Bi-Sparse Unsupervised Feature Selection

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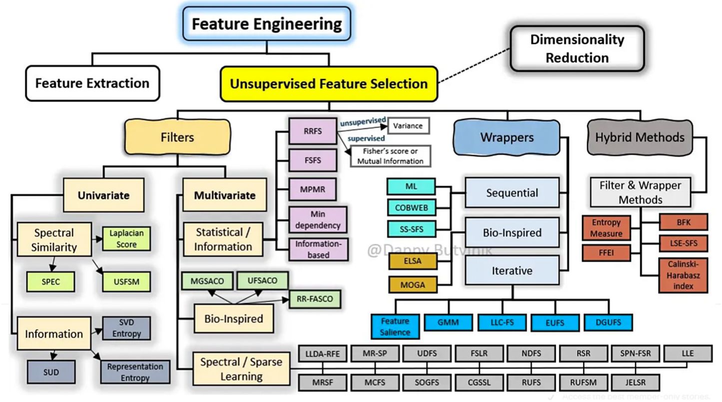
Joint work with Chenyi Huang (SHU), Pan Shang (CAS) and Wanquan Liu (SYSU)

Outline

Unsupervised Feature Selection

- Select a subset of input features without labels
- `https://dannybutvinik.medium.com`



Related Works

- Yang-Shen-Huang-Zhou, IJCAI, 2011

$$\begin{aligned} \min_{W} \ & -\mathrm{Tr}(W^\top S W) + \lambda \|W\|_{2,1} \\ \text{s.t. } & W^\top W = I \end{aligned}$$

- Tian-Nie-Wang-Li, NIPS, 2020

$$\begin{aligned} \min_{W} \ & -\mathrm{Tr}(W^\top S W) + \lambda \|W\|_{2,0} \\ \text{s.t. } & W^\top W = I \end{aligned}$$

- Li-Nie-Bian-Wu-Li, IEEE TPAMI, 2023

$$\begin{aligned} \min_{W} \ & -\mathrm{Tr}(W^\top S W) + \lambda \|W\|_{2,p}^{p} \ (0 < p < 1) \\ \text{s.t. } & W^\top W = I \end{aligned}$$

Related Works

- Zhu-Zhang-Wen-He-Cheng, MTA, 2017

$$
\begin{aligned}
&\min_{W} \; -\mathrm{Tr}(W^\top S W) + \lambda_1 \|W\|_{2,1} + \lambda_2 \|W\|_1 \\
&\text{s.t. } W^\top W = I
\end{aligned}
$$

- Other fields
  - Rubinstein-Zibulevsky-Huang-Elad, IEEE TSP, 2010
  - Hu-Liu-Gao-Shang, IEEE TCBB, 2021
  - Bian-Xu-Wang, IEEE PIMRC, 2022
  - Zhang-Liu-Li, IEEE TIP, 2023

Can non-convex bi-sparse optimization benefit UFS?

Outline

New Formulation

- Bi-sparse unsupervised feature selection

$$\min_{W} \; -\mathrm{Tr}(W^\top SW) + \lambda \|W\|_{2,p}^p \; (0 < p < 1)$$
$$\text{s.t. } W^\top W = I$$

$$\Downarrow$$

$$\min_{W} \; -\mathrm{Tr}(W^\top SW) + \lambda_1 \|W\|_{2,p}^p + \lambda_2 \|W\|_q^q \; (0 \leq p, q < 1)$$
$$\text{s.t. } W^\top W = I$$

- Advantages
  - Bi-sparse optimization: $\lambda_1 \|W\|_{2,p}^p + \lambda_2 \|W\|_q^q$
  - A non-convex framework: $0 \leq p, q < 1$

