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From Feature Selection to Instance-wise Feature Acquisition¹

Tutorial @ SDM 2024

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Advanced Topics

Advanced Topics

- ▶ Feature Acquisition
 - ▶ Interpretability (e.g., [liy23])
 - ▶ Dealing with structure (e.g., multidimensional Bayesian network classification [ELZ21, EZ23])
 - ▶ Reducing label uncertainty or learning to defer (e.g., dynamic classifier selection [EYC23b, EYC23a])
- ▶ Feature Selection
 - ▶ Incorporating fairness constraints (e.g., [GSSV22])
 - ▶ Feature selection for hierarchical classification (e.g., [ZHYZ⁺19])

Is Instance-wise Feature Acquisition Interpretable? [liy23]

- ▶ Using sparse set of features to classify data instances is essential for model interpretability
 - ▶ Observe which features contribute to each model output
- ▶ Sparsity can be achieved
 - ▶ globally by incorporating regularizer to objective function
 - ▶ instance-level, e.g., evaluate features along different decision paths in decision trees
- ▶ Goal: assess interpretability of IFCO [LZ21]

Interpretability of IFCO

- ▶ Model-based interpretability: humans can understand how model behaves and which factors influence its decision-making process
- ▶ Post-hoc interpretability: relationships learned by model from given dataset

Dataset & Baselines

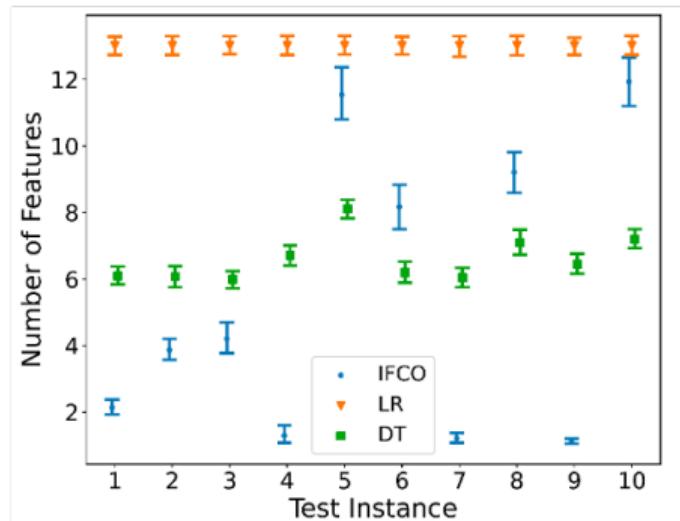
- ▶ For demonstration purpose, we use the **German credit-risk dataset**: classify people as high or low credit risk

Feature	Description	Feature	Description
F_1	Checking account status	F_{11}	Present residence
F_2	Duration in months	F_{12}	Property
F_3	Credit history	F_{13}	Age in years
F_4	Purpose of the credit	F_{14}	Other installment plans
F_5	Credit amount	F_{15}	Housing
F_6	Savings account status	F_{16}	Existing credits
F_7	Present employment (years)	F_{17}	Job
F_8	Installment rate	F_{18}	Number of dependents
F_9	Personal status	F_{19}	Telephone
F_{10}	Other debtors	F_{20}	Foreign worker

- ▶ Standard interpretable models:
 - ▶ Logistic regression with L1-norm regularizer (LR)
 - ▶ Decision tree (DT)

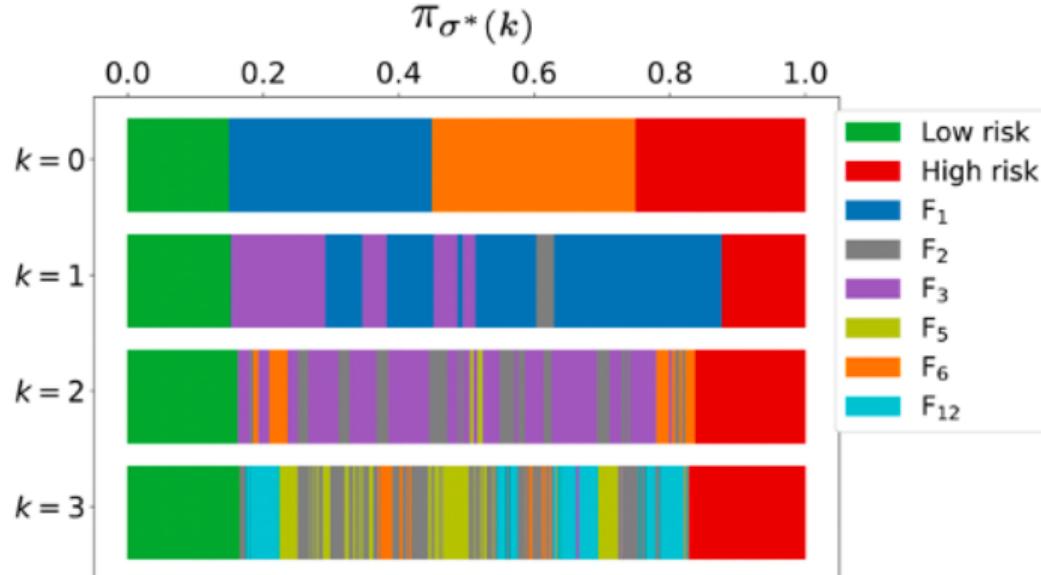
Model-based Interpretability

- ▶ Sparsity: use sparse set of features for classification
 - ▶ LR: global sparsity by using the L1-norm penalty
 - ▶ DT: instance-level sparsity by evaluating features along different branches (greedy learning of tree structure)
 - ▶ IFCO: instance-level sparsity by using feature acquisition cost $\sum_{k=1}^R e(F_{\sigma(k)})$
- ▶ Sparsity stability: interpretations are meaningless if sparsity varies drastically due to small perturbation in training dataset



Model-based Interpretability

- ▶ Simulability: human can reason about decision-making process
 - ▶ LR: dot product between feature vector and weight vector
 - ▶ DT: hierarchical decision-making
 - ▶ IFCO:



Model-based Interpretability

- ▶ **Modularity**: ability to interpret meaningful portions of decision-making process independently
 - ▶ LR: **affine transformation** of input feature space (i.e., $w_i F_i$)
 - ▶ DT: each tree node is **modular block** that contributes to final classification decision
 - ▶ IFCO: sequential decision-making process based on **sufficient statistic**

