Learning to Select Features

Xianchao Xiu

Department of Automation

上海大学 Shanghai University

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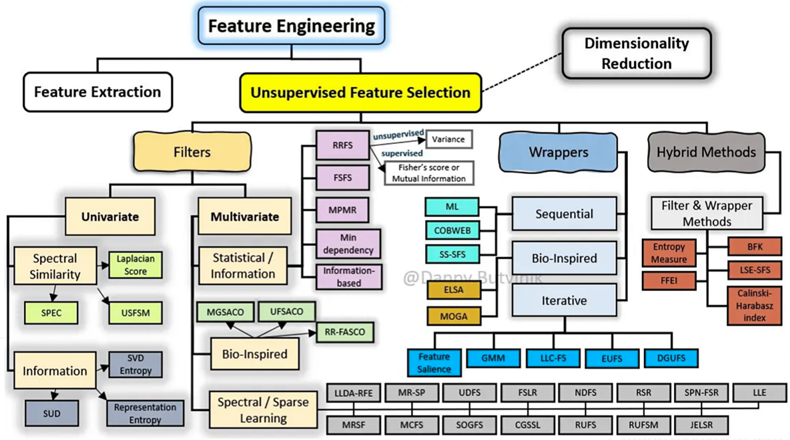
Joint work with Anning Yang (SHU), Long Chen (SHU), Jianhao Li (SHU) and others

Outline

UFS

- Unsupervised feature selection *vs.* Feature extraction
- Select a subset of input features without labels



PCA

- Given $X = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n) \in \mathbb{R}^{d\times n}$, principal component analysis (PCA) is

$$\begin{aligned} \min_{W\in\mathbb{R}^{d\times p}} \quad & \frac{1}{2}\|X - WW^\top X\|_{\mathrm{F}}^2 \\ \text{s.t.} \quad & W^\top W = I_p \end{aligned}$$

$$\Updownarrow$$

$$\begin{aligned} \min_{W\in\mathbb{R}^{d\times p}} \quad & -\mathrm{Tr}(W^\top XX^\top W) \\ \text{s.t.} \quad & W^\top W = I_p \end{aligned}$$

- Unsupervised feature selection by sparse PCA

$$\begin{aligned} \min_{W\in\mathbb{R}^{d\times p}} \quad & -\mathrm{Tr}(W^\top XX^\top W) \\ \text{s.t.} \quad & W^\top W = I_p, \ \|W\|_{2,0} \le s \end{aligned}$$

- The i-th feature can be measured by $\|\mathbf{w}^i\|$ since $\mathbf{z}_i = (\mathbf{w}^{1\top}, \ \mathbf{w}^{2\top}, \ \ldots \ , \mathbf{w}^{d\top})\mathbf{x}_i$
- The dimension number is often omitted when it does not cause ambiguity

SOTA

- Li-Nie-Bian et al, Sparse PCA via $\ell_{2,p}$-Norm Regularization for Unsupervised Feature Selection, IEEE TPAMI, 2023

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

- Li-Sun-Zhang, Unsupervised Feature Selection via Nonnegative Orthogonal Constrained Regularized Minimization, arXiv:2403.16966

$$\begin{aligned} \min_{W,Y} \quad & \mathrm{Tr}(Y^\top L Y) + \alpha \|Y - X^\top W\|_{2,1} + \beta \|W\|_{2,1} + \gamma \|W\|_{\mathrm{F}}^2 \\ \text{s.t.} \quad & Y^\top Y = I, \ Y \geq 0 \end{aligned}$$

- Hu-Wang-Zhang et al, Bi-Level Spectral Feature Selection, IEEE TNNLS, 2025
- Jiao-Xue-Zhang, Sparse Learning-Based Feature Selection in Classification: A Multi-Objective Perspective, IEEE TETCI, 2025
- Li-Yu-Yang et al, Exploring Feature Selection With Limited Labels: A Comprehensive Survey of Semi-Supervised and Unsupervised Approaches, IEEE TKDE, 2024

Contribution

- (Q1) How to learn feature structures $\Rightarrow$ Sparse coding

  Xiu-Yang-Huang et al, Enhancing Unsupervised Feature Selection via Double Sparsity Constrained Optimization, 2025
- (Q2) How to learn data distributions $\Rightarrow$ Contrastive learning

  Xiu-Yang-Li, Sparse PCA Meets Contrastive Learning: A New Method for Unsupervised Feature Selection, 2025
- (Q3) How to learn regularization parameters $\Rightarrow$ Deep unfolding networks

  Chen-Xiu, Tuning-Free Structured Sparse PCA via Deep Unfolding Networks, 2025
- (Q4) How to learn feature selection $\Rightarrow$ Large language models

  Li-Xiu, LLM4FS: Leveraging Large Language Models for Feature Selection and How to Improve It, 2025

Outline

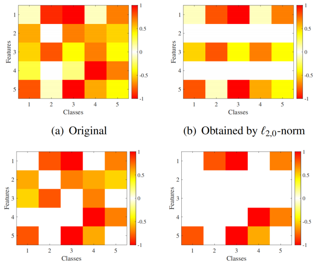
Model

- (Q1) How to learn feature structures

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

$$\Downarrow$$

$$\begin{aligned} \min_{W} \quad & -\mathrm{Tr}(W^\top X X^\top W) \\ \text{s.t.} \quad & W^\top W = I, \ \|W\|_{2,0} \le s_1, \ \|W\|_0 \le s_2 \end{aligned}$$



(a) Original (b) Obtained by $\ell_{2,0}$-norm

(c) Obtained by ℓ_0-norm (d) Obtained by double sparsity

- Double Sparsity Constrained Optimization for Feature Selection (DSCOFS)
  - $\|W\|_{2,0} \le s_1$: Global feature selection
  - $\|W\|_0 \le s_2$: Local feature selection

Algorithm

- Proximal alternating method (PAM)
- Model reformulation

$$
\begin{aligned}
\min_{W} \quad & -\mathrm{Tr}(W^\top X X^\top W) \\
\text{s.t.} \quad & W^\top W = I, \ \|W\|_{2,0} \le s_1, \ \|W\|_0 \le s_2
\end{aligned}
$$

$$\Downarrow$$

$$
\begin{aligned}
\min_{W,Y,Z} \quad & -\mathrm{Tr}(W^\top X X^\top W) \\
\text{s.t.} \quad & W^\top W = I, \ \|Y\|_{2,0} \le s_1, \ \|Z\|_0 \le s_2 \\
& W = Y, \ W = Z
\end{aligned}
$$

$$\Downarrow$$

$$
\begin{aligned}
\min_{W,Y,Z} \quad & -\mathrm{Tr}(W^\top X X^\top W) + \mu_1 \|W - Y\|_{\mathrm{F}}^2 + \mu_2 \|W - Z\|_{\mathrm{F}}^2 \\
\text{s.t.} \quad & W^\top W = I, \ \|Y\|_{2,0} \le s_1, \ \|Z\|_0 \le s_2
\end{aligned}
$$

Algorithm

- Input: X, μ_1, μ_2, s_1, s_2, τ_1, τ_2, τ_3
- Initialize: (W^0, Y^0, Z^0)
- While not converged do
  - Update W^{k+1} by

$$\begin{aligned} \min_{W} \quad & -\mathrm{Tr}(W^\top X X^\top W) + \mu_1 \|W - Y^k\|_\mathrm{F}^2 + \mu_2 \|W - Z^k\|_\mathrm{F}^2 + \tau_1 \|W - W^k\|_\mathrm{F}^2 \\ \text{s.t.} \quad & W^\top W = I \end{aligned}$$