Optimization Algorithm

- First-order algorithm: PAM (Proximal Alternating Method)
- Model reformulation

$$\begin{aligned} \min_{W} \quad & -\mathrm{Tr}(W^\top S W) + \lambda_1 \|W\|_{2,p}^p + \lambda_2 \|W\|_q^q \\ \text{s.t.} \quad & W^\top W = I \end{aligned}$$

$$\Downarrow$$

$$\begin{aligned} \min_{W,U,V} \quad & -\mathrm{Tr}(W^\top S W) + \lambda_1 \|V\|_{2,p}^p + \lambda_2 \|U\|_q^q \\ \text{s.t.} \quad & W^\top W = I, V = W, U = W \end{aligned}$$

$$\Downarrow$$

$$\begin{aligned} \min_{W,U,V} \quad & -\mathrm{Tr}(W^\top S W) + \lambda_1 \|V\|_{2,p}^p + \lambda_2 \|U\|_q^q \\ & + \frac{\beta_1}{2}\|W - U\|_{\mathrm{F}}^2 + \frac{\beta_2}{2}\|W - V\|_{\mathrm{F}}^2 + \Phi(W) \end{aligned}$$

Optimization Algorithm

- Input: X, λ_1, λ_2, β_1, β_2, p,q, τ_1, τ_2, τ_3
- Initialize: W^0, U^0, V^0
- While not converged do
  - Update W^{k+1} by

$$\begin{aligned}&\min_{W} \; -\mathrm{Tr}(W^\top S W) + \frac{\beta_1}{2}\|W - U^k\|_{\mathrm{F}}^2 + \frac{\beta_2}{2}\|W - V^k\|_{\mathrm{F}}^2 + \frac{\tau_1}{2}\|W - W^k\|_{\mathrm{F}}^2 \\ &\text{s.t. } W^\top W = I\end{aligned}$$

  - Update U^{k+1} by

$$\min_{U} \; \lambda_2\|U\|_q^q + \frac{\beta_1}{2}\|W^{k+1} - U\|_{\mathrm{F}}^2 + \frac{\tau_2}{2}\|U - U^k\|_{\mathrm{F}}^2$$

  - Update V^{k+1} by

$$\min_{V} \; \lambda_1\|V\|_{2,p}^p + \frac{\beta_2}{2}\|W^{k+1} - V\|_{\mathrm{F}}^2 + \frac{\tau_3}{2}\|V - V^k\|_{\mathrm{F}}^2$$

- Output: $W^{k+1}, U^{k+1}, V^{k+1}$

Update W

- Riemannian gradient

$$\begin{aligned}\min_{W} \quad & -\mathrm{Tr}(W^\top S W) + \frac{\beta_1}{2}\|W - U^k\|_{\mathrm{F}}^2 + \frac{\beta_2}{2}\|W - V^k\|_{\mathrm{F}}^2 + \frac{\tau_1}{2}\|W - W^k\|_{\mathrm{F}}^2 \\ \mathrm{s.t.} \quad & W^\top W = I\end{aligned}$$

$$\Downarrow$$

$$\nabla g(W) = -2SW + \beta_1(W - U^k) + \beta_2(W - V^k) + \tau_1(W - W^k)$$

$$\Downarrow$$

$$\begin{aligned}\operatorname{grad} g(W) &= \mathcal{P}_W(\nabla g(W)) \\ &= \nabla g(W) - W \,\mathrm{sym}(W^\top \nabla g(W))\end{aligned}$$

Update W

- Riemannian Hessian

$$\nabla^2 g(W) = -2I \otimes S + (\beta_1 + \beta_2 + \tau_1) I$$

$$\Downarrow$$

$$\begin{aligned} \operatorname{Hess} g(W) &= \mathcal{P}_W(\nabla^2 g(W)) \\ &= \nabla^2 g(W) - W \operatorname{sym}(W^\top \nabla^2 g(W)) \end{aligned}$$

$$\Downarrow$$

$$\operatorname{Hess} g(W) \approx \frac{\operatorname{grad} g(W + \varepsilon I) - \operatorname{grad} g(W)}{\varepsilon}$$

Update W

- Input: S, U^k, V^k, β_1, β_2, τ_1, ε, $\Delta' > 0$, $\rho' \in [0, \frac{1}{4})$
- While not converged do
  - Obtain η_i by solving trust domain subproblem

$$\begin{aligned} \min_{\eta \in \mathrm{T_W}\,\mathrm{St}(d,m)} \quad & m_W(\eta) = g(W) + \mathrm{Tr}(\eta^\top \operatorname{grad} g(W)) + \frac{1}{2}\operatorname{vec}(\eta)^\top \operatorname{Hess} g(W) \operatorname{vec}(\eta) \\ \text{s.t.} \quad & \mathrm{Tr}(\eta^\top W \eta^\top) \leq \Delta^2 \end{aligned}$$