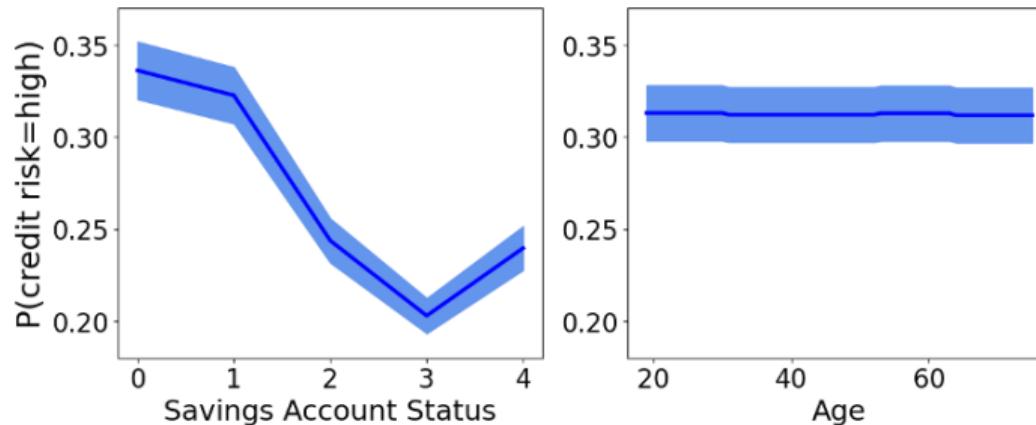
$$\pi_{\sigma^*(k)} = \frac{\left(\Delta(F_{\sigma^*(k)} | F_{\sigma^*(1)}, \dots, F_{\sigma^*(k-1)}, \mathcal{C}) \right) \pi_{\sigma^*(k-1)}}{\Delta^T(F_{\sigma^*(k)} | F_{\sigma^*(1)}, \dots, F_{\sigma^*(k-1)}, \mathcal{C}) \pi_{\sigma^*(k-1)}}$$

- ▶ **Conditional independence** assumption helps to decompose $\pi_{\sigma^*(k)}$ into simple and meaningful portions in terms of $P(F_{\sigma^*(k)} | \mathcal{C})$

Post-hoc Interpretability: Dataset-level Interpretations

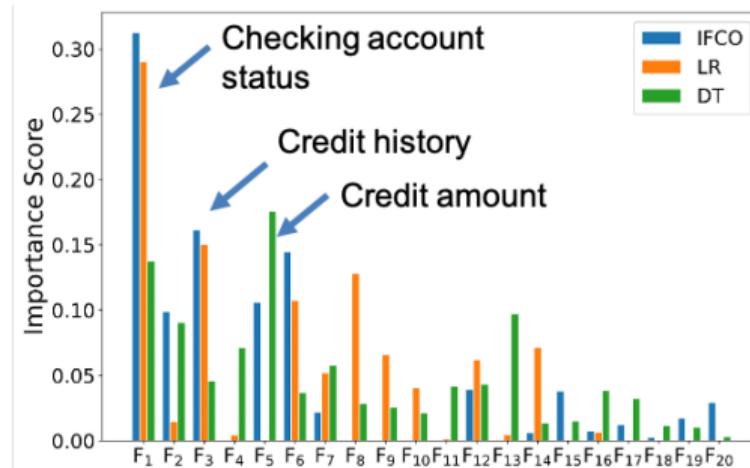
- ▶ Partial dependence: marginal effects of **individual feature** on **output** of machine learning model

$$PD(F_i) \approx \frac{1}{N} \sum_{n=1}^N \hat{f}(F_i, \bar{F}_i^{(n)})$$



Post-hoc Interpretability: Dataset-level Interpretations

- ▶ Feature importance: number of times specific feature contributes to specific classification decision



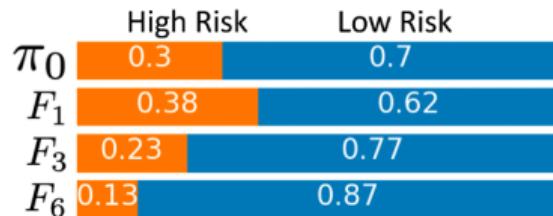
Post-hoc Interpretability: Dataset-level Interpretations

- ▶ Accuracy stability: test accuracy should be stable for any perturbations in training data

Method	Accuracy	Feat.
IFCO	0.754±0.040	5.85
DT	0.702±0.044	6.78
LR	0.740±0.034	14.0
XGB	0.755±0.037	19.9

- ▶ Gradient boosted trees (XGB) (black box) requires 3.4 times more features for a just 0.1% improvement

Post-hoc Interpretability: Prediction-level interpretations

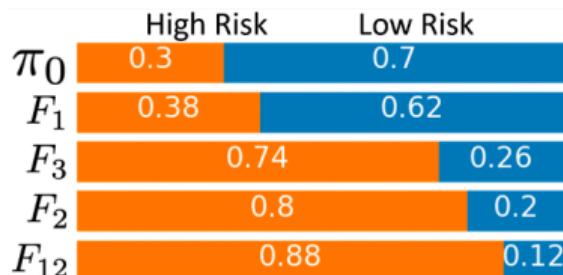


► bad checking account status

► good credit history

► good savings account status

Correctly predicted → low credit-risk



► bad checking account status

► bad credit history

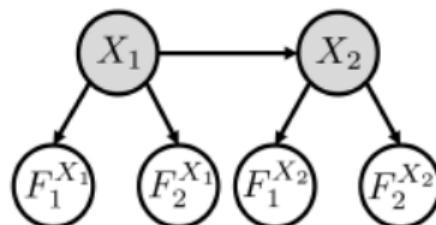
► credit history of 36 months

► no known property

Correctly predicted → high credit-risk

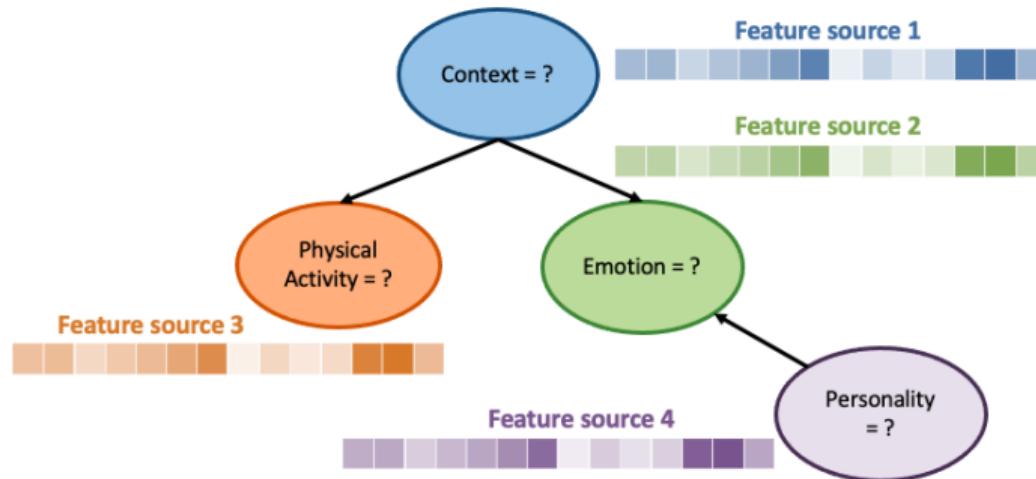
Instance-wise Multidimensional Classification [ELZ21, EZ23]

- ▶ Many real-world applications (e.g., medical diagnosis, behavioral analysis)
 - ▶ Bayesian networks used to describe relationships between variables
 - ▶ Variables not directly observable but can be inferred via features
- ▶ Multi-dimensional Bayesian network classification [GBBL21] learns underlying unknown Bayesian network structure between variables in X and features in F , and then performs inference to compute the values of variables in X



Problem Statement

- ▶ What happens if features are acquired at a cost?
- ▶ Goal: accurately classify each data instance during testing, while keeping **total feature acquisition cost minimum** when data instance label corresponds to known Bayesian network of multiple class variables



