ,  $n_1 = n_2 = n_3 = 100$   
 $\hat{\mathbf{A}}_{\gamma} := \underset{\mathbf{A} \in \mathcal{S}(\mathbf{X}^{\top}\mathbf{X})}{\arg \min} \phi_{\gamma}(\mathbf{A}; \mathbf{X}, \mathbf{W}_{\xi})$   
Error  $:= \phi_0(\hat{\mathbf{A}}_{\gamma}; \mathbf{X}, \mathbf{W}_0)$ 

Table: Avg. and s.d. of errors over 100 experiments when few associations are observed ( $\alpha = 0.05$ ).

St.Dev.	Method	$\xi = 0$	$\xi = 0.2$	$\xi = 0.6$	$\xi = 1.0$
<i>σ</i> = 0.4	CDMCA ( $\gamma = 0$ )	$\textbf{0.027} \pm 0.008$	$0.043\pm0.013$	$0.070\pm0.026$	$0.087\pm0.030$
	IR-CDMCA ( $\gamma = 0.5$ )	$\textbf{0.027} \pm 0.008$	$0.031\pm0.010$	$0.039\pm0.015$	$0.045\pm0.016$
	IR-CDMCA ( $\gamma = 1$ )	$\textbf{0.027} \pm 0.008$	$\textbf{0.028} \pm 0.009$	$\textbf{0.030} \pm 0.010$	$\textbf{0.033} \pm 0.011$
<i>σ</i> = 1.0	CDMCA ( $\gamma = 0$ )	$0.141\pm0.042$	$0.181\pm0.055$	$0.227\pm0.058$	$0.274\pm0.063$
	IR-CDMCA ( $\gamma = 0.5$ )	$\textbf{0.140} \pm 0.041$	$0.160\pm0.050$	$0.194\pm0.059$	$0.243\pm0.071$
	IR-CDMCA ( $\gamma = 1$ )	$0.141\pm0.041$	$\textbf{0.157} \pm 0.051$	$\textbf{0.187} \pm 0.063$	$\textbf{0.229} \pm 0.072$

IR-CDMCA is more robust than CDMCA in this experiment.

# Experiment 2: Comparison with existing methods (D = 2)

By resampling data vectors and links across views so that associations become one-to-one, we can apply existing methods:

- CCA: Canonical Correlation Analysis (Hotelling, 1936)
- KCCA: Kernel CCA (Lai and Fyfe, 2000)
- RCCA: CCA with robust covariance estimators
  - ▶ MCD: Minimum Covariance Discriminator (Rousseeuw, 1985)
  - OGK: Orthogonal Gnenendian Kettering (Maronna and Zammar, 2002)
  - MVE: Minimum Volume Ellipsoid (Rousseeuw, 1985)
  - S-bi: S-estimator with biweight (Huber, 2011)

We assess these methods by mean Average Precision score (Baeza-Yates and Ribeiro-Neto, 1999; mAP). Higher mAP indicates better retrieval precision.

## Experiment 2: Comparison with existing methods (D = 2)

Table: Many associations are observed ( $\alpha = 0.5$ ) and  $\sigma = 1.0$ .

mAP	$\xi = 0$	$\xi = 0.25$	$\xi = 0.5$	$\xi = 0.75$	$\xi = 1$
CCA	$0.484\pm0.055$	$0.408\pm0.066$	$0.346\pm0.061$	$0.291\pm0.056$	$0.256\pm0.054$
KCCA ( $\beta = 1$ )	$\mathbf{\underline{0.616}} \pm 0.060$	$\underline{\textbf{0.530}} \pm 0.054$	$0.453\pm0.062$	$0.415\pm0.066$	$0.372\pm0.049$
KCCA ( $\beta = 1.5$ )	$0.556\pm0.076$	$0.444\pm0.058$	$0.371\pm0.052$	$0.337\pm0.055$	$0.310\pm0.050$
RCCA (MCD)	$0.443\pm0.059$	$0.384\pm0.072$	$0.313\pm0.070$	$0.270\pm0.056$	$0.230\pm0.047$
RCCA (OGK)	$0.477\pm0.054$	$0.434\pm0.065$	$0.379\pm0.068$	$0.327\pm0.052$	$0.285\pm0.059$
RCCA (MVE)	$0.454\pm0.057$	$0.388\pm0.076$	$0.323\pm0.064$	$0.272\pm0.059$	$0.240\pm0.048$
RCCA (S-bi)	$0.488\pm0.057$	$0.436\pm0.059$	$0.384\pm0.061$	$0.336\pm0.062$	$0.293\pm0.053$
CDMCA ( $\gamma = 0$ )	$0.518\pm0.054$	$0.509 \pm 0.053$	$0.499 \pm 0.053$	$0.494\pm0.049$	$0.487\pm0.048$
IR-CDMCA ( $\gamma = 0.5$ )	$0.519\pm0.052$	$0.518\pm0.052$	$0.512\pm0.053$	$0.511\pm0.052$	$0.507\pm0.050$
IR-CDMCA $(\gamma = 1)$	$0.521\pm0.051$	$\textbf{0.519} \pm \textbf{0.052}$	$0.516\pm0.052$	$0.516\pm0.052$	$0.514\pm0.051$
IR-CDMCA ( $\gamma = 1.5$ )	$0.522\pm0.051$	$0.520\pm0.052$	$\underline{\textbf{0.517}}\pm0.052$	$\underline{\textbf{0.517}}\pm0.052$	$\underline{\textbf{0.515}}\pm0.051$