  - Update Y^{k+1} by

$$\begin{aligned} \min_{Y} \quad & \|W^{k+1} - Y\|_\mathrm{F}^2 + \tau_2 \|Y - Y^k\|_\mathrm{F}^2 \\ \text{s.t.} \quad & \|Y\|_{2,0} \leq s_1 \end{aligned}$$

  - Update Z^{k+1} by

$$\begin{aligned} \min_{Z} \quad & \|W^{k+1} - Z\|_\mathrm{F}^2 + \tau_3 \|Z - Z^k\|_\mathrm{F}^2 \\ \text{s.t.} \quad & \|Z\|_0 \leq s_2 \end{aligned}$$

Convergence

- Denote the objective function as

$$f(W, Y, Z) = -\operatorname{Tr}(W^\top X X^\top W X) + \mu_1 \|W - Y\|_{\mathrm{F}}^2 + \mu_2 \|W - Z\|_{\mathrm{F}}^2$$

- Suppose that $\beta \geq \max\{2(\lambda_0 + \lambda_1), 2m\lambda_2\}$
- (Theorem) Let $\{(W^k, Y^k, Z^k)\}$ be the generated sequence. Then the following properties hold:
  - $\{f(W^k, Y^k, Z^k)\}$ is strictly nonincreasing
  - The sequence $\{(W^k, Y^k, Z^k)\}$ is bounded
  - $\lim_{k\to\infty} \|(W^{k+1}, Y^{k+1}, Z^{k+1}) - (W^k, Y^k, Z^k)\|_{\mathrm{F}} = 0$
  - Any accumulation point (W^*, Y^*, Z^*) of the sequence $\{(W^k, Y^k, Z^k)\}$ is a stationary point in the sense that

$$0 \in \nabla f(W^*, Y^*, Z^*) + \mathrm{N}(W^*, Y^*, Z^*)$$

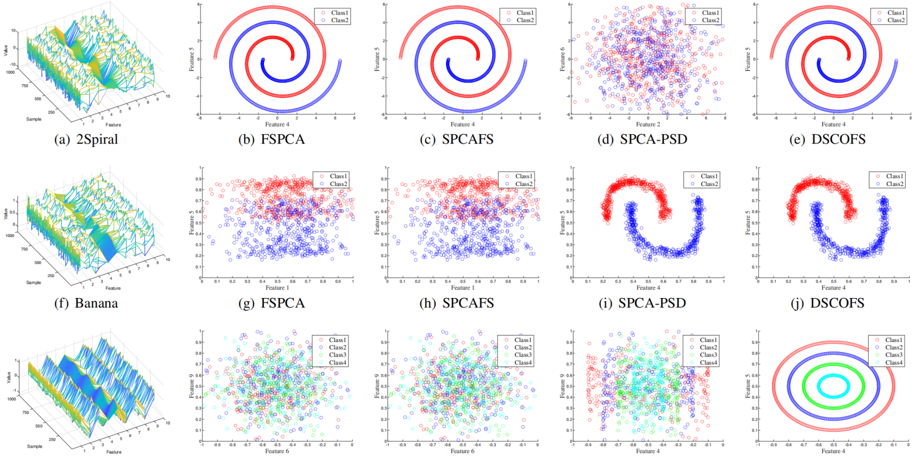
Experiments

- Compared methods
  - LapScore: He-Cai-Niyogi, NIPS, 2005
  - UDFS: Yang-Shen-Ma et al, IJCAI, 2011
  - SOGFS: Nie-Zhu-Li, IEEE TKDE, 2021
  - RNE: Liu-Ye-Li-Wang et al, KBS, 2020
  - SPCAFS: Li-Nie-Bian-Wu et al, IEEE TPAMI, 2023
  - FSPCA: Nie-Tian-Wang et al, IEEE TPAMI, 2023
  - SPCA-PSD: Zheng-Zhang-Liu et al, arXiv:2309.06202
- Implementation setups
  - Initialization: RandOrthhMat
  - Sparsity level: $s_1 \in \{10, 20, \ldots, 100\}$, $s_2 \in \{0.1, 0.2, \ldots, 0.9\}dp$
  - Stopping criteria:

$$\frac{|f(X^{k+1}, Y^{k+1}, Z^{k+1}) - f(X^k, Y^k, Z^k)|}{1 + |f(X^k, Y^k, Z^k)|} \leq 10^{-3}$$

Experiments

- Synthetic datasets



(a) 2Spiral (b) FSPCA (c) SPCAFS (d) SPCA-PSD (e) DSCOFS

(f) Banana (g) FSPCA (h) SPCAFS (i) SPCA-PSD (j) DSCOFS

(k) Dartboard (l) FSPCA (m) SPCAFS (n) SPCA-PSD (o) DSCOFS

Experiments

- Real datasets: Accuracy (ACC) ↑

Datasets	ALLfea	LapScore	UDFS	SOGFS	RNE	FSPCA	SPCAFS	SPCA-PSD	DSCOFS
COIL20	57.74±4.93	54.82±3.91 (100)	**58.71±3.47 (100)**	49.66±4.81 (100)	55.84±4.41 (90)	50.15±4.70 (100)	54.39±3.67 (100)	56.57±3.05 100)	**60.51±4.63 (100)**
USPS	65.12±4.95	62.02±4.09 (90)	59.52±2.97 (60)	55.58±3.07 (100)	46.04±2.69 (100)	**67.38±4.36 (60)**	67.34±4.49 (100)	65.38±4.26 (100)	**69.67±4.97 (100)**
lung_discrete	65.10±6.44	59.29±6.33 (70)	68.58±6.99 (100)	65.12±6.89 (100)	64.05±6.65 (100)	60.19±6.55 (40)	71.37±7.68 (100)	**72.22±8.02 (80)**	**73.12±8.48 (100)**
GLIOMA	56.84±5.24	58.88±3.96 (90)	56.80±4.85 (100)	57.44±6.16 (70)	58.32±7.31 (90)	47.92±4.61 (80)	50.60±5.02 (20)	**59.28±5.01 (90)**	**60.88±6.31 (80)**
UMIST	41.07±2.38	40.13±2.79 (100)	47.12±2.49 (40)	41.70±3.17 (100)	40.35±2.26 (90)	46.70±2.29 (100)	46.78±2.51 (90)	**47.98±2.91 (90)**	**48.10±3.01 (70)**
warpPIE10P	25.67±1.90	28.94±1.66 (100)	41.42±3.18 (20)	46.90±3.89 (20)	29.57±2.96 (90)	28.01±2.27 (50)	**48.76±3.86 (50)**	43.74±3.91 (70)	**49.00±3.88 (40)**
Isolet	57.89±3.82	52.21±2.76 (100)	41.95±2.07 (100)	49.31±2.32 (100)	47.12±2.06 (90)	**53.62±2.36 (100)**	53.04±2.33 (100)	51.91±2.15 (70)	**59.67±3.46 (100)**
MSTAR	77.04±7.98	67.87±3.49 (90)	78.15±5.80 (90)	73.74±5.89 (100)	69.16±6.03 (100)	75.52±6.22 (70)	**80.80±5.95 (100)**	79.70±6.43 (90)	**82.59±7.41 (100)**
Average	55.81±4.71	53.02±3.62	56.53±4.04	54.93±4.53	51.31±4.30	53.69±4.47	59.14±4.44	**59.60±4.47**	**62.94±5.27**