Optimization Setup

- ▶ $\mathcal{G} = (X, E)$: known Bayesian network structure
- ▶ $X \triangleq \{X_1, X_2, \dots, X_n\}$: set of nodes corresponding to categorical variables
- ▶ E : set of **directed edges** to represent relationships between categorical variables
- ▶ $F \triangleq \{F_1^{X_1}, \dots, F_{K_1}^{X_1}, F_1^{X_2}, \dots, F_{K_2}^{X_2}, \dots, F_1^{X_n}, \dots, F_{K_n}^{X_n}\}$: set of features, where $F_k^{X_i}$ is k th feature associated with variable X_i
- ▶ e_k^i : cost of acquiring k th feature associated with variable X_i
- ▶ $C_l^{X_i}$: class value for variable X_i

Optimization Setup

- ▶ Introduce random variables
 - ▶ $R_i \in \{0, \dots, K_i\}$: last feature acquired before classification decision for variable X_i
 - ▶ $D_{R_i} \in \{1, \dots, N_i\}$: classification decision based on R_i features for variable X_i

$$\min_{\mathbf{R}, \mathbf{D}_{\mathbf{R}}} J(\mathbf{R}, \mathbf{D}_{\mathbf{R}})$$
$$J(\mathbf{R}, \mathbf{D}_{\mathbf{R}}) = \mathbb{E} \left\{ \sum_{i=1}^n \sum_{k=1}^{R_i} e_k^i + \sum_{\mathbf{j}} \sum_{\mathbf{m}} M_{\mathbf{m}\mathbf{j}} P(\mathbf{D}_{\mathbf{R}} = \mathbf{j}, \mathbf{C} = \mathbf{c}_{\mathbf{m}}) \right\}$$

- ▶ The computational complexity of directly solving the above problem is high

Alternative Approach

- ▶ Determine features to be acquired and classification decision for each categorical variable X_i in \mathcal{G}

$$J(R_i, D_{R_i}) = \mathbb{E} \left[\sum_{k=1}^{R_i} e_k^i + \sum_{l=1}^{N_i} \sum_{m=1}^{N_i} M_{lm}^i P(D_{R_i} = l, \mathcal{C}_i = C_m^{X_i}) \right],$$

- ▶ How to account for relationships between categorical variables? propagate decisions across \mathcal{G}
 - ▶ Initially, acquire features and make classification decisions for in-degree 0 nodes
 - ▶ Use such decisions to drive feature acquisition and classification decisions for each in-degree greater than 0 node

ISEC Algorithm

$$F_1^{X_1} F_2^{X_1} F_3^{X_1} \dots F_{K_1}^{X_1} \quad F_1^{X_2} F_2^{X_2} F_3^{X_2} \dots F_{K_2}^{X_2}$$

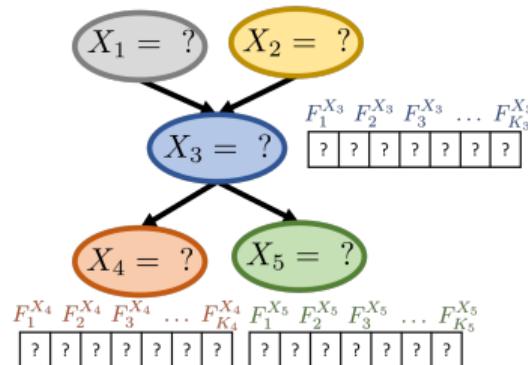
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$$F_1^{X_1} F_2^{X_1} F_3^{X_1} \dots F_{K_1}^{X_1} \quad F_1^{X_2} F_2^{X_2} F_3^{X_2} \dots F_{K_2}^{X_2}$$

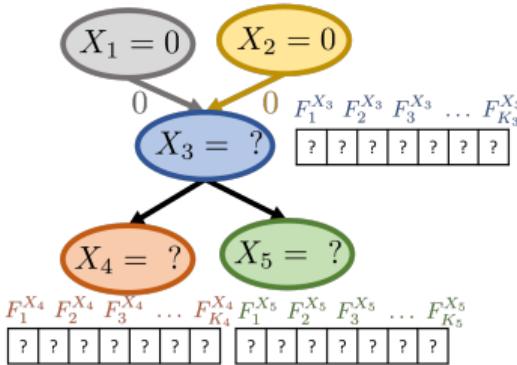
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$$F_1^{X_1} F_2^{X_1} F_3^{X_1} \dots F_{K_1}^{X_1} \quad F_1^{X_2} F_2^{X_2} F_3^{X_2} \dots F_{K_2}^{X_2}$$

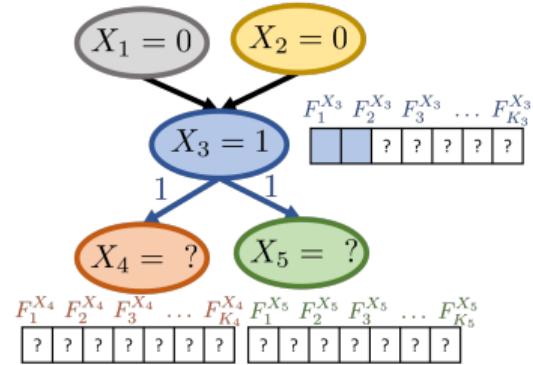
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(a)



(b)



(c)

Figure 6: (a) Original Bayesian network; (b) Feature acquisition and classification for variables of in-degree 0; (c) Feature acquisition and classification for variables of in-degree > 0

Some Results

TABLE II: Comparison of global accuracy (GA), mean accuracy (MA), and the average number of features (AF). The highest and the second highest accuracy values are bolded and gray-shaded, and gray-shaded, respectively. The smallest and the second smallest AF values are bolded and gray-shaded, and gray-shaded, respectively.

