

Bi-Sparse Unsupervised Feature Selection

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Outline

Introduction

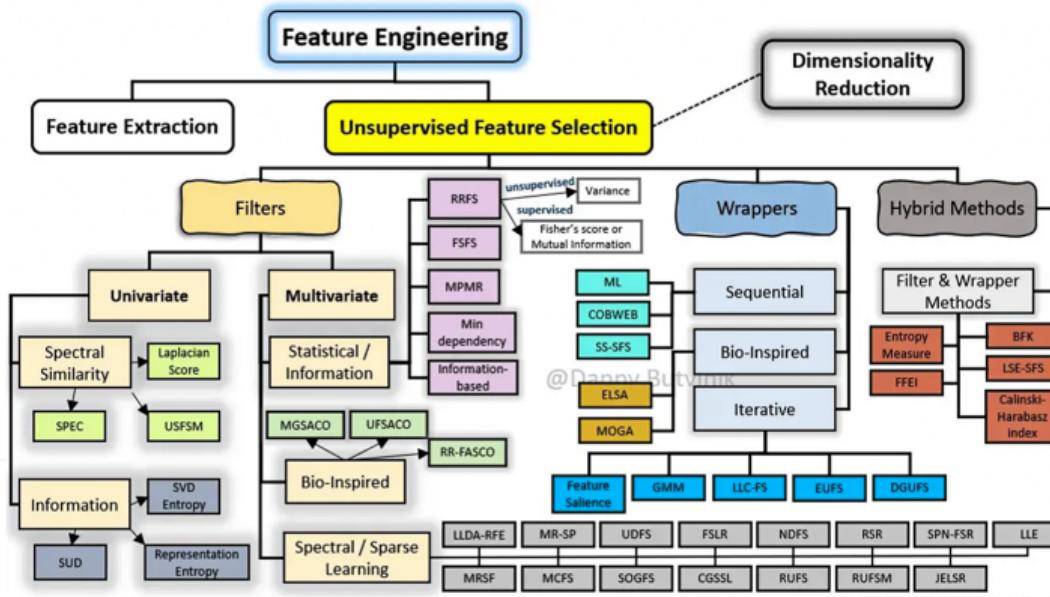
Proposed Method

Numerical Experiments

Conclusions and Future Work

Unsupervised Feature Selection

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



@DannyButvinik

Related Works

- ▶ Yang-Shen-Huang-Zhou, IJCAI, 2011

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

- ▶ Tian-Nie-Wang-Li, NIPS, 2020

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

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

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

Related Works

- ▶ Zhu-Zhang-Wen-He-Cheng, MTA, 2017

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

- ▶ 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?

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New Formulation

- Bi-sparse unsupervised feature selection

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

↓

$$\begin{aligned} \min_W \quad & -\text{Tr}(W^\top SW) + \lambda_1 \|W\|_{2,p}^p + \lambda_2 \|W\|_q^q \quad (0 \leq p, q < 1) \\ \text{s.t. } \quad & W^\top W = I \end{aligned}$$

- 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

$$\min_W -\text{Tr}(W^\top SW) + \lambda_1 \|W\|_{2,p}^p + \lambda_2 \|W\|_q^q$$

$$\text{s.t. } W^\top W = I$$

\Downarrow

$$\min_{W,U,V} -\text{Tr}(W^\top SW) + \lambda_1 \|V\|_{2,p}^p + \lambda_2 \|U\|_q^q$$

$$\text{s.t. } W^\top W = I, V = W, U = W$$

\Downarrow

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

Optimization Algorithm

- ▶ Input: $X, \lambda_1, \lambda_2, \beta_1, \beta_2, p, q, \tau_1, \tau_2, \tau_3$
- ▶ Initialize: W^0, U^0, V^0
- ▶ While not converged do
 - ▶ Update W^{k+1} by

$$\begin{aligned} \min_W \quad & -\text{Tr}(W^\top SW) + \frac{\beta_1}{2} \|W - U^k\|_F^2 + \frac{\beta_2}{2} \|W - V^k\|_F^2 + \frac{\tau_1}{2} \|W - W^k\|_F^2 \\ \text{s.t. } & W^\top W = I \end{aligned}$$

- ▶ Update U^{k+1} by

$$\min_U \lambda_2 \|U\|_q^q + \frac{\beta_1}{2} \|W^{k+1} - U\|_F^2 + \frac{\tau_2}{2} \|U - U^k\|_F^2$$