Experiments

- Real datasets: Normalized mutual information (NMI) ↑

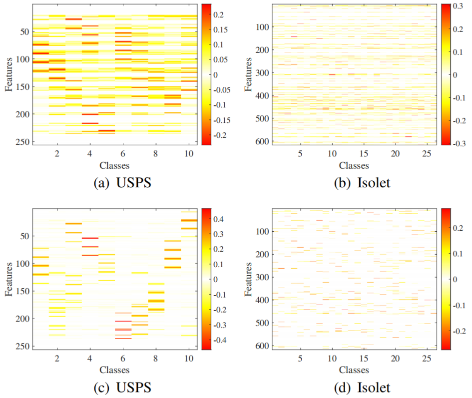
Datasets	ALLfea	LapScore	UDFS	SOGFS	RNE	FSPCA	SPCAFS	SPCA-PSD	DSCOFS
COIL20	75.37±1.96	69.59±1.48 (100)	**73.54±1.76 (100)**	68.92±1.84 (100)	70.43±1.92 (100)	68.50±1.56 (100)	69.98±1.45 (100)	69.85±1.41 (100)	**76.25±1.71 (100)**
USPS	61.12±2.01	59.46±1.80 (100)	54.69±2.11 (100)	52.96±1.54 (100)	45.36±1.93 (90)	**62.00±1.87 (60)**	60.98±2.37 (100)	60.90±2.02 (100)	**64.06±2.58 (100)**
lung_discrete	62.85±5.13	56.79±3.99 (100)	64.84±5.09 (100)	59.70±5.24 (100)	61.63±5.83 (70)	58.26±6.39 (40)	69.09±5.61 (100)	**70.93±5.46 (80)**	**70.98±7.00 (100)**
GLIOMA	48.86±5.72	51.03±2.48 (100)	47.22±3.53 (10)	48.67±10.98 (100)	48.62±6.32 (100)	21.94±5.28 (100)	24.14±6.97 (100)	**51.44±5.62 (90)**	**51.06±6.19 (80)**
UMIST	63.67±1.85	61.16±1.71 (100)	62.00±1.58 (100)	60.79±1.54 (100)	55.92±1.57 (70)	65.27±1.58 (100)	66.23±1.60 (90)	**66.25±1.72 (100)**	**67.24±1.85 (100)**
warpPIE10P	25.07±2.88	25.13±1.73 (90)	46.18±3.30 (20)	52.12±3.25 (20)	32.67±3.31 (90)	23.90±2.01 (50)	**52.63±3.33 (50)**	46.02±3.70 (70)	**52.65±3.29 (50)**
Isolet	75.72±1.70	69.77±1.20 (100)	56.29±1.11 (100)	67.40±1.44 (100)	64.27±0.95 (90)	**70.79±1.12 (100)**	67.71±1.33 (100)	69.69±0.80 (100)	**75.01±1.35 (100)**
MSTAR	82.42±3.31	74.10±1.76 (100)	76.45±2.47 (90)	76.39±1.70 (100)	66.87±1.99 (80)	78.39±2.17 (90)	**80.33±2.50 (100)**	79.17±2.77 (90)	**81.14±3.13 (100)**
Average	61.89±3.07	58.38±2.02	60.15±2.62	60.87±3.44	55.72±2.98	56.13±2.75	61.39±3.15	**64.28±2.94**	**67.30±3.39**

Experiments

- Ablation studies: Feature similarity rate (FSR)

$$\mathrm{FSR} = \frac{|\mathbb{T}_{\mathrm{our}} \cap \mathbb{T}_{2,0}|}{n}$$

Datasets	$\|W\|_0 \leq s_2$	ACC ↑	NMI ↑	FSR
COIL20	×	60.25±4.52	75.89±1.58	84
	√	60.51±4.42	76.25±1.71	
USPS	×	68.69±4.79	61.25±2.39	68
	√	69.67±4.97	64.06±2.58	
lung_discrete	×	71.42±7.95	69.74±6.11	92
	√	73.12±8.48	70.98±7.00	
GLIOMA	×	58.24±5.04	49.76±6.12	85
	√	60.88±6.31	51.06±6.19	
UMIST	×	47.33±3.05	67.44±1.88	95
	√	48.10±3.01	67.24±1.85	
warpPIE10P	×	47.91±4.99	51.19±3.79	89
	√	49.00±3.88	52.65±3.29	
Isolet	×	57.29±3.44	72.82±1.87	52
	√	59.67±3.46	75.01±1.35	
MSTAR	×	82.06±6.87	81.01±2.41	99
	√	82.59±7.41	81.14±3.13	



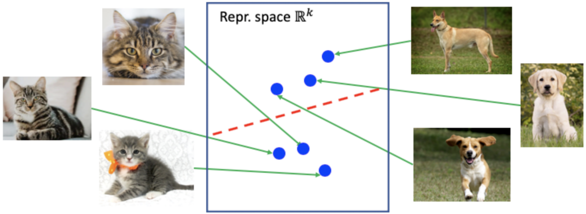
Outline

Motivation

- (Q2) How to learn data distributions

$$
\begin{aligned}
\min_{W} \quad & \frac{1}{2}\|X - WW^\top X\|_{\mathrm{F}}^2 \\
\text{s.t.} \quad & W^\top W = I, \ \|W\|_{2,0} \le s_1, \ \|W\|_0 \le s_2
\end{aligned}
$$

  - Convex loss: ℓ_1-norm, $\ell_{2,1}$-norm, quantile, Huber
  - Nonconvex loss: ℓ_p-norm, $\ell_{2,p}$-norm, SCAD, MCP, capped ℓ_1
- Contrastive learning: learn a discrimination model between positive and negative pairs



Motivation

- Let $X = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$ and $Y = (\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n)$ be two different pairs, the contrastive loss is defined as

$$L_c(X, Y) = \frac{1}{2n} \sum_{i=1}^{n} (L_c(\mathbf{x}_i) + L_c(\mathbf{y}_i))$$

$$L_c(\mathbf{x}_i) = -\log \frac{\exp(s(\mathbf{x}_i, \mathbf{y}_i)/\tau)}{\sum_{j=1, j\neq i}^{n} \exp(s(\mathbf{x}_i, \mathbf{x}_j)/\tau) + \sum_{j=1}^{n} \exp(s(\mathbf{x}_i, \mathbf{y}_j)/\tau)}$$

$$L_c(\mathbf{y}_i) = -\log \frac{\exp(s(\mathbf{y}_i, \mathbf{x}_i)/\tau)}{\sum_{j=1, j\neq i}^{n} \exp(s(\mathbf{y}_i, \mathbf{y}_j)/\tau) + \sum_{j=1}^{n} \exp(s(\mathbf{y}_i, \mathbf{x}_j)/\tau)}$$

- $s(\mathbf{x}, \mathbf{y}) = \mathbf{x}^\top \mathbf{y}$ is the similarity metric, τ is the temperature parameter

A simple framework for contrastive learning of visual representations

T Chen, S Kornblith, M Norouzi… - … on machine learning, 2020 - proceedings.mlr.press

… In our contrastive learning, as positive pairs are computed in the same device, the model can exploit the local information leakage to improve prediction accuracy without improving …

Model

- DSCOFS with contrastive learning (DSCOFS-CL)

$$\begin{aligned} \min_{W} \quad & \frac{1}{2}\|X - WW^\top X\|_{\mathrm{F}}^2 \\ \text{s.t.} \quad & W^\top W = I, \ \|W\|_{2,0} \le s_1, \ \|W\|_0 \le s_2 \end{aligned}$$

$$\Downarrow$$

$$\begin{aligned} \min_{W} \quad & L_c(X, WW^\top X) \\ \text{s.t.} \quad & W^\top W = I, \ \|W\|_{2,0} \le s_1, \ \|W\|_0 \le s_2 \end{aligned}$$