Dataset	Metric	ISEC	IC-NB	IC-ETANA	PC-NB	BCC	MD-KNN	IC-SVM	PC-SVM
Edm	GA	0.5905	0.3890	0.4668	0.5443	0.3905	0.3864	0.3578	0.4483
	MA	0.7401	0.6491	0.6500	0.7101	0.6952	0.6209	0.6755	0.7013
	AF	5.8654	16.0000	8.6333	16.0000	16.0000	16.0000	16.0000	16.0000
Voice	GA	0.8753	0.6897	0.8224	0.6824	0.2735	0.8359	0.7663	0.7220
	MA	0.9364	0.8243	0.8748	0.8343	0.5210	0.9142	0.8780	0.8514
	AF	2.5127	19.0000	2.2719	19.0000	19.0000	19.0000	19.0000	19.0000
Jura	GA	0.4402	0.3036	0.3481	0.4010	0.1588	0.2591	0.2562	0.2393
	MA	0.6352	0.5405	0.5845	0.6016	0.4764	0.4889	0.5307	0.4830
	AF	7.0517	9.0000	8.2394	9.0000	9.0000	9.0000	9.0000	9.0000
Song	GA	0.3299	0.2114	0.2509	0.2611	0.3082	0.4229	0.3471	0.3548
	MA	0.7134	0.6012	0.6709	0.6360	0.6802	0.7565	0.6728	0.6724
	AF	16.3172	98.0000	16.6072	98.0000	98.0000	98.0000	98.0000	98.0000
Flare	GA	0.8173	0.0277	0.7800	0.0463	0.8204	0.7802	0.8202	0.8202
	MA	0.9205	0.2194	0.8906	0.5736	0.9226	0.9035	0.9225	0.9225
	AF	1.3040	10.0000	7.0573	10.0000	10.0000	10.0000	10.0000	10.0000
Student	GA	0.6099	0.5742	0.5914	0.0815	0.5469	0.5208	0.5334	0.5021
	MA	0.7409	0.7227	0.5529	0.5418	0.6522	0.6546	0.6560	0.6084
	AF	8.4940	30.0000	14.9458	30.0000	30.0000	30.0000	30.0000	30.0000
Emotion	GA	0.3121	0.1820	0.2378	0.2731	0.0000	0.1164	0.2631	0.3203
	MA	0.7783	0.7391	0.7641	0.7700	0.6885	0.7026	0.7934	0.7718
	AF	8.5983	72.0000	15.3432	72.0000	72.0000	72.0000	72.0000	72.0000
Child	GA	0.5620	0.5509	0.5350	0.4800	0.3910	0.5098	0.3909	0.3909
	MA	0.8197	0.8156	0.8069	0.7783	0.7106	0.7799	0.7106	0.7106
	AF	4.4293	17.0000	5.8147	17.0000	17.0000	17.0000	17.0000	17.0000
Hepar2	GA	0.4200	0.0900	0.4170	0.0350	0.4180	0.4150	0.4230	0.4150
	MA	0.7807	0.4260	0.7757	0.4193	0.7813	0.7792	0.7813	0.7747
	AF	12.6213	67.0000	31.9470	67.0000	67.0000	67.0000	67.0000	67.0000
Sachs	GA	0.7920	0.7770	0.6000	0.3000	0.7920	0.7880	0.7920	0.7920
	MA	0.8420	0.8345	0.7250	0.5765	0.8420	0.8399	0.8420	0.8420
	AF	1.8575	9.0000	8.4295	9.0000	9.0000	9.0000	9.0000	9.0000
Insurance	GA	0.8270	0.6920	0.8100	0.6150	0.4320	0.6062	0.7240	0.7310
	MA	0.9050	0.8350	0.9030	0.7840	0.5870	0.7841	0.8540	0.8520
	AF	2.9115	25.0000	5.4565	25.0000	25.0000	25.0000	25.0000	25.0000

Joint Feature Acquisition & Classifier Selection [EZZC23b, EZZC23a]

- ▶ ML models **cannot accurately** predict all test instances
- ▶ Problematic, especially in risk-sensitive applications (e.g., autonomous vehicles, medical diagnosis)
- ▶ To the best of our knowledge, instance-wise feature acquisition assumes single loss function
- ▶ How to jointly acquire the subset of features based on which each example is to be classified and the appropriate classifier to be used for this task?
 - ▶ Assess **difficulty** of classifying data instances to guide decision making process
 - ▶ Easy-to-classify data instances: few features and simple classifier
 - ▶ Hard-to-classify data instances: more features and powerful classifier

Problem Description

- ▶ $X \triangleq [X_1, \dots, X_F]^\top$: feature vector containing F features
- ▶ c_f : cost of acquiring f th feature
- ▶ $Y \in \{1, \dots, N\}$: label
- ▶ $C \triangleq \{C_1, \dots, C_Z\}$: set of Z classifiers

Objective: jointly determine subset of features to be acquired, classifier to be used and the label of each example

Optimization Setup

- ▶ Introduce **random variables**

- ▶ $S \in \{0, \dots, F\}$: last feature acquired before label assignment
- ▶ $U_S \in \{0, \dots, Z\}$: classifier selected after S features have been acquired
- ▶ $D_S \in \{1, \dots, N\}$: classification decision for data instance under consideration based on S features

$$\min_{S, U_S, D_S} L(S, U_S, D_S)$$

$$L(S, U_S, D_S) = \mathbb{E} \left\{ \sum_{f=1}^S c_f + \sum_{z=1}^Z \lambda_z \mathbb{I}_{\{U_S=z\}} h_S^z + \gamma \mathbb{I}_{\{U_S=0\}} \right. \\ \left. \times \sum_{j=1}^N \sum_{i=1}^N \Omega_{ij} P(D_S = j, Y = i) \right\},$$

Optimum Solution

- ▶ $\phi_f \triangleq [\phi_f^1, \dots, \phi_f^N]^T$: posterior probability vector with $\phi_f^i \triangleq P(Y = i|x_1, \dots, x_f)$
- ▶ Optimum label assignment strategy

$$D_S^* =_{1 \leq j \leq N} [\Omega_j^T \phi_S].$$

- ▶ Optimum classifier selection strategy

$$U_S^* =_{0 \leq t \leq Z} [\lambda_t H_S^t(\phi_S)].$$

- ▶ Optimum feature acquisition strategy via dynamic programming

$$\bar{L}_f(\phi_f) = \min \left[l(\phi_f), \bar{I}_f(\phi_f) \right]$$

$$l(\phi_f) = \min_{0 \leq t \leq Z} [\lambda_t H_f^t(\phi_f)]$$

$$\bar{I}_f(\phi_f) = c_{f+1} + \sum_{x_{f+1}} \bar{L}_{f+1}(\phi_{f+1}) \Pi_{f+1}^T(x_{f+1}) \phi_f$$