- MCD Minimum Covariance Discriminator (Rousseeuw, 1985)
- OGK Orthogonal Gnenendian Kettenring (Maronna and Zamar, 2002)
- MVE Minimum Volume Ellipsoid (Rousseeuw, 1985)
- S-bi biweight-type S-estimator (Huber, 2011)

## Experiment 2: Comparison with existing methods (D = 2)

Table: Few associations are observed ( $\alpha = 0.05$ ) and  $\sigma = 1.0$ .

mAP	$\xi = 0$	$\xi = 0.25$	$\xi = 0.5$	$\xi = 0.75$	$\xi = 1$
CCA	$0.162\pm0.022$	$0.159\pm0.026$	$0.162\pm0.019$	$0.163\pm0.019$	$0.158\pm0.022$
KCCA ( $\beta = 1$ )	$0.171\pm0.018$	$0.173\pm0.017$	$0.171\pm0.018$	$0.165\pm0.012$	$0.173\pm0.018$
KCCA ( $\beta = 1.5$ )	$0.165\pm0.014$	$0.169\pm0.013$	$0.166\pm0.014$	$0.161\pm0.012$	$0.164\pm0.009$
RCCA (MCD)	$0.157\pm0.022$	$0.166\pm0.029$	$0.165\pm0.032$	$0.163\pm0.023$	$0.163\pm0.024$
RCCA (OGK)	$0.173\pm0.030$	$0.176\pm0.028$	$0.167\pm0.027$	$0.170\pm0.027$	$0.173\pm0.023$
RCCA (MVE)	$0.168\pm0.027$	$0.168\pm0.027$	$0.161\pm0.022$	$0.164\pm0.018$	$0.164\pm0.023$
RCCA (S-bi)	$0.162\pm0.022$	$0.166\pm0.023$	$0.170\pm0.026$	$0.174\pm0.029$	$0.173\pm0.027$
<b>CDMCA</b> $(\gamma = 0)$	$0.412\pm0.073$	$0.331\pm0.066$	$0.300\pm0.060$	$0.282\pm0.060$	$0.262\pm0.052$
IR-CDMCA ( $\gamma = 0.5$ )	$0.418\pm0.073$	$0.377\pm0.070$	$0.358\pm0.071$	$0.339\pm0.076$	$0.321\pm0.061$
<b>IR-CDMCA</b> $(\gamma = 1)$	$0.419\pm0.071$	$0.402\pm0.072$	$0.383\pm0.073$	$0.379\pm0.076$	$0.366\pm0.072$
IR-CDMCA ( $\gamma = 1.5$ )	<b><u>0.420</u></b> ± 0.070	$\underline{\textbf{0.408}} \pm 0.071$	$\underline{\textbf{0.395}} \pm 0.072$	$\underline{\textbf{0.394}} \pm 0.073$	$\underline{\textbf{0.387}} \pm 0.075$

- MCD Minimum Covariance Discriminator (Rousseeuw, 1985)
- OGK Orthogonal Gnenendian Kettenring (Maronna and Zamar, 2002)
- MVE Minimum Volume Ellipsoid (Rousseeuw, 1985)
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# Conclusion

- We propose Iteratively-Reweighted CDMCA (IR-CDMCA), which is a robust extension of CDMCA.
- We prove the convergence of IR-CDMCA.
- ► IR-CDMCA outperforms CDMCA in numerical experiments.



Figure: CDMCA with cont.

Figure: IR-CDMCA with cont.

## References I

- Yan, S., Xu, D., Zhang, B., Zhang, H. J., Yang, Q. and Lin, S. (2007). Graph embedding and extensions: A general framework for dimensionality reduction. *IEEE transactions on pattern analysis and machine intelligence*, **29**(1), 40-51.
- Huang, Z., Shan, S., Zhang, H., Lao, S. and Chen, X. (2012). Cross-view graph embedding. In *Asian Conference on Computer Vision* (pp. 770-781). Springer Berlin Heidelberg.
- [3] Fujisawa, H. and Eguchi, S. (2008). Robust parameter estimation with a small bias against heavy contamination. *Journal of Multivariate Analysis*, **99**(9), 2053-2081.
- [4] Rousseeuw, P. J. (1985). Multivariate estimation with high breakdown point. *Mathematical statistics and applications*, 8, 283-297.