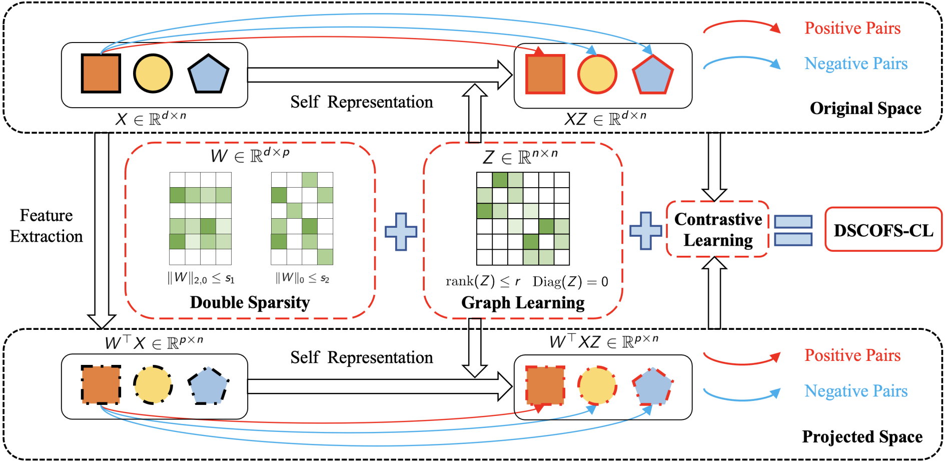
$$\Downarrow$$

$$\begin{aligned} \min_{W,Z} \quad & \lambda L_c(X, XZ) + (1-\lambda) L_c(W^\top X, W^\top XZ) \\ \text{s.t.} \quad & W^\top W = I, \ \|W\|_{2,0} \le s_1, \ \|W\|_0 \le s_2 \\ & \mathrm{rank}(Z) \le r, \ \mathrm{Diag}(Z) = 0 \end{aligned}$$

  - $\mathrm{rank}(Z) \le r$ represents the global structure
  - $\mathrm{Diag}(Z) = 0$ avoids the case where $Z = E$

Architecture

- DSCOFS-CL = Double Sparsity + Graph Learning + Contrastive Learning



Algorithm

- Proximal alternating method (PAM)

$$
\begin{aligned}
\min_{W,Z} \quad & \lambda L_c(X, XZ) + (1-\lambda) L_c(W^\top X, W^\top XZ) \\
\text{s.t.} \quad & W^\top W = I,\ \|W\|_{2,0} \le s_1,\ \|W\|_0 \le s_2 \\
& \operatorname{rank}(Z) \le r,\ \operatorname{Diag}(Z) = 0
\end{aligned}
$$

$$\Downarrow$$

$$
\begin{aligned}
\min_{W,Z,Y,P,Q} \quad & \lambda L_c(X, XZ) + (1-\lambda) L_c(W^\top X, W^\top XZ) \\
\text{s.t.} \quad & \|P\|_{2,0} \le s_1,\ \|Q\|_0 \le s_2, \operatorname{rank}(Y) \le r,\ \operatorname{Diag}(Z) = 0 \\
& W^\top W = I,\ Z = Y, W = P,\ W = Q
\end{aligned}
$$

$$\Downarrow$$

$$
\begin{aligned}
\min_{W,Z,Y,P,Q} \quad & \lambda L_c(X, XZ) + (1-\lambda) L_c(W^\top X, W^\top XZ) + \mu \|W^\top W - I\|_F^2 \\
& + \alpha \|Z - Y\|_F^2 + \beta \|W - P\|_F^2 + \gamma \|W - Q\|_F^2 \\
\text{s.t.} \quad & \|P\|_{2,0} \le s_1,\ \|Q\|_0 \le s_2,\ \operatorname{rank}(Y) \le r,\ \operatorname{Diag}(Z) = 0
\end{aligned}
$$

Algorithm

- Input: X, λ, μ, α, β, γ, s_1, s_2, r, τ_1, τ_2, τ_3, τ_4, τ_5
- Initialize: $(W^0, Z^0, Y^0, P^0, Q^0)$
- While not converged do
  - Update W^{k+1} by

$$\begin{aligned}\min_{W} \quad & (1-\lambda)L_c(W^\top X, W^\top XZ^k) + \mu\|W^\top W - I\|_{\mathrm{F}}^2 \\ & + \beta\|W - P^k\|_{\mathrm{F}}^2 + \gamma\|W - Q^k\|_{\mathrm{F}}^2 + \tau_1\|W - W^k\|_{\mathrm{F}}^2\end{aligned}$$

  - Update Z^{k+1} by

$$\begin{aligned}\min_{Z} \quad & \lambda L_c(X, XZ) + (1-\lambda)L_c(W^{k+1,\top}X, W^{k+1,\top}XZ) \\ & + \alpha\|Z - Y^k\|_{\mathrm{F}}^2 + \tau_2\|Z - Z^k\|_{\mathrm{F}}^2 \\ \text{s.t.} \quad & \mathrm{Diag}(Z) = 0\end{aligned}$$

  - Update Y^{k+1}
  - Update P^{k+1}
  - Update Q^{k+1}

Algorithm

- Define

$$
\begin{aligned}
f(W,Z,Y,P,Q) = {} & \lambda L_c(X,XZ) + (1-\lambda)L_c(W^\top X, W^\top XZ) \\
& + \mu\|W^\top W - I\|_{\mathrm{F}}^2 + \alpha\|Z-Y\|_{\mathrm{F}}^2 + \beta\|W-P\|_{\mathrm{F}}^2 + \gamma\|W-Q\|_{\mathrm{F}}^2 \\
& + \delta(Z) + \delta(Y) + \delta(P) + \delta(Q)
\end{aligned}
$$

- We call (W,Z,Y,P,Q) is a critical point if $0 \in \partial f(W,Z,Y,P,Q)$
- (Theorem) For each k, the sequence $\{(W^k, Z^k, Y^k, P^k, Q^k)\}$ generated by our PAM algorithm converges and $0 \in \partial f(W^*, Z^*, Y^*, P^*, Q^*)$ with

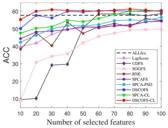
$$
\lim_{k\to+\infty}(W^k, Z^k, Y^k, P^k, Q^k) = (W^*, Z^*, Y^*, P^*, Q^*)
$$

  - Sufficient decreasing
  - Lower bounds for iterations
  - Kurdyka-Lojasiewicz properties

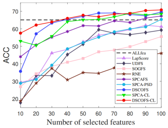
Experiments

- Real datasets: Accuracy (ACC) ↑

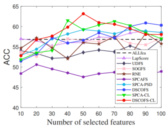
Datasets	ALLfea	LapScore	UDFS	SOGFS	RNE	SPCAFS	SPCA-PSD	DSCOFS	SPCA-CL	DSCOFS-CL
COIL20	57.74±4.93	54.82±3.91 (100)	58.71±3.47 (100)	49.66±4.81 (100)	55.84±4.41 (90)	54.39±3.67 (100)	56.57±3.05 (100)	**60.51±4.63 (100)**	60.31±3.49 (90)	**61.32±5.18 (80)**
USPS	65.12±4.95	62.02±4.09 (90)	59.52±2.97 (60)	55.58±3.07 (100)	46.04±2.69 (100)	67.34±4.49 (100)	65.38±4.26 (100)	**69.67±4.97 (100)**	68.88±4.05 (80)	**70.82±4.77 (100)**
GLIOMA	56.84±5.24	58.88±3.96 (90)	56.80±4.85 (100)	57.44±6.16 (70)	58.32±7.31 (90)	50.60±5.02 (20)	59.28±5.01 (90)	60.88±6.31 (80)	**61.48±6.20 (40)**	**63.16±7.46 (50)**
UMIST	41.07±2.38	40.13±2.79 (100)	47.12±2.49 (40)	41.70±3.17 (100)	40.35±2.26 (90)	46.78±2.51 (90)	47.98±2.91 (90)	48.10±3.01 (70)	**49.55±3.00 (60)**	**50.95±3.15 (70)**
Isolet	57.89±3.82	52.21±2.76 (100)	41.95±2.07 (100)	49.31±2.32 (100)	47.12±2.06 (90)	53.04±2.33 (100)	51.91±2.15 (70)	59.67±3.46 (100)	**60.53±3.75 (90)**	**63.22±3.50 (90)**
MSTAR	77.04±7.98	67.87±3.49 (90)	78.15±5.80 (90)	73.74±5.89 (100)	69.16±6.03 (100)	80.80±5.95 (100)	79.70±6.43 (90)	**82.59±7.41 (100)**	**81.57±6.28 (100)**	81.22±5.59 (100)
Average	59.28±4.88	55.99±3.50	57.04±3.69	54.57±4.24	52.81±4.13	58.83±4.00	60.14±3.97	63.57±4.96	**63.72±4.46**	**65.12±4.94**