Intuition

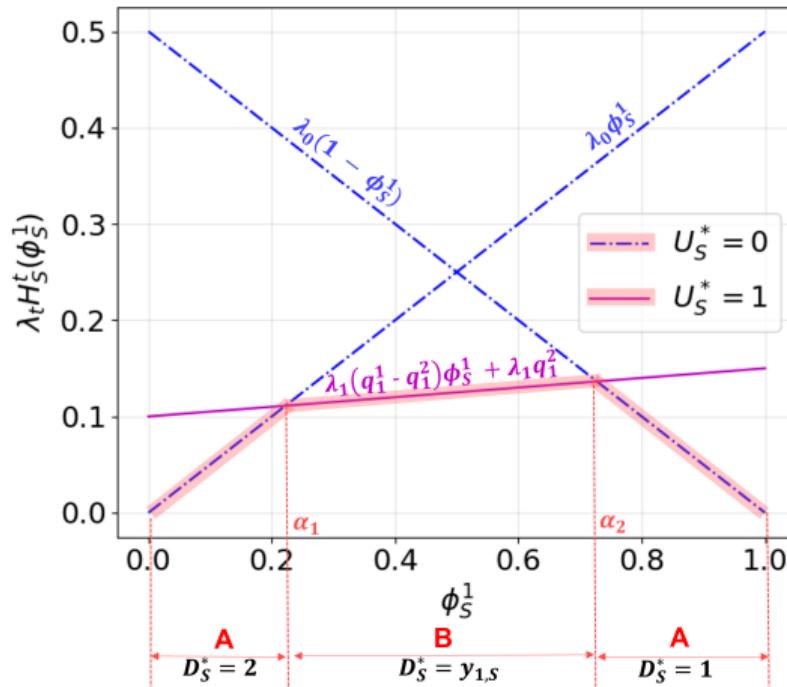
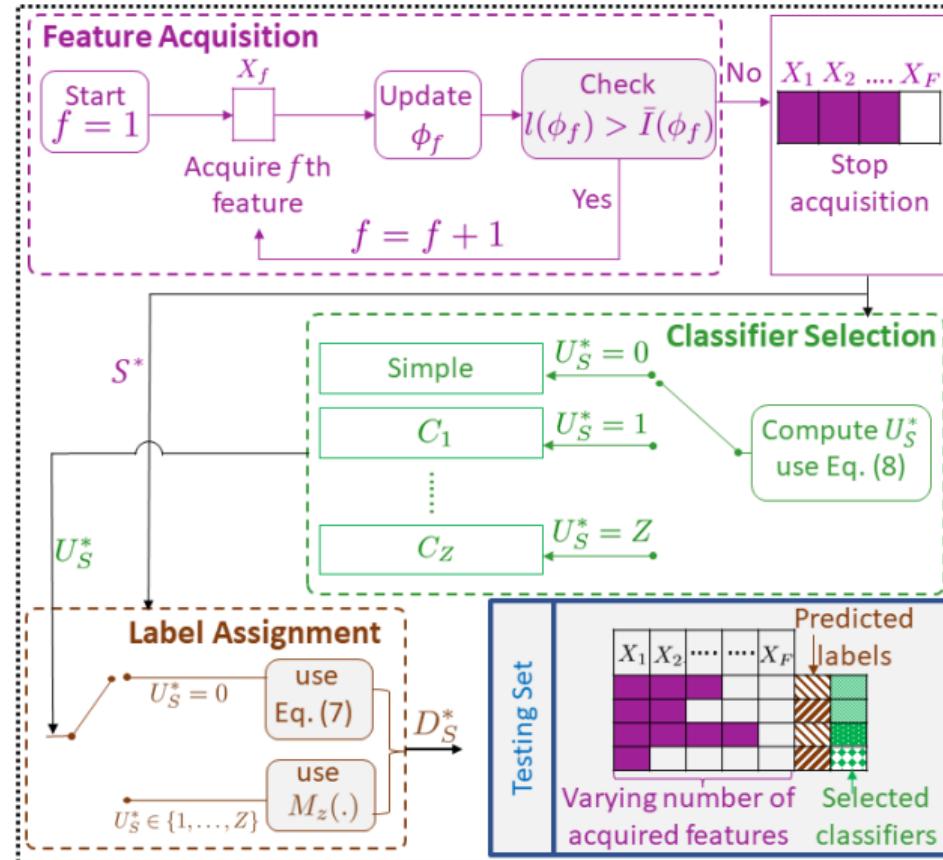


Figure 7: Illustration of classifier selection and label assignment processes in the case of two label values (i.e., $N = 2$), a simple classifier (region A), and a single powerful classifier (region B).

SFCS Algorithm

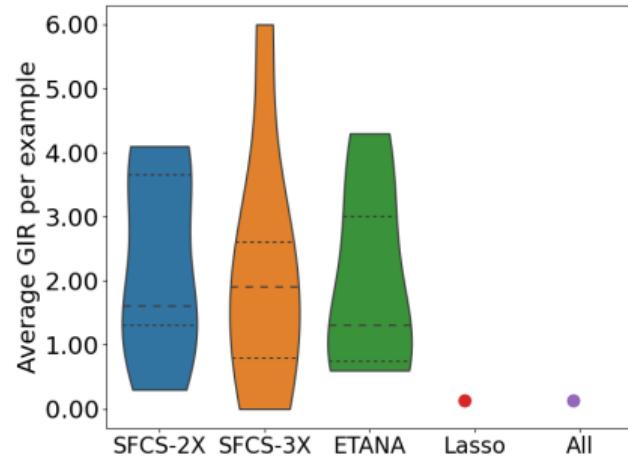


Some Results

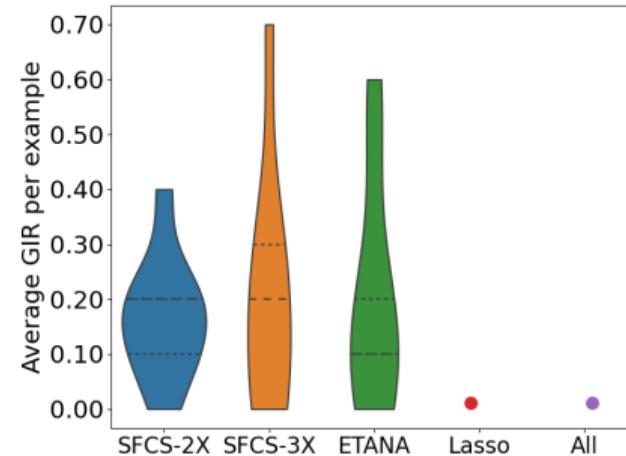
Method	Monks Problem		Diabetes		EEG Eye State		MagicTelescope		Student		German Credit	
	Acc	Feat	Acc	Feat	Acc	Feat	Acc	Feat	Acc	Feat	Acc	Feat
SFCS-SVM	0.536	5.722	0.753	6.056	0.536	3.315	0.794	6.316	0.864	4.656	0.732	12.081
SFCS-DT	0.795	5.722	0.753	6.056	0.485	3.315	0.807	6.316	0.869	4.656	0.732	12.081
ETANA	0.529	5.188	0.749	5.935	0.500	12.261	0.775	6.302	0.864	4.617	0.714	11.846
NB	0.591	6.000	0.751	8.000	0.437	14.000	0.727	11.000	0.827	32.000	0.700	20.000
SVM	0.657	6.000	0.674	8.000	0.551	14.000	0.806	11.000	0.787	32.000	0.700	20.000
DT	0.922	6.000	0.706	8.000	0.475	14.000	0.819	11.000	0.838	32.000	0.664	20.000
Lasso	0.654	4.800	0.766	8.000	0.551	13.400	0.789	9.000	0.851	14.600	0.734	17.800

- ▶ Good balance between accuracy and average number of acquired features
- ▶ Classifier selection in instance-wise feature acquisition enhances accuracy, but in most cases, increases average number of acquired features
- ▶ Why does SFCS-DT performs worse than DT?

Some Results



(a) Diabetes dataset.



(b) Magic dataset.