- ▶ Update V^{k+1} by

$$\min_V \lambda_1 \|V\|_{2,p}^p + \frac{\beta_2}{2} \|W^{k+1} - V\|_F^2 + \frac{\tau_3}{2} \|V - V^k\|_F^2$$

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

Update W

► Riemannian gradient

$$\min_W -\text{Tr}(W^\top SW) + \frac{\beta_1}{2} \|W - U^k\|_{\text{F}}^2 + \frac{\beta_2}{2} \|W - V^k\|_{\text{F}}^2 + \frac{\tau_1}{2} \|W - W^k\|_{\text{F}}^2$$

$$\text{s.t. } W^\top W = I$$



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



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

Update W

► Riemannian Hessian

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

\Downarrow

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

\Downarrow

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

Update W

- ▶ Input: $S, U^k, V^k, \beta_1, \beta_2, \tau_1, \varepsilon, \Delta' > 0, \rho' \in [0, \frac{1}{4})$
- ▶ While not converged do
 - ▶ Obtain η_i by solving trust domain subproblem

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

- ▶ 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
$$W_{i+1}^k = R_W(\eta_i)$$
 - ▶ else
$$W_{i+1}^k = W_i^k$$
- ▶ Output: W

Update U

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

↓

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

↓

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

↓

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

Lemma

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

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

where

$$c(\lambda, q) = (2\lambda(1-q))^{\frac{1}{2-q}} > 0$$

$$\kappa(\lambda, q) = (2-q)\lambda^{\frac{1}{2-q}}(2(1-q))^{\frac{q+1}{q-2}}$$

$$\varpi_q(a) \in \{x : x - a + \lambda q \operatorname{sgn}(x)x^{q-1} = 0, x > 0\}$$

Update V

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

\Downarrow

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

\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

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

Convergence

- ▶ $f(Q)$ is proper and lower semicontinuous.
- ▶ $f(Q)$ satisfies the K-L property at each $Q \in \text{dom } f$.
- ▶ Assume the sequence $\{Q^k\}_{k \in \mathbb{N}}$ is generated by above algorithm. Then the following inequality holds

$$f(Q^{k+1}) + \tau \|Q^{k+1} - Q^k\|_F^2 \leq f(Q^k)$$

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

$$\|V\|_F \leq a \|Q^{k+1} - Q^k\|_F$$

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

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

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

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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