  - Compute the trust ratio ρ_i
  - if $\rho_i < \frac{1}{4}$ then
    $\Delta_{i+1} = \frac{1}{4}\Delta_i$
  - else if $\rho_i > \frac{3}{4}$ and $\|\eta_i\| = \Delta_i$ then
    $\Delta_{i+1} = \min(2\Delta_i, \Delta')$
  - else
    $\Delta_{i+1} = \Delta_i$
  - if $\rho_i > \rho'$ then
    $W^k_{i+1} = R_W(\eta_i)$
  - else
    $W^k_{i+1} = W^k_i$
- Output: W

Update U

$$\min_{U} \ \lambda_2 \|U\|_q^q + \frac{\beta_1}{2}\|W^{k+1} - U\|_{\mathrm{F}}^2 + \frac{\tau_2}{2}\|U - U^k\|_{\mathrm{F}}^2$$

$$\Downarrow$$

$$\min_{U} \ \lambda_2 \|U\|_q^q + \frac{\beta_1 + \tau_2}{2}\|U - \frac{\beta_1}{\beta_1 + \tau_2} W^{k+1} + \frac{\tau_2}{\beta_1 + \tau_2} U^k\|_{\mathrm{F}}^2$$

$$\Downarrow$$

$$\min_{u_{ij}} \ \lambda_2 |u_{ij}|^q + \frac{\beta_1 + \tau_2}{2}(u_{ij} - y_{ij})^2$$

$$\Downarrow$$

$$u_{ij} = \mathrm{Prox}(y_{ij}, \lambda_2/(\beta_1 + \tau_2))$$

Lemma

- Revisiting ℓ_q $(0 \leq q<1)$ Norm Regularized Optimization, arXiv:2306.14394

$$\mathrm{Prox}(a,\lambda) = \mathrm{argmin}_x \frac{1}{2}(x-a)^2 + \lambda|x|^q \ (0 \leq q < 1)$$
$$= \begin{cases} \{0\}, & |a| < \kappa(\lambda,q) \\ \{0, \mathrm{sgn}(a)c(\lambda,q)\}, & |a| = \kappa(\lambda,q) \\ \{\mathrm{sgn}(a)\varpi_q(|a|)\}, & |a| > \kappa(\lambda,q) \end{cases}$$

where

$$c(\lambda,q) = (2\lambda(1-q))^{\frac{1}{2-q}} > 0$$
$$\kappa(\lambda,q) = (2-q)\lambda^{\frac{1}{2-q}}(2(1-q))^{\frac{q+1}{q-2}}$$
$$\varpi_q(a) \in \left\{x : x - a + \lambda q\,\mathrm{sgn}(x)x^{q-1} = 0, x > 0\right\}$$

Update V

$$\min_{V} \;\; \lambda_1 \|V\|_{2,p}^{p} + \frac{\beta_2}{2}\|W^{k+1} - V\|_{\mathrm{F}}^2 + \frac{\tau_3}{2}\|V - V^k\|_{\mathrm{F}}^2$$

$$\Downarrow$$

$$\min_{V} \;\; \lambda_1 \|V\|_{2,p}^{p} + \frac{\beta_2+\tau_3}{2}\|V - \frac{\beta_2}{\beta_2+\tau_3}W^{k+1} + \frac{\tau_3}{\beta_2+\tau_3}V^k\|_{\mathrm{F}}^2$$

$$\Downarrow$$

$$\min_{\mathbf{v}^i} \;\; \lambda_1 \sum_{i=1}^{d} \|\mathbf{v}^i\|_2^p + \frac{\beta_2+\tau_3}{2}\|\mathbf{v}^i - \mathbf{z}^i\|_2^2$$

$$\Downarrow$$

$$\mathbf{v}^i = \mathrm{Prox}(\|\mathbf{z}^i\|_2, \lambda_1/(\beta_2+\tau_3)) \cdot \frac{\mathbf{z}^i}{\|\mathbf{z}^i\|_2}$$