Figure 8: Distribution of average Gini impurity reduction (GIR) per example. “All” denotes baselines that use all features (e.g., SVM, DT)

- ▶ Feature with higher GIR is **more significant** than a feature with lower GIR, since latter cannot be used to effectively separate labels

Some Results

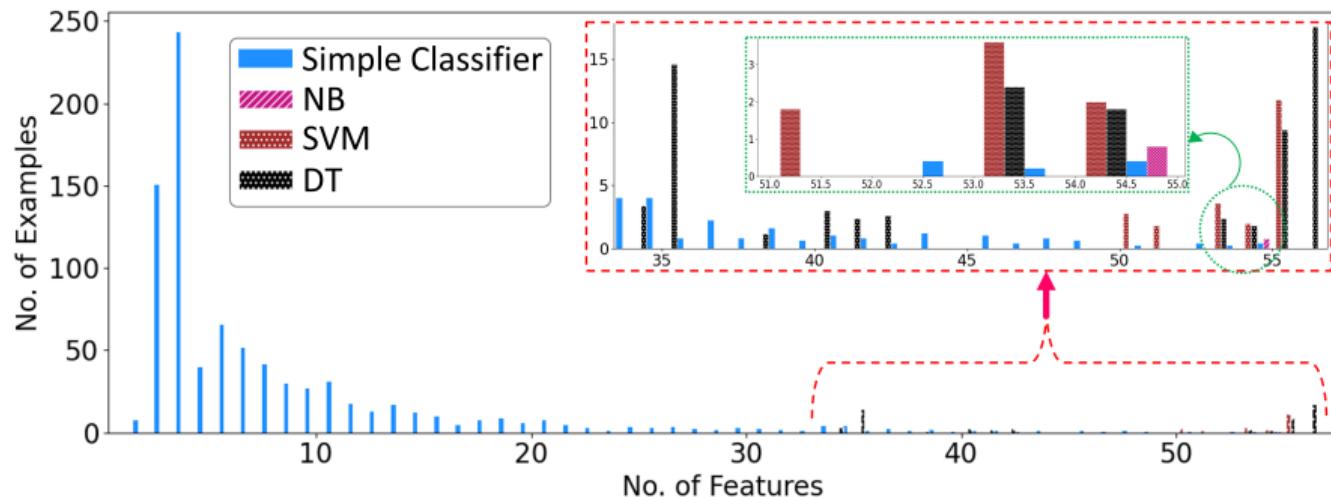


Figure 9: Distribution of number of acquired features during testing for the Spambase dataset using SFCS-3X (NB, SVM, DT).

- ▶ Classify most instances using simple classifier with few features
- ▶ When number of acquired features increases, SFCS switches to other classifiers (difficult-to-classify instances)

Causal Feature Selection for Algorithmic Fairness [GSSV22]

- ▶ Algorithmic fairness is critical when supervised classification models are used to support decisions in high-stake domains
- ▶ Not discrimination-aware feature selection methods prefer features that improve accuracy
- ▶ Goal: identify subset of new features to include in a dataset without worsening its biases against protected groups
 - ▶ Meant to be used during training dataset creation time
 - ▶ Key challenge: one or more non-protected features can facilitate reconstruction of protected information (e.g., infer race from zip code)
 - ▶ Main idea: perform conditional independence tests between different subsets of features

Causal Feature Selection for Algorithmic Fairness [GSSV22]

- ▶ Input dataset comprises:
 - ▶ Target variable Y (e.g., credit score)
 - ▶ Set of protected/sensitive features S (e.g., gender and race)
 - ▶ Set of admissible features A (e.g., expected monthly usage)
 - ▶ Protected variables can affect the outcome through admissible features
 - ▶ Features that are neither admissible nor sensitive (e.g., age and education)
- ▶ Two-phase method using conditional independence tests
 - ▶ Identify features that do not capture information about sensitive attributes
 - ▶ Ensure fairness even if features capture some information about sensitive attributes

Causal Feature Selection for Algorithmic Fairness [GSSV22]

Algorithm 1 SeqSel

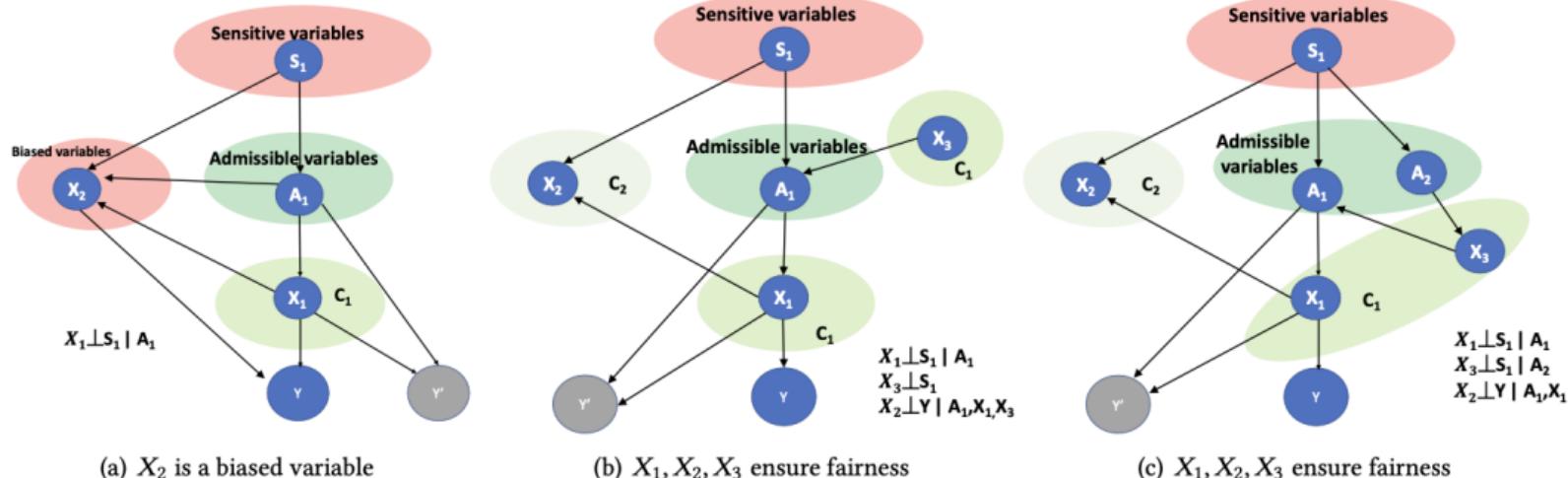
```
1: Input: Variables  $\mathbf{A}, \mathbf{S}, \mathbf{X}, Y$ 
2:  $C_1 \leftarrow \emptyset$ 
3: for  $X \in \mathbf{X}$  do
4:   if  $\exists A \subseteq \mathbf{A}$  such that  $(X \perp\!\!\!\perp \mathbf{S}|A)$  then
5:      $C_1 \leftarrow C_1 \cup \{X\}$ 
6:  $C_2 \leftarrow \emptyset$ 
7:  $\mathbf{X} \leftarrow \mathbf{X} \setminus C_1$ 
8: for  $X \in \mathbf{X}$  do
9:   if  $(X \perp\!\!\!\perp Y|\mathbf{A} \cup C_1)$  then
10:     $C_2 \leftarrow C_2 \cup \{X\}$ 
11: return  $C_1 \cup C_2$ 
```

- ▶ Find variables X_i independent of \mathbf{S} by performing conditional independence test
- ▶ Variables whose paths from \mathbf{S} are blocked by \mathbf{A} do not provide any new information about \mathbf{S}
 - ▶ Check if X_i is conditionally independent of \mathbf{S} given \mathbf{A}
- ▶ Variables X_i not independent of \mathbf{S} even given \mathbf{A} can leak sensitive information
 - ▶ If independent of Y given \mathbf{A} , no effect on the classifier
- ▶ Any variable that is not independent of \mathbf{S} and Y even after intervening on \mathbf{A} should not be added

Causal Feature Selection for Algorithmic Fairness [GSSV22]