# References II

- [5] Maronna, R. A. and Zamar, R. H. (2002). Robust estimates of location and dispersion for high-dimensional datasets. *Technometrics*, **44**(4), 307-317.
- [6] Huber, P. J. (2011). Robust statistics. Springer Berlin Heidelberg.
- [7] Salibian-Barrera, M. and Yohai, V. J. (2006). A fast algorithm for S-regression estimates. Journal of Computational and Graphical Statistics, 15(2), 414-427.
- [8] Todorov V and Filzmoser P (2009) An object-oriented framework for robust multivariate analysis. *Journal of Statistical Software* **32**(1):1-47,
- [9] Lai, P. L., and Fyfe, C. (2000). Kernel and nonlinear canonical correlation analysis. *International Journal of Neural Systems*, 10(05), 365-377.
- [10] Hotelling, H. (1936). Relations between two sets of variates. *Biometrika*, 28(3/4), 321-377.

# Solution of CDMCA

$$\begin{split} \mathbf{X} &= \mathsf{Diag}[\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \cdots, \mathbf{X}^{(D)}] \in \mathbb{R}^{n \times p}, \\ \mathbf{W} &= [\mathbf{W}^{(de)}] \in \mathbb{R}^{n \times n} \left( \mathbf{W}^{(de)} = (w_{ij}^{(de)}) \in \mathbb{R}^{n_d \times n_e} \right), \\ \hat{\mathbf{G}} &= \mathbf{X}^\top \mathsf{diag}(\mathbf{W1}) \mathbf{X} \in \mathbb{R}^{p \times p}, \\ \hat{\mathbf{H}} &= \mathbf{X}^\top \mathbf{WX} \in \mathbb{R}^{p \times p}, \\ \mathbf{A} &= (\mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \cdots, \mathbf{A}^{(D)})^\top \in \mathbb{R}^{p \times K}, \end{split}$$

where  $p = p_1 + p_2 + \cdots + p_D$ ,  $n = n_1 + n_2 + \cdots + n_D$ .

Solution of CDMCA is

$$\hat{\mathbf{A}} = \hat{\mathbf{G}}^{-1/2}(\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_2, \dots, \hat{\mathbf{u}}_K),$$

where  $\hat{\mathbf{G}}^{-1/2} \hat{\mathbf{H}} \hat{\mathbf{G}}^{-1/2} = \sum_{k=1}^{p} \hat{\lambda}_k \hat{\mathbf{u}}_k \hat{\mathbf{u}}_k^{\top}$  is eigendecomposition satisfying  $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \cdots \geq \hat{\lambda}_p$ .

# Simulation settings

- Number of views: D = 3
- Dimension:  $p_1 = p_2 = p_3 = 10$
- Sample size:  $n_1 = n_2 = n_3 = 100$
- Scatter within cluster:  $\sigma > 0$
- Resampling rate:  $\alpha \in (0, 1]$
- Contamination rate:  $\xi \ge 0$



## mean Average Precision (mAP)

For a query  $\mathbf{x}_i^1 \in \mathbb{R}^{p_1}$ , we rank view-2 data vectors  $\{\mathbf{x}_j^2\}_{j=1}^{n_2} \subset \mathbb{R}^{p_2}$  by considering euclidean distances from the query  $\{\|(\hat{\mathbf{A}}^1)^\top \mathbf{x}_i^1 - (\hat{\mathbf{A}}^2)^\top \mathbf{x}_j^2\|_2\}_{j=1}^{n_2}$ . We define an index set of associated vectors  $\mathcal{S}_i := \{1 \leq j \leq n_2 \mid w_{ij}^{12} = 1\}$ , and we sort the ranking of  $\{\mathbf{x}_j^2 \mid j \in \mathcal{S}_i\}$  so as to be  $q_1^{(i)} \leq q_2^{(i)} \leq \cdots \leq q_{|\mathcal{S}_i|}^{(i)}$ . Then Average Precision (AP) for a query  $\mathbf{x}_i^1$  is defined by AP<sub>i</sub> :=  $|\mathcal{S}_i|^{-1} \sum_{j=1}^{|\mathcal{S}_i|} (j/q_j^{(i)})$ , and a sample mean of AP scores over all queries,

$$\mathsf{mAP} := \frac{1}{n_1} \sum_{i=1}^{n_1} \underbrace{\frac{1}{|\mathcal{S}_i|} \sum_{j=1}^{|\mathcal{S}_i|} \frac{j}{q_j^{(i)}}}_{=:\mathsf{AP}_i},$$

is called mean Average Precision (mAP). Higher mAP indicates better retrieval precision.