Convergence

- $f(Q)$ is proper and lower semicontinuous.
- $f(Q)$ satisfies the K-L property at each $Q \in \operatorname{dom} f$.
- Assume the sequence $\{Q^k\}_{k\in\mathbb{N}}$ is generated by above algorithm. Then the following inequality holds
$$f(Q^{k+1}) + \tau\|Q^{k+1} - Q^k\|_{\mathrm{F}}^2 \leq f(Q^k)$$
where $\tau = \frac{1}{2}\min\{\tau_1, \tau_2, \tau_3\}$.
- Assume that $\{Q^k\}_{k\in\mathbb{N}}$ is generated by above algorithm. Then, $\{Q^k\}_{k\in\mathbb{N}}$ is bounded. In addition, there exists $V \in \partial f(Q^{k+1})$ such that
$$\|V\|_{\mathrm{F}} \leq a\|Q^{k+1} - Q^k\|_{\mathrm{F}}$$
where $a = \max\{\tau_1, \beta_1 + \tau_2, \beta_2 + \tau_3\}$.

Convergence

- Assume $\{(W^k, U^k, V^k)\}_{k\in\mathbb{N}}$ is generated by above algorithm. Then, the sequence $\{(W^k, U^k, V^k)\}_{k\in\mathbb{N}}$ globally converges to a critical point of $f(W, U, V)$, *i.e.*,

$$0 \in \partial f(W^*, U^*, V^*)$$

with

$$\lim_{k\to+\infty}(W^k, U^k, V^k) = (W^*, U^*, V^*)$$

and $\partial f(\cdot)$ being the limiting subdifferential set.

Outline

Experimental Details

- Compared methods
  - LapScore: He-Cai-Niyogi, NIPS, 2005
  - MCFS: Cai-Zhang-He, SIGKDD, 2010
  - UDFS: Yang-Shen-Ma, IJCAI, 2011
  - SOGFS: Nie-Zhu-Li, IEEE TKDE, 2021
  - RNE: Liu-Ye-Li-Wang, KBS, 2020
  - FSPCA: Tian-Nie-Wang-Li, NIPS, 2020
  - SPCAFS: Li-Nie-Bian, IEEE TPAMI, 2023
  - GSPCA: Zhu-Zhang-Wen, MTA, 2017
- Implementation setups
  - Initialization: QR decomposition
  - Stopping criteria:

$$\frac{|f(W^{k+1}, U^{k+1}, V^{k+1}) - f(W^k, U^k, V^k)|}{\max\{1, |f(W^k, U^k, V^k)|\}} \leq 10^{-4}$$

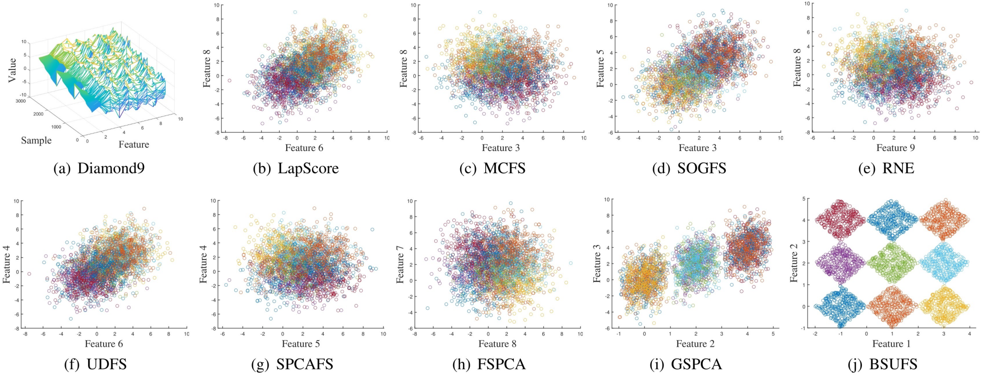
Experimental Details

- Selected datasets

Type	Datasets	Features	Samples	Classes
Synthetic datasets	Dartboard1	9	1000	4
	Diamond9	9	3000	9
Real-world datasets	COIL20	1024	1440	20
	USPS	256	1000	10
	LUNG	325	73	7
	GLIOMA	4434	50	4
	UMIST	644	575	20
	pie	1024	1166	53
	Isolet	617	1560	26
	MSTAR	1024	2425	10