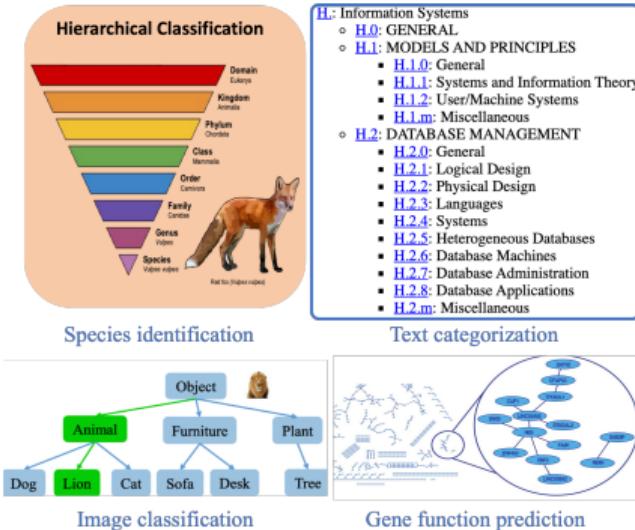
- ▶ Causal DAG G captures functional dependencies between variables
 - ▶ Variable X_1 causes X_2 iff $X_1 \rightarrow X_2$ in G
 - ▶ Joint probability distribution can be decomposed similar to Bayesian networks
- ▶ Variables X and Y are d -separated given Z , if all paths between X and Y are blocked by Z
 - ▶ Ideally, the prediction and protected attributes should be d -separated in G
- ▶ do-operator: assign value x to variable X ($do(X) = x$) in G' induced by G , with the difference that all incoming edges of X have been removed
- ▶ A classifier is considered **fair** if for any collection of values α of \mathbf{A} and output y' $P(Y' = y | do(\mathbf{S}) = \mathbf{s}, do(\mathbf{A}) = \alpha) = P(Y' = y | do(\mathbf{S}) = \mathbf{s}', do(\mathbf{A}) = \alpha), \forall \mathbf{A}, \mathbf{S}, Y'$
- ▶ Testing for causal fairness requires fully specified causal graphs (not available in practise)
 - ▶ Use conditional mutual information instead

Causal Feature Selection for Algorithmic Fairness [GSSV22]



- Given \mathbf{A} , $D = \mathbf{A} \cup \mathbf{T}$ is **causally fair** if the Bayes optimal predictor Y' , trained on D satisfies causal fairness with respect to sensitive attributes \mathbf{S}
- Goal: identify largest subset \mathbf{T} such that Y' , trained using these variables is fair
- New node Y' is added to G
- All features that impact the classifier output are made parents of Y'

Feature Selection for Hierarchical Classification [ZH^Z⁺19]



- ▶ Large-scale classification tasks comprise hundreds, thousands, or even tens of thousands of class labels
- ▶ Class labels are structured (often in a tree)
 - ▶ Class hierarchy divides the classification task into small and easy subtasks
- ▶ Goal: Feature selection for hierarchical classification tasks
 - ▶ Relevant features may differ among classes
 - ▶ Need to select different features for different subtasks

Feature Selection for Hierarchical Classification [ZH^Z⁺19]

- ▶ Feature selection as penalized optimization

- ▶ $\min_{\mathbf{W}} L(\mathbf{X}\mathbf{W}, \mathbf{Y}) + \lambda R(\mathbf{W})$

- ▶ Empirical loss L (e.g., logistic, hinge, cross-entropy loss)

- ▶ Regularizer R and positive constant λ

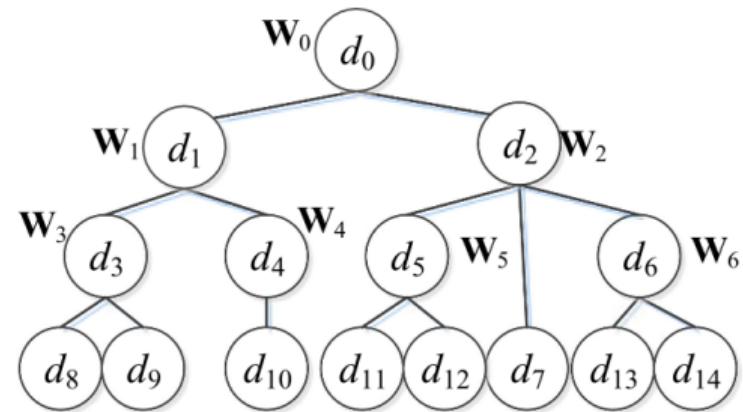
- ▶ Structural sparsity with $\ell_{2,1}$ -norm

- ▶ Goal: minimize $\sum_{i=0}^N (\|\mathbf{X}_i \mathbf{W}_i - \mathbf{Y}_i\|_F^2 + \lambda \|\mathbf{W}_i\|_{2,1})$

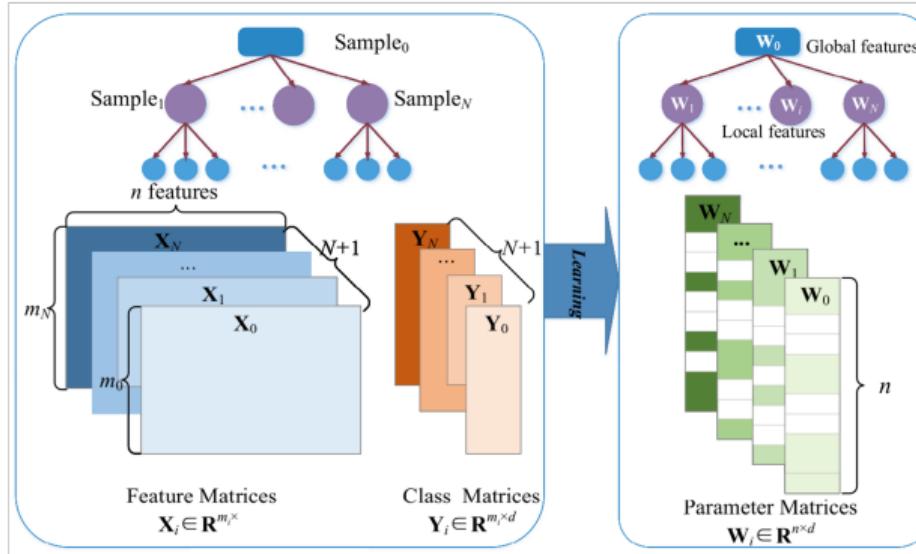
- ▶ Closed form solution obtained for least squares loss

- ▶ Feature weight matrix \mathbf{W}_i is computed for each internal node i

- ▶ Data instances of the i th node: $\mathbf{X}_i = [\mathbf{x}_1; \mathbf{x}_2; \dots; \mathbf{x}_{m_i}]$



Feature Selection for Hierarchical Classification [ZH^Z⁺19]



Algorithm 1. Hierarchical Feature Selection (Hier-FS)

Input: Input data $\mathbf{X}_i \in \mathbb{R}^{m_i \times n}$ and labels $\mathbf{Y} \in \{0, 1\}^{m_i \times d}$, where $i = 0, 1, \dots, N$, and N is the number of internal nodes. To facilitate the calculation, we let d be the maximum number of classes of internal nodes. Regularization parameter is λ , and the maximal iteration number is T .