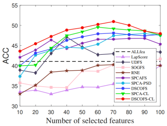
(a) COIL20



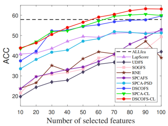
(b) USPS



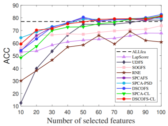
(c) GLIOMA



(d) UMIST



(e) Isolet

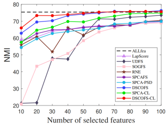


(f) MSTAR

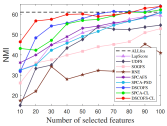
Experiments

- Real datasets: Normalized mutual information (NMI) ↑

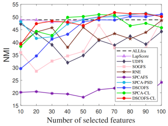
Datasets	ALLfea	LapScore	UDFS	SOGFS	RNE	SPCAFS	SPCA-PSD	DSCOFS	SPCA-CL	DSCOFS-CL
COIL20	75.37±1.96	69.59±1.48 (100)	73.54±1.76 (100)	68.92±1.84 (100)	70.43±1.92 (100)	69.98±1.45 (100)	69.85±1.41 (100)	**76.25±1.71 (100)**	74.79±1.48 (100)	**75.76±1.76 (90)**
USPS	61.12±2.01	59.46±1.80 (100)	54.69±2.11 (100)	52.96±1.54 (100)	45.36±1.93 (90)	60.98±2.37 (100)	60.90±2.02 (100)	**64.06±2.58 (100)**	62.29±2.40 (100)	**63.95±2.67 (100)**
GLIOMA	48.86±5.72	51.03±2.48 (100)	47.22±3.53 (10)	48.67±10.98 (100)	48.62±6.32 (100)	24.14±6.97 (100)	**51.44±5.62 (90)**	51.06±6.19 (80)	50.95±4.10 (60)	**51.71±5.03 (70)**
UMIST	63.67±1.85	61.16±1.71 (100)	62.00±1.58 (100)	60.79±1.54 (100)	55.92±1.57 (70)	66.23±1.60 (90)	66.25±1.72 (100)	67.24±1.85 (100)	**69.98±1.84 (80)**	**70.54±1.70 (70)**
Isolet	75.72±1.70	69.77±1.20 (100)	56.29±1.11 (100)	67.40±1.44 (100)	64.27±0.95 (90)	67.71±1.33 (100)	69.69±0.80 (100)	75.01±1.35 (100)	**75.41±1.51 (100)**	**77.32±1.37 (100)**
MSTAR	82.42±3.31	74.10±1.76 (100)	76.45±2.47 (90)	76.39±1.70 (100)	66.87±1.99 (80)	**80.33±2.50 (100)**	79.17±2.77 (90)	**81.14±3.13 (100)**	78.63±2.50 (100)	78.88±1.60 (100)
Average	67.86±2.76	64.19±1.74	61.70±2.09	62.52±3.17	58.58±2.45	61.56±2.70	66.22±2.39	**69.13±2.80**	68.68±2.31	**69.69±2.36**



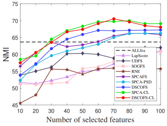
(a) COIL20



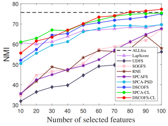
(b) USPS



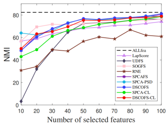
(c) GLIOMA



(d) UMIST



(e) Isolet



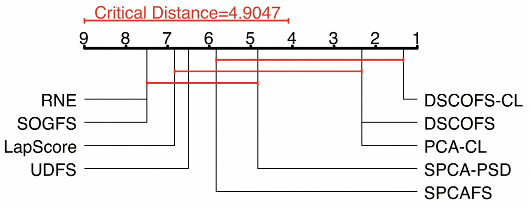
(f) MSTAR

Experiments

- Friedman tests ($\mathcal{H}_0$: There is no significant difference of compared methods)

Methods	Ranking	P-value	Hypothesis
LapScore	6.83	0.00001	Reject
UDFS	6.50		
SOGFS	7.50		
RNE	7.50		
SPCAFS	5.83		
SPCA-PSD	4.83		
DSCOFS	2.33		
SPCA-CL	2.33		
DSCOFS-CL	1.33		

- Post-hoc Nemenyi tests



Outline

Motivation

- (Q3) How to learn regularization parameters

$$
\begin{aligned}
\min_{W,Z,Y,P,Q} \quad & \lambda L_c(X, XZ) + (1-\lambda) L_c(W^\top X, W^\top XZ) + \mu \|W^\top W - I\|_{\mathrm{F}}^2 \\
& + \alpha \|Z - Y\|_{\mathrm{F}}^2 + \beta \|W - P\|_{\mathrm{F}}^2 + \gamma \|W - Q\|_{\mathrm{F}}^2 \\
\text{s.t.} \quad & \|P\|_{2,0} \le s_1, \ \|Q\|_0 \le s_2, \ \mathrm{rank}(Y) \le r, \ \mathrm{Diag}(Z) = 0
\end{aligned}
$$

  - $\mu, \alpha, \beta, \gamma \in \{10^{-6}, 10^{-4}, 10^{-2}, 10^0, 10^2, 10^4, 10^6\}$
  - $s_1 \in \{10, 20, \ldots, 100\}$
  - $s_2 \in \{0.1, 0.2, \ldots, 0.5\} dp$
  - $r = 0.1d$
  - $\lambda = 0.5$
- From iterative optimization to deep unfolding networks
  - Gregor-LeCun, Learning Fast Approximations of Sparse Coding, ICML, 2010
  - Chen-Liu-Yin, Learning to optimize: A Tutorial for Continuous and Mixed-Integer Optimization, SCCM, 2024

Model

- Consider structured sparse PCA

$$
\begin{aligned}
\min_{W} \quad & \frac{1}{2}\|X - WW^\top X\|_\mathrm{F}^2 + \lambda\|W\|_{2,1} + \mu\|W\|_1 \\
\mathrm{s.t.} \quad & W^\top W = I
\end{aligned}
$$

- Alternating direction method of multipliers (ADMM)

$$
\begin{aligned}
\min_{W} \quad & \frac{1}{2}\|X - WW^\top X\|_\mathrm{F}^2 + \lambda\|Y\|_{2,1} + \mu\|Z\|_1 \\
\mathrm{s.t.} \quad & W^\top W = I, \ W = Y, \ W = Z
\end{aligned}
$$

$$\Downarrow$$

$$
\begin{aligned}
\mathcal{L}(W, Y, Z, \Lambda, \Pi) = {} & \frac{1}{2}\|X - WW^\top X\|_\mathrm{F}^2 + \lambda\|Y\|_{2,1} + \mu\|Z\|_1 \\
& + \langle \Lambda, W - Y \rangle + \frac{\alpha}{2}\|W - Y\|_\mathrm{F}^2 + \langle \Pi, W - Z \rangle + \frac{\beta}{2}\|W - Z\|_\mathrm{F}^2
\end{aligned}
$$