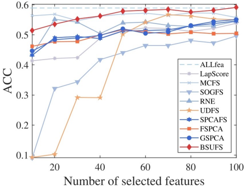
- Evaluation metrics
  - ACC: Accuracy
  - NMI: Normalized mutual information

Synthetic Experiments

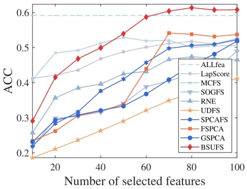


Real Experiments

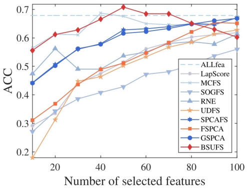
- ACC comparisons



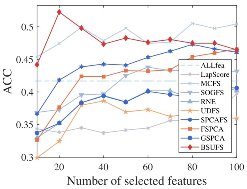
(a) COIL20



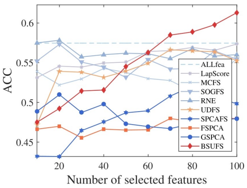
(b) Isolet



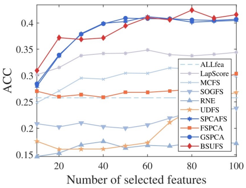
(c) USPS



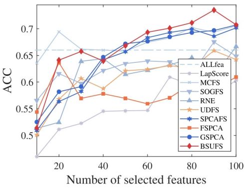
(d) umist



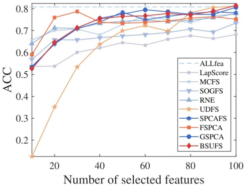
(e) GLIOMA



(f) pie



(g) LUNG



(h) MSTAR

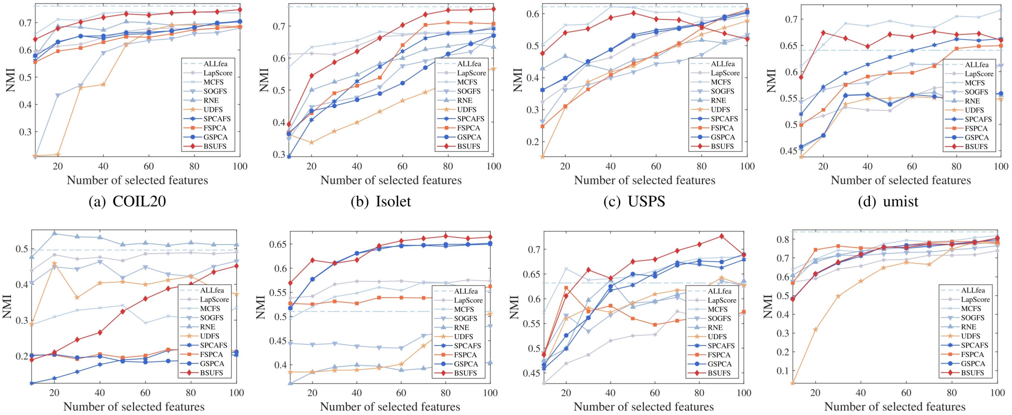
Real Experiments

- ACC comparisons

Datasets	ALLfea	LapScore	MCFS	SOGFS	RNE	UDFS	SPCAFS	FSPCA	GSPCA	BSUFS
COIL20	58.97±4.99 (10)	53.91±3.61 (100)	**57.35±3.83 (80)**	49.66±3.63 (100)	55.16±3.35 (20)	56.77±3.09 (70)	54.63±3.64 (100)	51.71±3.05 (50)	55.12±2.67 (100)	**59.18±3.49 (100)**
Isolet	59.18±3.19 (10)	52.55±2.83 (100)	52.87±2.87 (50)	48.93±2.69 (100)	47.39±2.91 (80)	41.11±1.71 (100)	52.26±2.81 (100)	**54.15±2.69 (70)**	51.84±2.82 (100)	**61.34±3.33 (80)**
USPS	67.79±4.96 (10)	61.76±4.52 (100)	**68.70±4.10 (40)**	56.00±3.48 (100)	61.28±3.46 (100)	62.83±3.79 (100)	66.98±3.92 (100)	65.43±4.90 (90)	66.79±4.10 (100)	**70.77±3.73 (50)**
umist	41.68±2.46 (10)	39.71±3.28 (100)	**50.54±4.16 (80)**	43.81±2.98 (60)	41.01±2.25 (90)	38.64±1.61 (40)	47.32±3.48 (80)	46.58±2.34 (100)	40.65±2.29 (90)	**52.29±3.61 (20)**
GLIOMA	57.44±6.40 (10)	57.36±3.60 (100)	55.52±9.25 (100)	57.32±6.47 (20)	**57.80±2.98 (20)**	56.64±6.47 (70)	52.08±3.64 (80)	48.04±5.26 (90)	51.00±5.08 (20)	**61.28±9.01 (100)**
pie	25.79±1.39 (10)	34.86±1.43 (60)	31.46±1.47 (70)	23.78±1.19 (100)	17.49±0.76 (40)	26.82±1.32 (100)	**41.16±2.46 (60)**	30.39±1.43 (100)	40.90±1.85 (50)	**42.45±1.74 (80)**
LUNG	66.03±7.23 (10)	60.93±8.02 (70)	70.55±7.66 (100)	67.53±7.73 (90)	66.68±8.32 (100)	65.89±7.43 (90)	70.16±7.71 (100)	63.62±5.45 (20)	**70.68±7.41 (100)**	**73.51±6.80 (90)**
MSTAR	80.81±8.76 (10)	68.21±4.57 (100)	77.60±8.32 (100)	73.46±5.61 (100)	77.82±6.16 (100)	**81.25±7.48 (100)**	78.63±8.68 (90)	78.74±5.20 (30)	80.65±6.47 (100)	**81.43±6.89 (100)**
Average	57.21±4.92	53.66±3.98	**58.07±5.21**	52.56±4.22	53.08±3.77	53.74±4.11	57.90±4.54	54.83±3.79	57.21±4.09	**62.78±4.83**