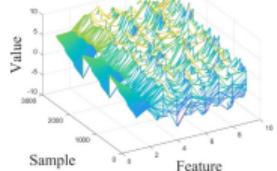
- ▶ Selected datasets

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

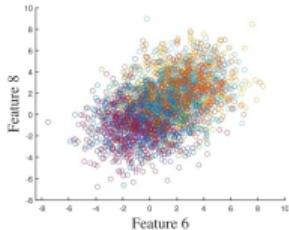
- ▶ Evaluation metrics

- ▶ ACC: Accuracy
- ▶ NMI: Normalized mutual information

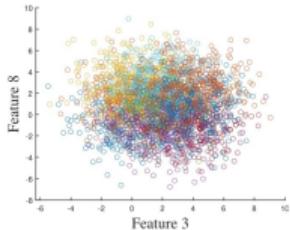
Synthetic Experiments



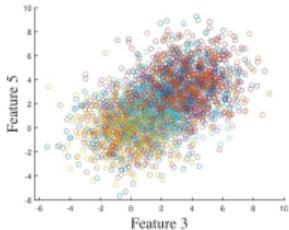
(a) Diamond9



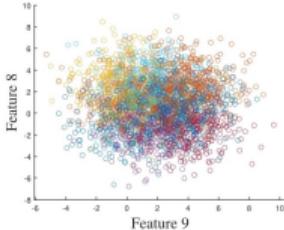
(b) LapScore



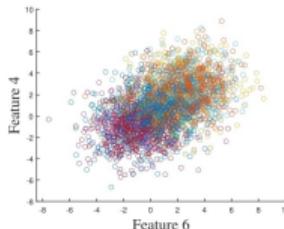
(c) MCFS



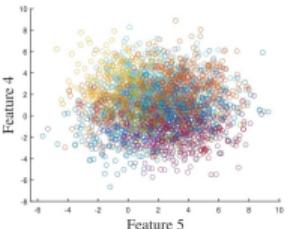
(d) SOGFS



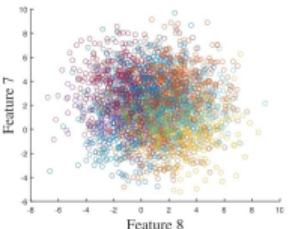
(e) RNE



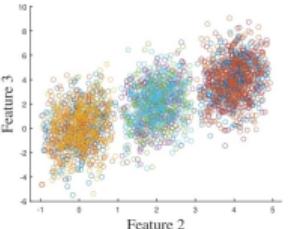
(f) UDFS



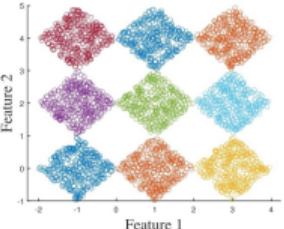
(g) SPCAFS



(h) FSPCA

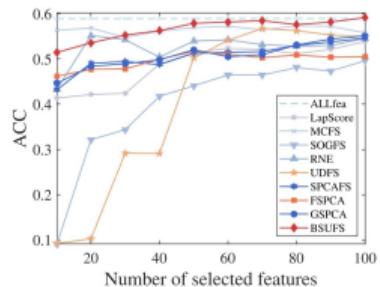


(i) GSPCA

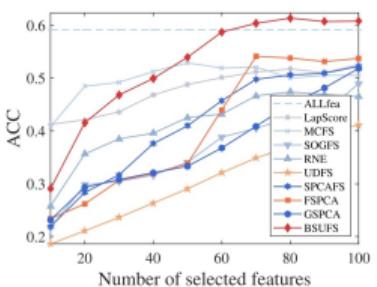


(j) BSUFS

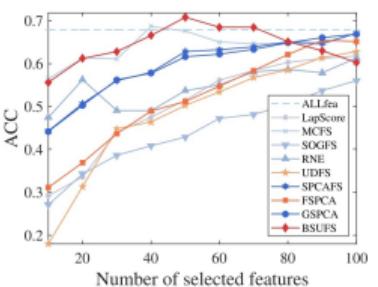
Real-world Experiments — ACC



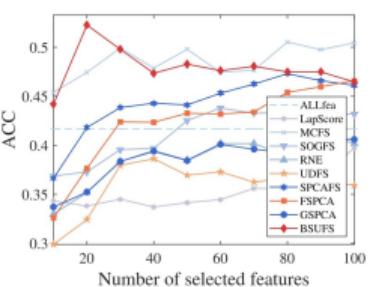
(a) COIL20



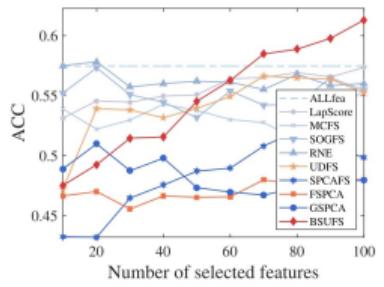
(b) Isolet



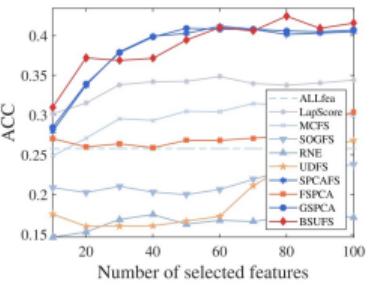
(c) USPS



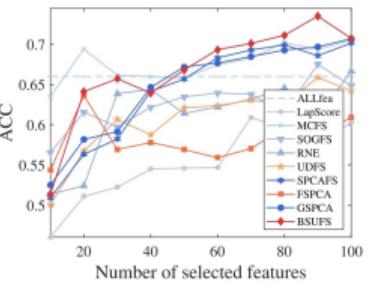