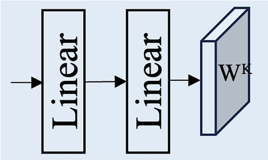
SPCA-Net

- Update W-block

$$
\begin{aligned}
\min_{W} \quad & f(W) := \frac{1}{2}\|X - WW^\top X\|_\mathrm{F}^2 + \frac{\alpha}{2}\|W - Y^k + \Lambda^k/\alpha\|_\mathrm{F}^2 + \frac{\beta}{2}\|W - Z^k + \Pi^k/\beta\|_\mathrm{F}^2 \\
\text{s.t.} \quad & W^\top W = I
\end{aligned}
$$

$$\Downarrow$$

$$
\begin{aligned}
\min_{W} \quad & f(W^k) + \langle \nabla f(W^k), W - W^k \rangle + \frac{1}{2\eta}\|W - W^k\|_\mathrm{F}^2 \\
\text{s.t.} \quad & W^\top W = I
\end{aligned}
$$



$$\Downarrow$$

$$W^{k+1} = UV^\top$$

$$\Downarrow$$

$$W^{k+1} = \textbf{LargNet}(U, V^\top)$$

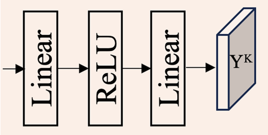
SPCA-Net

- Update Y-block

$$\min_{Y} \ \lambda\|Y\|_{2,1} + \frac{\alpha}{2}\|X^{k+1} - Y + \Lambda^k/\alpha\|_{\mathrm{F}}^2$$

$$\Downarrow$$

$$Y^{k+1} = \mathrm{sign}(\|X^{k+1} + \Lambda^k/\alpha\|_2) \circ \max(\|X^{k+1} + \Lambda^k/\alpha\|_2 - \lambda/\alpha, 0)$$



$$\Downarrow$$

$$Y^{k+1} = \frac{X^{k+1} + \Lambda^k/\alpha}{\|X^{k+1} + \Lambda^k/\alpha\|_2}\mathrm{ReLU}(\|X^{k+1} + \Lambda^k/\alpha\|_2 - \lambda/\alpha)$$

$$\Downarrow$$

$$Y^{k+1} = \textbf{GSoftNet}(X^{k+1} + \Lambda^k/\alpha, \lambda/\alpha)$$

SPCA-Net

- Update Z-block

$$\min_{Z} \;\; \mu\|Z\|_1 + \frac{\beta}{2}\|X^{k+1} - Z + \Pi^k/\beta\|_{\mathrm{F}}^2$$

$$\Downarrow$$

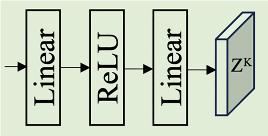
$$Z^{k+1} = \mathrm{sign}(X^{k+1} + \Pi^k/\beta) \circ \max(|X^{k+1} + \Pi^k/\beta| - \mu/\beta, 0)$$

$$\Downarrow$$

$$Z^{k+1} = \frac{X^{k+1} + \Pi^k/\beta}{|X^{k+1} + \Pi^k/\beta|}\mathrm{ReLU}(|X^{k+1} + \Pi^k/\beta| - \mu/\beta)$$

$$\Downarrow$$

$$Z^{k+1} = \textbf{SoftNet}(X^{k+1} + \Pi^k/\beta, \mu/\beta)$$



SPCA-Net

- Input: X, $\lambda, \mu, \alpha, \beta$
- Initialize: $(W^0,\ Y^0,\ Z^0,\ \Lambda^0,\ \Pi^0)$
- While $k = 1, \ldots, K$ do
  - Update W^{k+1} by

$$W^{k+1} = \textbf{LargNet}(U, V^\top)$$

  - Update Y^{k+1} by

$$Y^{k+1} = \textbf{GSoftNet}(X^{k+1} + \Lambda^k/\alpha, \lambda/\alpha)$$

  - Update Z^{k+1} by

$$Z^{k+1} = \textbf{SoftNet}(X^{k+1} + \Pi^k/\beta, \mu/\beta)$$

  - Update Λ^{k+1}, Π^{k+1} by

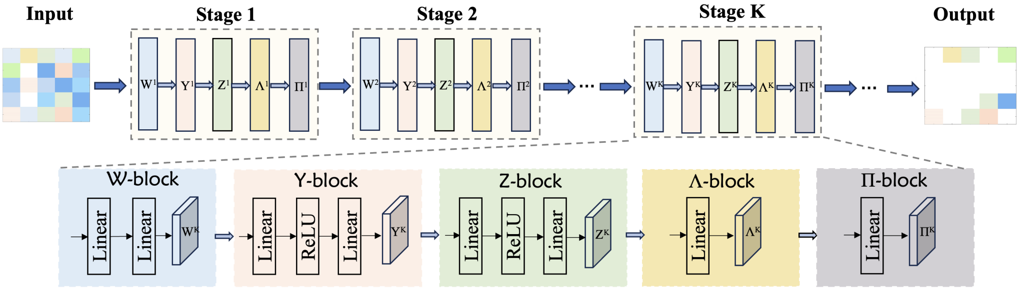
$$\Lambda^{k+1} = \textbf{Linear}(W^{k+1}, Y^{k+1}, \Lambda^k, \alpha),\ \ \Pi^{k+1} = \textbf{Linear}(W^{k+1}, Z^{k+1}, \Pi^k, \beta)$$

- Output: Trained W

Architecture

- All papameters $(\lambda, \mu, \alpha, \beta)$ are trained in an end-to-end manner
- The loss is defined as

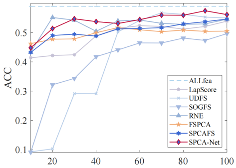
$$\mathrm{Loss} = \frac{1}{2}\|X - \bar{W}\bar{W}^\top X\|_{\mathrm{F}}^2 + \lambda\|\bar{W}\|_{2,1} + \mu\|\bar{W}\|_1$$



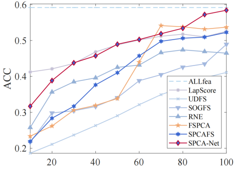
Experiments

- Real datasets: Accuracy (ACC) $\uparrow$

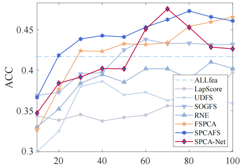
Datasets	ALLfea	LapScore	UDFS	SOGFS	RNE	FSPCA	SPCAFS	SPCA-Net
COIL20	58.97±4.99 (10)	53.91±3.61 (100)	**56.70±3.09 (70)**	49.66±3.63 (100)	55.16±3.35 (20)	51.71±3.05 (50)	54.63±3.64 (100)	**57.46±2.76 (90)**
Isolet	59.18±3.19 (10)	52.55±2.83 (100)	41.11±1.71 (100)	48.93±2.69 (100)	47.39±2.91 (80)	**54.15±2.69 (70)**	52.26±2.81 (100)	**58.43±4.31 (100)**
UMIST	41.68±2.46 (10)	39.71±3.28 (100)	38.64±1.61 (40)	43.81±2.98 (80)	41.01±2.25 (90)	46.58±2.34 (100)	**47.32±3.48 (80)**	**47.58±4.97 (70)**
MSTAR	80.81±8.76 (10)	68.21±4.57 (100)	**81.25±7.48 (100)**	73.46±5.61 (100)	77.82±6.16 (100)	78.74±5.20 (30)	78.63±8.68 (90)	**81.90±6.87 (100)**