Real Experiments

- NMI comparisons



(a) COIL20 (b) Isolet (c) USPS (d) umist

(e) GLIOMA (f) pie (g) LUNG (h) MSTAR

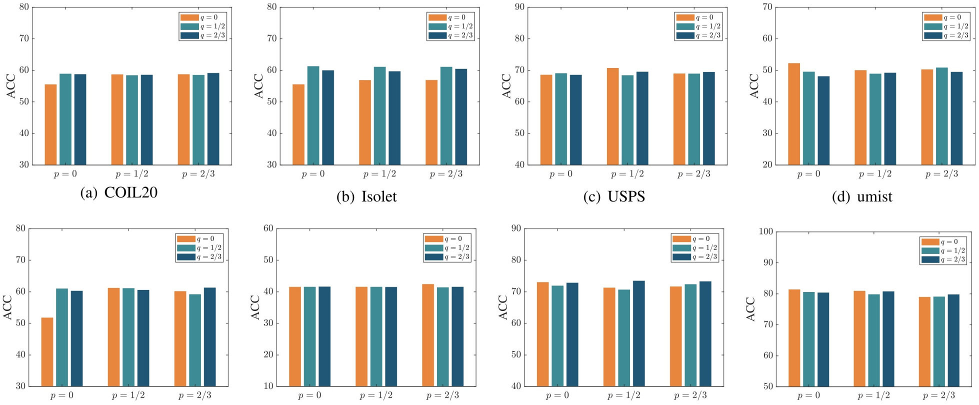
Real Experiments

- NMI comparisons

Datasets	ALLfea	LapScore	MCFS	SOGFS	RNE	UDFS	SPCAFS	FSPCA	GSPCA	BSUFS
COIL20	76.04±1.69 (10)	69.01±1.53 (100)	**73.98±1.79 (80)**	68.03±1.59 (100)	70.76±2.07 (100)	69.12±1.17 (80)	70.29±1.31 (100)	68.41±1.60 (100)	70.44±1.37 (100)	**74.78±1.79 (100)**
Isolet	76.09±1.77 (10)	69.86±1.26 (100)	68.29±1.05 (50)	67.15±1.45 (90)	64.74±1.28 (100)	56.73±1.05 (100)	69.18±1.33 (100)	**71.12±1.11 (80)**	67.02±1.43 (100)	**75.32±1.22 (100)**
USPS	62.11±2.24 (10)	59.37±1.98 (100)	**62.18±2.01 (40)**	53.36±1.83 (100)	52.77±2.01 (100)	57.76±2.02 (100)	60.28±2.17 (100)	**61.14±1.87 (100)**	60.54±2.29 (100)	60.16±1.68 (50)
umist	64.07±1.76 (10)	61.23±2.15 (100)	**71.71±2.29 (100)**	61.46±2.03 (70)	56.08±1.80 (60)	55.43±1.50 (80)	66.26±1.74 (100)	64.94±1.65 (100)	55.88±1.62 (100)	**67.62±1.91 (70)**
GLIOMA	49.59±6.76 (10)	**48.96±3.59 (100)**	34.15±9.10 (50)	46.51±9.11 (20)	**54.21±2.23 (100)**	45.86±8.08 (20)	22.01±4.88 (80)	22.17±5.17 (90)	21.09±4.65 (100)	45.14±8.66 (100)