(d) umist



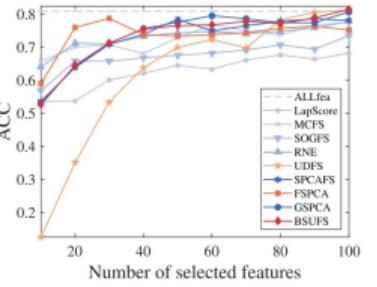
(e) GLIOMA



(f) pie



(g) LUNG

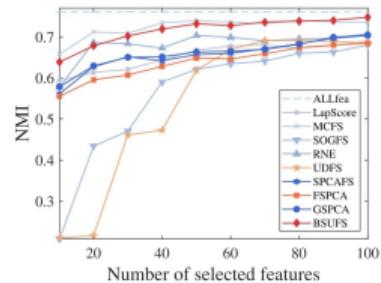


(h) MSTAR

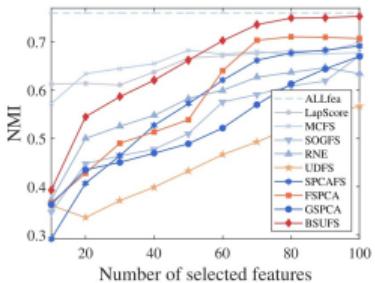
Real-world Experiments — ACC

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

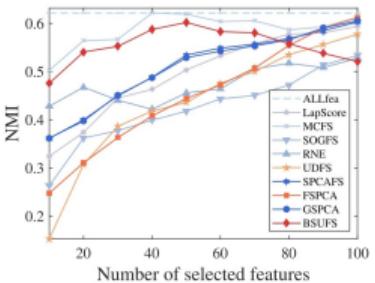
Real-world Experiments —— NMI



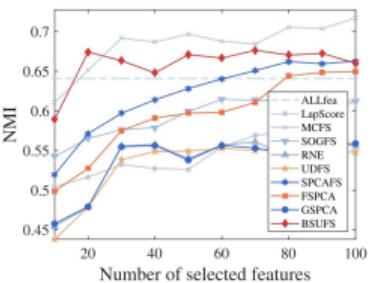
(a) COIL20



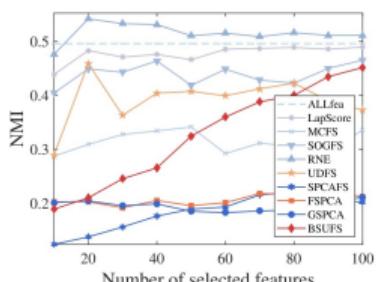
(b) Isolet



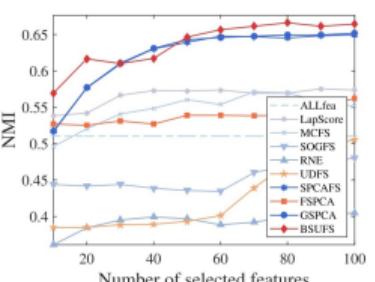
(c) USPS



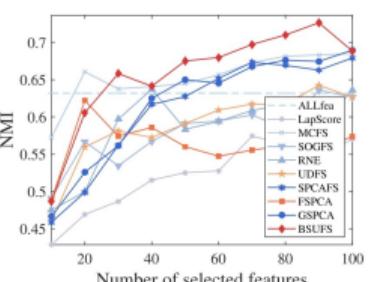
(d) umist



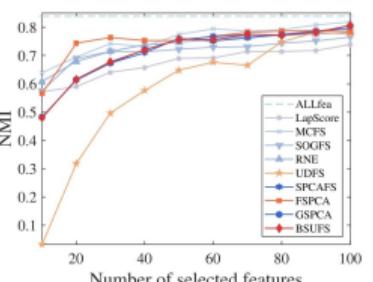
(e) GLIOMA



(f) pie



(g) LUNG

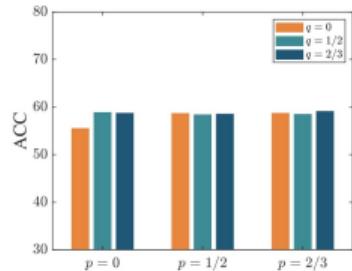


(h) MSTAR

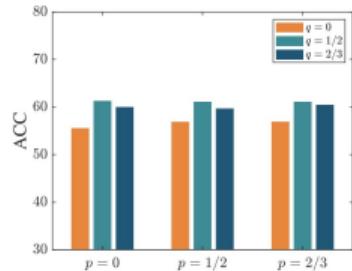
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COIL20	76.04±1.69 (10)	69.01±1.53 (100)	73.98±1.79 (80)	68.03±1.59 (100)	70.76±2.07 (100)	69.12±1.17 (80)	70.29±1.31 (100)	68.41±1.60 (100)	70.44±1.37 (100)	74.78±1.79 (100)
Isolet	76.09±1.77 (10)	69.86±1.26 (100)	68.29±1.05 (50)	67.15±1.45 (90)	64.74±1.28 (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