Output: Matrix $\mathbf{W} \in \mathbb{R}^{n \times d(N+1)}$.

```
1: Set  $t = 0$  and initialize  $\mathbf{W}_i \in \mathbb{R}^{n \times d}$  randomly;  
2:  $\mathbf{W} = [\mathbf{W}_0, \mathbf{W}_1, \dots, \mathbf{W}_N]$ ;  
3: while  $t < T$  do  
4:   for  $i = 0 : N$  do  
5:     Compute the diagonal matrix  $\mathbf{D}_i^{(t)}$  according to  
       
$$d_{jj}^i = \frac{1}{2\|\mathbf{w}_j^i\|_2^2};$$
  
6:   end for  
     // Update the root node and internal nodes.  
7:   for  $i = 0 : N$  do  
8:     Update  $\mathbf{W}_i$  by  $\mathbf{W}_i^{(t+1)} = (\mathbf{X}_i^T \mathbf{X}_i + \lambda \mathbf{D}_i^{(t)})^{-1} (\mathbf{X}_i^T \mathbf{Y}_i)$ ;  
9:   end for  
10:  Update  $\mathbf{W}^{(t+1)} = [\mathbf{W}_0, \mathbf{W}_1, \dots, \mathbf{W}_N]$ ;  
11:   $t = t + 1$ ;  
12: end while  
13: return  $\mathbf{W}$ ;
```

- Top-down recursive strategy
- Node i th's top-ranked (w.r.t $\|\mathbf{w}_j^i\|_F$) features are selected

Feature Selection for Hierarchical Classification [ZH^Z⁺¹⁹]

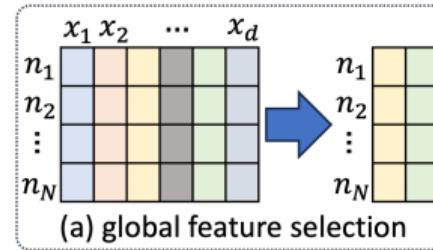
- ▶ Hierarchical regularization with parent–child relationship
 - ▶ Parent–child classes are similar to each other; should share common features
 - ▶ Relationship is incorporated into regularizer: $\sum_{i=1}^N \|\mathbf{W}_i - \mathbf{W}_{p_i}\|_F^2$
- ▶ Hierarchical regularization with sibling relationship
 - ▶ Siblings come from different subtrees
 - ▶ Discriminative features must be selected for each sibling
 - ▶ Hilbert–Schmidt Independence Criterion to penalize dependence between selected features at sibling nodes
- ▶ Hierarchical regularization with family relationship
 - ▶ Both parent–child and sibling relationships between categories incorporated into the optimization problem

Summary and Conclusion

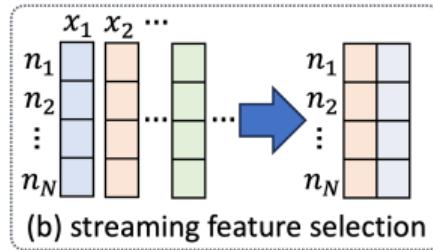
Still 🤔 about Feature Selection vs Feature Acquisition?

- ▶ Global Feature Selection
 - ▶ Identify, during **training**, a subset of features (**common** across instances)
 - ▶ Online/streaming methods when full feature set unavailable at training
- ▶ Active Feature Acquisition
 - ▶ During **training** (related to feature selection with missing values)
 - ▶ During **testing**, learned model is used
- ▶ Instance-wise Feature Selection
 - ▶ Identify, during **testing**, small subset of features for each data instance (**varies** between instances)
 - ▶ Given a test instance, **all of its features** must be available
- ▶ Instance-wise Feature Acquisition
 - ▶ Different features acquired, during **testing**, for each data instance
 - ▶ Classification with costly features / Dynamic instance-wise feature acquisition

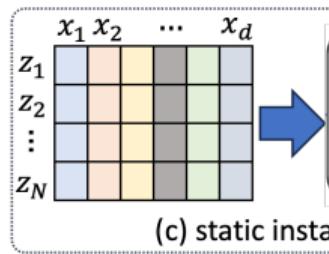
Feature Selection vs Feature Acquisition Visualized



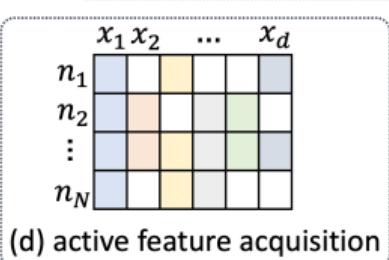
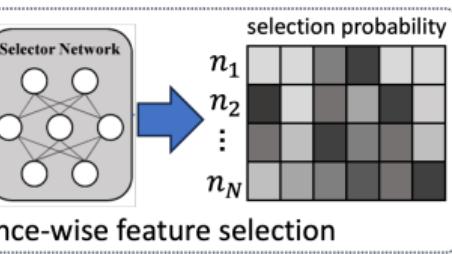
(a) global feature selection



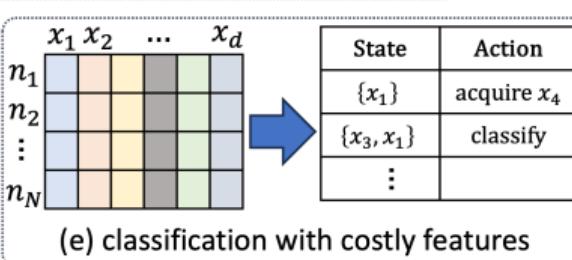
(b) streaming feature selection



(c) static instance-wise feature selection



(d) active feature acquisition



(e) classification with costly features

Key Takeaways

- ▶ Traditional feature selection is conducted during training
- ▶ Feature acquisition \neq feature selection
 - ▶ can be performed either during training or testing
- ▶ Instance-wise feature selection \neq instance-wise feature acquisition
- ▶ Both feature selection and feature acquisition approaches face significant challenges
- ▶ Instance-wise feature acquisition has broader implications to ML

(Non Exhaustive List of) Topics This Tutorial Didn't Cover

- ▶ Feature acquisition in both training and testing [DMW10]
- ▶ Group feature acquisition during testing [AJD24]
- ▶ Multiview/multimodal feature selection [YGSC15, LMF16, KAH20] and acquisition [NZC20]
- ▶ Active feature acquisition for time series data [LO21, BBS22, KCV⁺23]
- ▶ Feature selection (prompting) for large language models
- ▶ Knowledge–driven feature acquisition
- ▶ Causality and feature selection
- ▶ Feature selection/acquisition for non–linear models
 - ▶ Quantifying feature importance is difficult
 - ▶ Interpreting findings becomes challenging

Tutorial Slides

- ▶ Our coverage of state-of-the-art and challenges we identify are not exhaustive
- ▶ The slides can be found at: <https://www.cs.albany.edu/~cchelmis/tutorials/sdm/2024/>
- ▶ Suggested citation:
Daphney-Stavroula Zois, Charalampos Chelmis, “[From Feature Selection to Instance-wse Feature Acquisition](#)”, Minitutorial at SIAM International Conference on Data Mining (SDM), Houston, TX, April 2024.

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