pie	51.01±1.02 (10)	57.53±0.73 (90)	57.16±1.01 (70)	48.05±0.76 (100)	40.45±0.79 (100)	50.55±1.03 (100)	64.94±1.30 (100)	56.21±0.90 (100)	**65.20±1.42 (100)**	**66.66±1.14 (80)**
LUNG	63.18±5.48 (10)	57.44±6.44 (70)	68.53±5.20 (100)	63.62±5.41 (40)	63.74±5.30 (90)	64.27±5.35 (90)	67.91±6.23 (100)	62.23±4.80 (20)	**68.96±5.71 (100)**	**72.64±4.69 (90)**
MSTAR	83.96±3.14 (10)	73.90±1.62 (100)	**81.85±2.91 (100)**	76.56±1.54 (100)	78.26±2.51 (100)	78.18±3.64 (90)	79.62±2.30 (100)	78.87±2.52 (90)	80.53±2.41 (100)	**80.66±2.68 (100)**
Average	65.76±2.98	62.16±2.41	**64.73±3.17**	60.59±2.96	60.13±2.25	59.74±2.98	62.56±2.66	60.64±2.45	61.21±2.61	**67.87±2.97**

Effects of p and q

- ACC comparisons

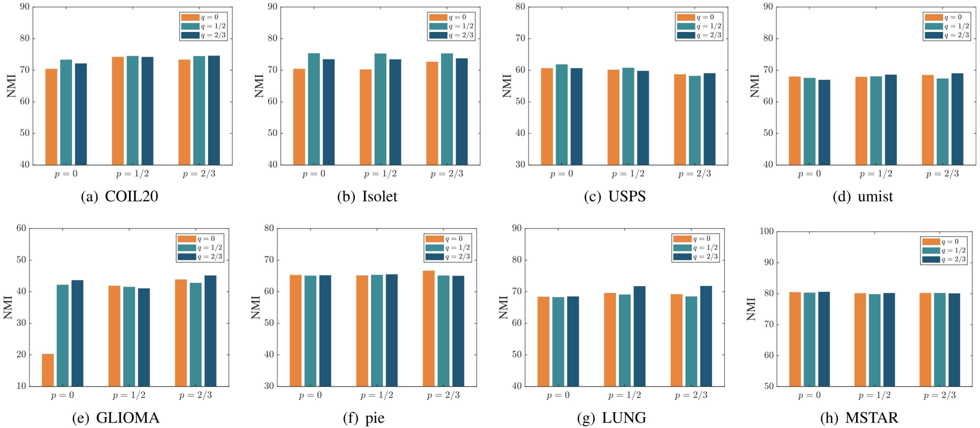


(a) COIL20 (b) Isolet (c) USPS (d) umist

(e) GLIOMA (f) pie (g) LUNG (h) MSTAR

Effects of p and q

- NMI comparisons



Ablation Experiments

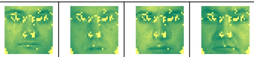
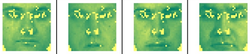
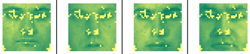
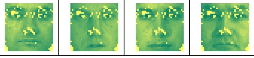
- ACC comparisons