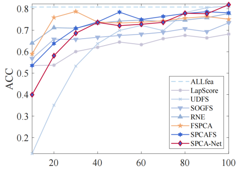
(a) COIL20



(b) Isolet



(c) UMIST

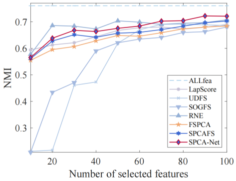


(d) MSTAR

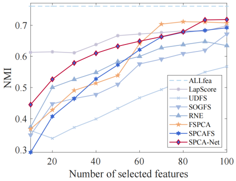
Experiments

- Real datasets: Normalized mutual information (NMI) ↑

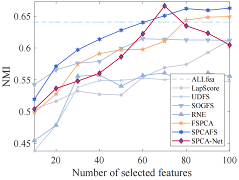
Datasets	ALLfea	LapScore	UDFS	SOGFS	RNE	FSPCA	SPCAFS	SPCA-Net
COIL20	76.04±1.69 (10)	69.01±1.53 (100)	69.12±1.17 (80)	68.03±1.59 (100)	**70.76±2.07 (100)**	68.41±1.60 (100)	70.29±1.31 (100)	**72.21±2.68 (90)**
Isolet	76.09±1.77 (10)	69.86±1.26 (100)	56.73±1.05 (100)	67.15±1.45 (100)	64.74±1.28 (90)	**71.12±1.11 (80)**	69.18±1.33 (100)	**71.80±1.59 (100)**
UMIST	64.07±1.76 (10)	61.23±2.15 (100)	55.43±1.50 (80)	61.46±2.03 (70)	56.08±1.80 (60)	64.94±1.65 (100)	**66.26±1.74 (100)**	**66.62±7.52 (70)**
MSTAR	83.96±3.14 (10)	73.90±1.62 (100)	78.18±3.64 (90)	76.56±1.54 (100)	78.26±2.51 (100)	78.87±2.52 (90)	**79.62±2.30 (100)**	**80.67±3.47 (90)**



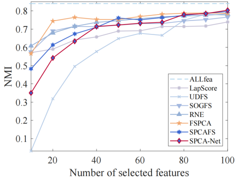
(a) COIL20



(b) Isolet



(c) UMIST



(d) MSTAR

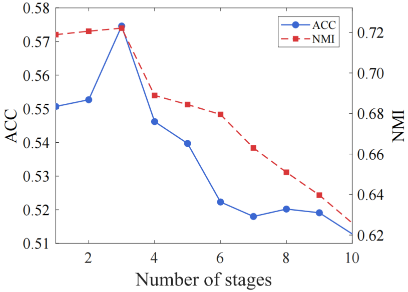
Experiments

- Ablation studies

Datasets	Network	ACC ↑	NMI ↑
COIL20	×	**55.12±2.67**	**70.44±1.37**
	√	**57.46±2.76**	**72.21±2.68**
Isolet	×	**51.84±2.82**	**67.02±1.43**
	√	**58.43±4.31**	**71.80±1.59**
UMIST	×	**40.65±2.29**	**55.88±1.62**
	√	**47.58±4.97**	**66.62±7.52**
MSTAR	×	**80.65±6.47**	**80.53±2.41**
	√	**81.90±6.87**	**80.67±3.47**

Datasets	Dynamic	ACC ↑	NMI ↑
COIL20	×	**56.71±3.83**	**71.49±3.67**
	√	**57.46±2.76**	**72.21±2.68**
Isolet	×	**52.06±3.71**	**68.91±2.36**
	√	**58.43±4.31**	**71.80±1.59**
UMIST	×	**42.63±2.78**	**60.12±1.69**
	√	**47.58±4.97**	**66.62±7.52**
MSTAR	×	**80.74±5.28**	**80.59±3.67**
	√	**81.90±6.87**	**80.67±3.47**

- Effect of deep unfolding stages



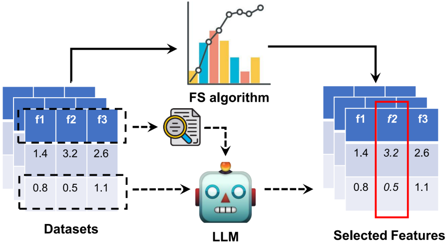
Outline

Motivation

- (Q4) How to learn feature selection

$$\min_{W} \quad -\mathrm{Tr}(W^\top X X^\top W)$$
$$\text{s.t.} \quad W^\top W = I, \ \|W\|_{2,0} \le s$$

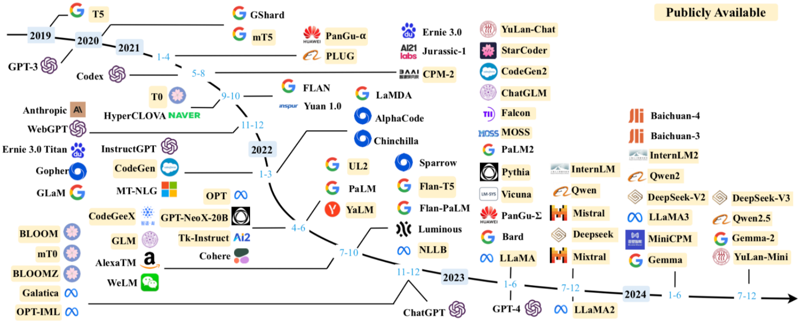
$\Rightarrow$



- From deep learning to large language models (LLMs)
  - Cho-Cund-Srivastava et al, LMPriors: Pre-Trained Language Models as Task-Specific Priors, NeurIPS, 2022
  - Han-Yoon-Arik et al, Large Language Models Can Automatically Engineer Features for Few-Shot Tabular Learning, ICML, 2024
  - Li-Tan-Liu, Exploring Large Language Models for Feature Selection: A Data-centric Perspective, SIGKDD, 2025

DeepSeek

- Guo-Yang-Zhang et al, DeepSeek-R1: Incentivizing Reasoning Capability in LLMs via Reinforcement Learning, arXiv:2501.12948
- Arrieta-Ugarte-Valle et al, o3-mini vs DeepSeek-R1: Which One is Safer? arXiv:2501.18438
- Muennighoff-Yang-Shi et al, S1: Simple Test-time Scaling, arXiv:2501.19393
- Gao-Jin-Ke et al, A Comparison of DeepSeek and Other LLMs, arXiv:2502.03688



Method

- **Dataset-specific Context**

  Using data collected via a telemarketing campaign at a Portuguese banking institution from 2008 to 2013, we wish to build a machine learning model that can predict whether a client will subscribe to a term deposit (target variable). The dataset contains a total of 16 features (e.g., age, marital status, whether the client has a housing loan). Prior to training the model, we first want to identify a subset of the 16 features that are most important for reliable prediction of the target variable.

- **Main System Prompt**

  For each feature input by the user, your task is to provide a feature importance score (between ⟨0.0⟩ and ⟨1.0⟩; larger value indicates greater importance) for predicting whether an individual will subscribe to a term deposit and a reasoning behind how the importance score was assigned. The results need to be written directly into a JSON file. Therefore, please do not include any extra text and return the results strictly in the given format. The scores for each feature should be different from one another.

- **Output Format Instruction**

  Here is an example output: "concept-1": "has credit in default ", "reasoning": "Clients with credits in default might be more hesitant to open new financial products due to their current financial situation and may be deemed a higher risk by the bank. Therefore, the score is 0.9.", "score": 0.9.