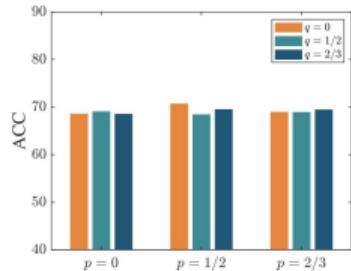
Effects of p and q



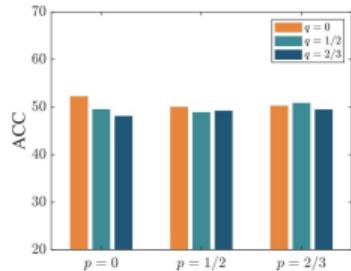
(a) COIL20



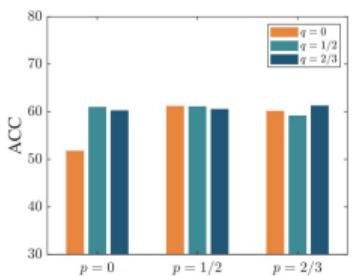
(b) Isolet



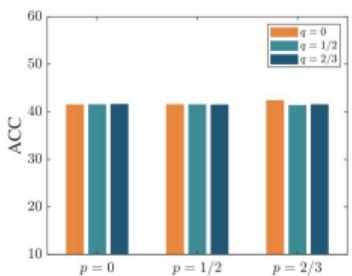
(c) USPS



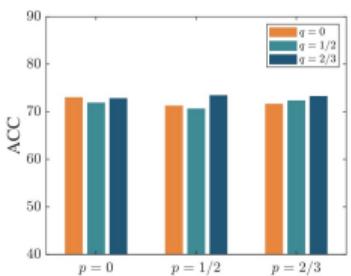
(d) umist



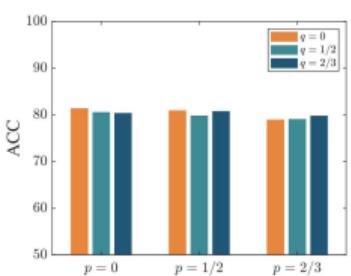
(e) GLIOMA



(f) pie

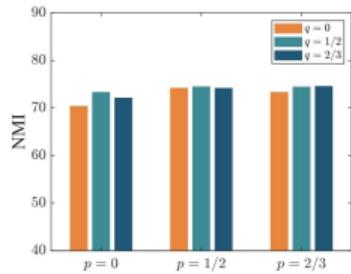


(g) LUNG

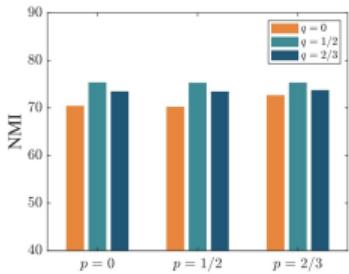


(h) MSTAR

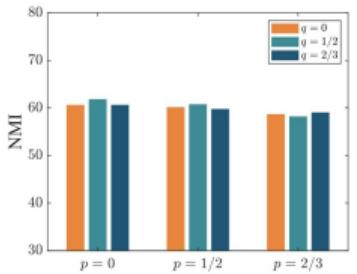
Effects of p and q



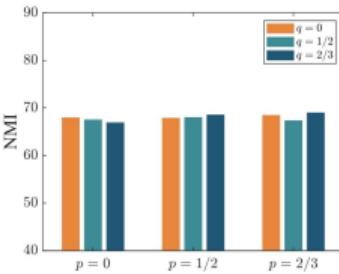
(a) COIL20



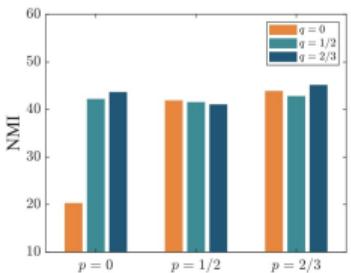
(b) Isolet



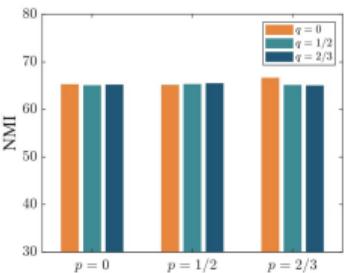
(c) USPS



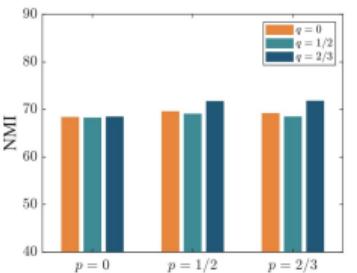
(d) umist



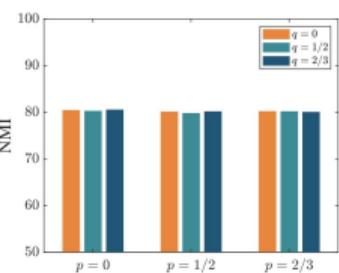
(e) GLIOMA



(f) pie



(g) LUNG



(h) MSTAR

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

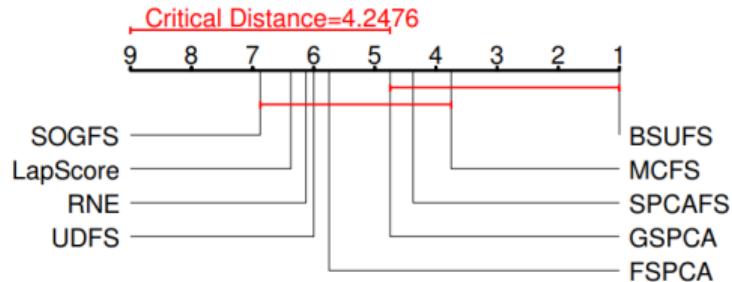
Methods	Samples				ACC	NMI
	Case I	Case II	Case III	Case IV		
Case I					40.98	65.02
Case II					40.79	65.11