Datasets	Case I	Case II	Case III	Case IV
COIL20	54.09	57.19	**58.76**	**59.18**
Isolet	51.77	**59.49**	56.19	**61.34**
USPS	67.06	67.58	**68.11**	**70.77**
umist	47.16	47.52	**49.23**	**52.29**
GLIOMA	49.76	59.16	**60.12**	**61.28**
pie	40.98	40.79	**41.15**	**42.45**
LUNG	71.34	70.30	**72.33**	**73.51**
MSTAR	79.25	78.63	**80.08**	**81.43**

- NMI comparisons

Datasets	Case I	Case II	Case III	Case IV
COIL20	69.94	72.31	**74.57**	**74.78**
Isolet	66.84	**73.18**	72.73	**75.32**
USPS	**60.65**	59.10	**61.14**	60.16
umist	66.48	67.14	**69.45**	**67.62**
GLIOMA	20.64	**44.74**	43.13	**45.14**
pie	65.02	65.13	**65.23**	**66.66**
LUNG	69.31	69.08	**71.94**	**72.64**
MSTAR	79.92	79.61	**79.97**	**80.66**

- Visual comparisons

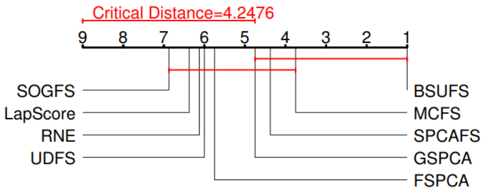
Methods	Samples	ACC	NMI
Case I		40.98	65.02
Case II		40.79	65.11
Case III		**41.15**	**65.23**
Case IV		**42.45**	**66.66**

Statistical Tests

- Friedman test

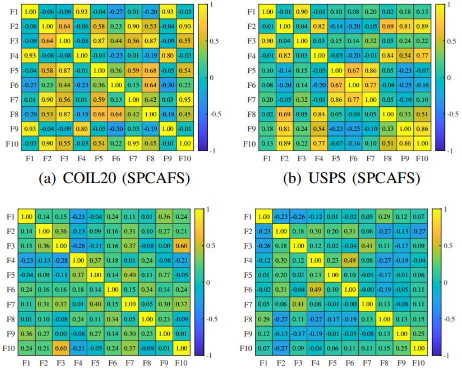
Methods	Ranking	P-value	Hypothesis
LapScore	5.670	0.0005	Reject
MCFS	**3.750**		
SOGFS	6.875		
RNE	6.125		
UDFS	6.000		
SPCAFS	4.375		
FSPCA	5.750		
GSPCA	4.750		
BSUFS	**1.000**		

- Post-hoc Nemenyi test



Discussion

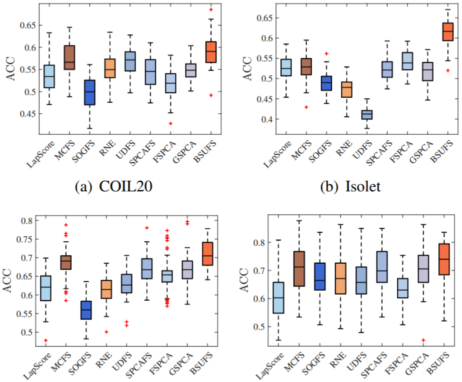
- Feature correlation



(a) COIL20 (SPCAFS) (b) USPS (SPCAFS)

(c) COIL20 (BSUFS) (d) USPS (BSUFS)

- Model stability



(a) COIL20 (b) Isolet

(c) USPS (d) LUNG

Outline

Conclusions and Future Work

- Conclusions
  - Construct bi-sparse optimization with $p, q \in [0, 1)$
  - Develop an efficient and convergent PAM algorithm
  - Perform sufficient experiments on real-word datasets
- Future work
  - Learn sparse via deep NNs
  - Extend to decentralized optimization
  - Apply to IoT anomaly detection

Thank you for your attention!

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