- **Main User Prompt**

  Provide a score and reasoning formatted according to the output schema above.

Method

- Dataset-specific Context

  Same as above

- Main System Prompt

  Please use the Random Forest (/ forward sequential selection / backward sequential selection / recursive feature elimination RFE / minimum redundancy maximum relevance selection MRMR / filtering by mutual information MI) model to directly analyze the dataset samples. This is a classification task, where "Class" represents the classification. Please analyze the importance scores of these features. The score range is [0.0, 1.0], and the score of each feature should be different. The output format is as follows, in JSON file format.

- Output Format Instruction

  Same as above

- Main User Prompt

  Same as above

Expriments

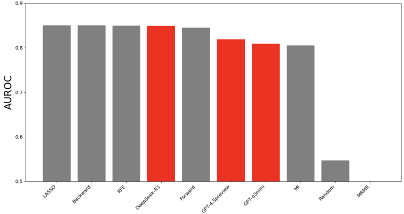
- Compared methods
  - DeepSeek-R1 (2025-01-20)
  - GPT-o3mini (2025-01-31)
  - GPT-4.5preview (2025-02-27)
  - LASSO
  - Forward sequential selection (Forward)
  - Backward sequential selection (Backward)
  - Recursive feature elimination (RFE)
  - Minimum redundancy maximum relevance selection (MRMR)
  - Mutual information (MI)
  - Random feature selection (Random)

- Statistics of datasets

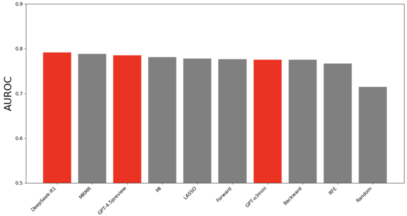
Datasets	Samples	Features
Bank	45211	16
Credit-G	1000	20
Pima Indians Diabetes	768	8
Give Me Some Credit	120269	10

Experiments

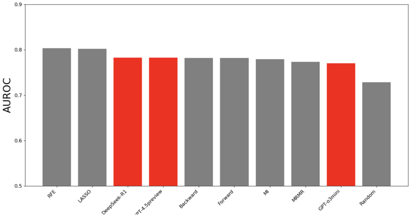
- LLMs vs. Data-driven methods



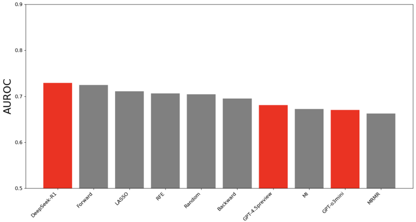
(a) Bank



(b) Credit-G



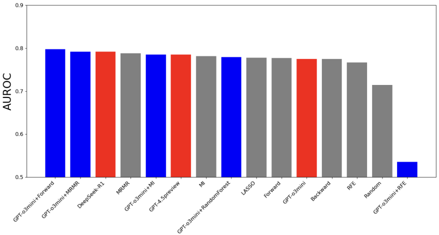
(c) Pima Indians Diabetes

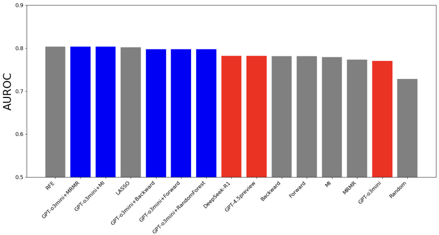


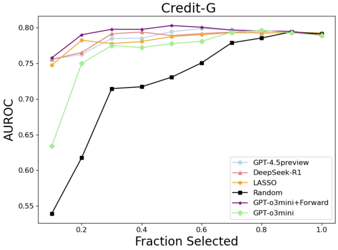
(d) Give Me Some Credit

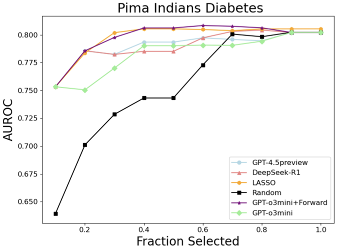
Experiments

- LLMs + Data-driven methods vs. LLMs vs. Data-driven methods



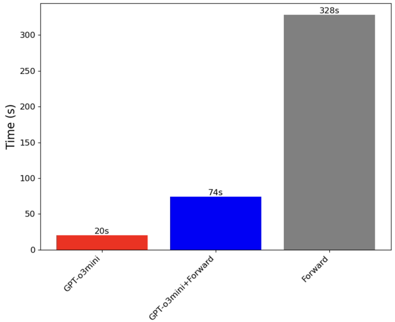


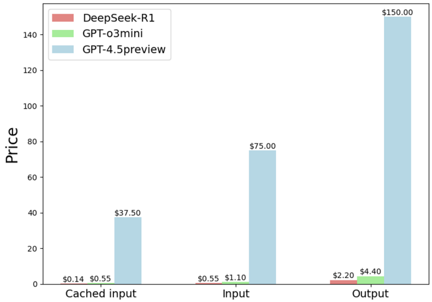




Experiments

- More interesting things should be investigated
  - Consider large datasets with more features, especially larger than thousands
  - Apply DeepSeek-R1 with different parameters, including 7B, 14B, 32B, 70B
  - Try RAG and fine-tuning to improve the stability and reliability
  - Expand to regression tasks, analyze feature correlation, etc

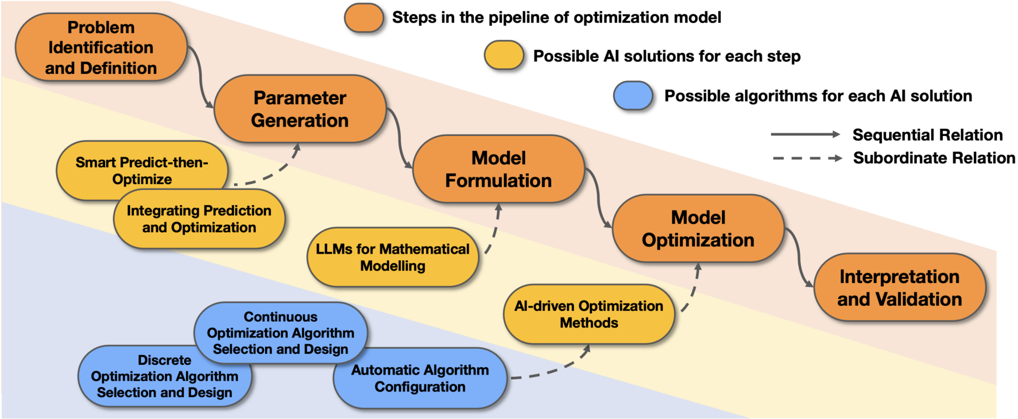




Outline

Future Work

- AI for optimization



Future Work

- Ramamonjison-Yu-Li et al, NL4Opt Competition: Formulating Optimization Problems Based on Their Natural Language Descriptions, NeurIPS, 2022
- Yang-Wang-Lu et al, Large Language Models as Optimizers, ICLR, 2024
- AhmadiTeshnizi-Gao-Udell, OptiMUS: Scalable Optimization Modeling with (MI)LP Solvers and Large Language Models, ICML, 2024
- Gao-Jiang-Cai et al, StrategyLLM: Large Language Models as Strategy Generators, Executors, Optimizers, and Evaluators for Problem Solving, NeurIPS, 2024
- Romera-Paredes-Barekatain et al, Mathematical Discoveries from Program Search with Large Language Models, Nature, 2024
- Jiang-Shu-Qian et al, LLMOPT: Learning to Define and Solve General Optimization Problems from Scratch, ICLR, 2025

Thank you for your attention

xcxiu@shu.edu.cn