Case III					41.15	65.23
Case IV					42.45	66.66

Statistical Tests

► Friedman test

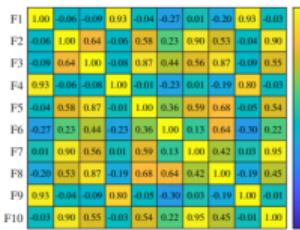
Methods	Ranking	P-value	Hypothesis
LapScore	5.670	0.0005	Reject
MCFS	3.750		
SOGFS	6.875		
RNE	6.125		
UDFS	6.000		
SPCAFS	4.375		
FSPCA	5.750		
GSPCA	4.750		
BSUFS	1.000		

► Post-hoc Nemenyi test

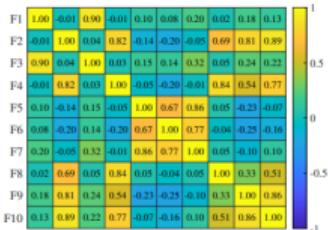


Discussion

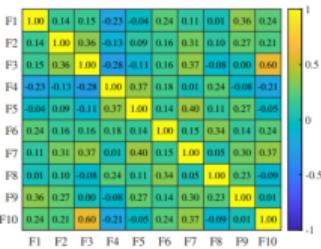
► Feature correlation



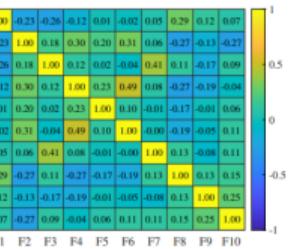
(a) COIL20 (SPCAFS)



(b) USPS (SPCAFS)

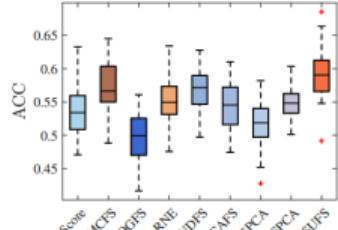


(c) COIL20 (BSUFS)

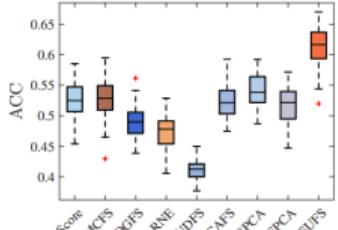


(d) USPS (BSUFS)

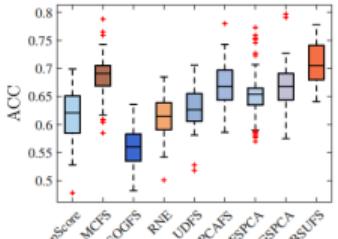
► Model stability



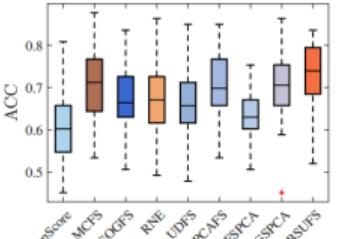
(a) COIL20



(b) Isolet



(c) USPS



(d) LUNG

Outline

Introduction

Proposed Method

Numerical Experiments

Conclusions and Future Work

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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