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# From Feature Selection to Instance-wise Feature Acquisition<sup>1</sup>

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 [EZC23b, EZC23a])
- ▶ Feature Selection
  - ▶ Incorporating fairness constraints (e.g., [GSSV22])
  - ▶ Feature selection for hierarchical classification (e.g., [ZHZ<sup>+</sup>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

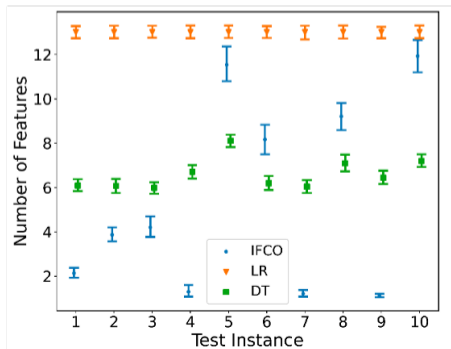
- ▶ For demonstration purpose, we use the **German credit-risk dataset**: classify people as high or low credit risk

Feature	Description	Feature	Description
F <sub>1</sub>	Checking account status	F <sub>11</sub>	Present residence
F <sub>2</sub>	Duration in months	F <sub>12</sub>	Property
F <sub>3</sub>	Credit history	F <sub>13</sub>	Age in years
F <sub>4</sub>	Purpose of the credit	F <sub>14</sub>	Other installment plans
F <sub>5</sub>	Credit amount	F <sub>15</sub>	Housing
F <sub>6</sub>	Savings account status	F <sub>16</sub>	Existing credits
F <sub>7</sub>	Present employment (years)	F <sub>17</sub>	Job
F <sub>8</sub>	Installment rate	F <sub>18</sub>	Number of dependents
F <sub>9</sub>	Personal status	F <sub>19</sub>	Telephone
F <sub>10</sub>	Other debtors	F <sub>20</sub>	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

- ▶ **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**

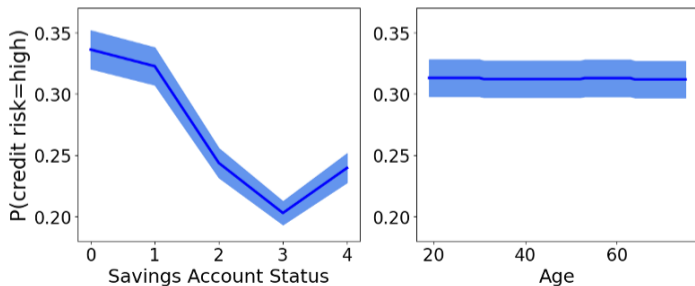
$$\pi_{\sigma^*(k)} = \frac{\left( \Delta(F_{\sigma^*(k)} | F_{\sigma^*(1)}, \dots, F_{\sigma^*(k-1)}, \mathcal{C}) \right) \pi_{\sigma^*(k-1)}}{\Delta^T(F_{\sigma^*(k)} | F_{\sigma^*(1)}, \dots, F_{\sigma^*(k-1)}, \mathcal{C}) \pi_{\sigma^*(k-1)}}$$

- ▶ **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

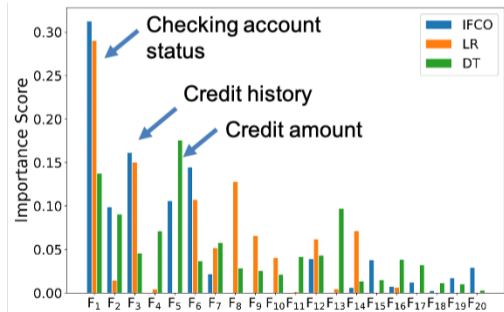
- ▶ **Partial dependence**: marginal effects of **individual feature** on **output** of machine learning model

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



## Post-hoc Interpretability: Dataset-level Interpretations

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



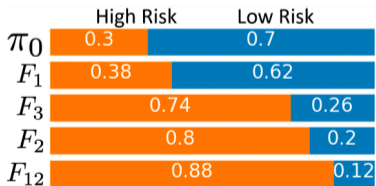
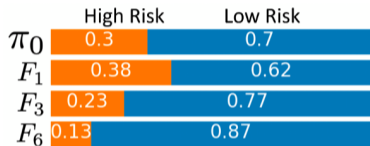
## Post-hoc Interpretability: Dataset-level Interpretations

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

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

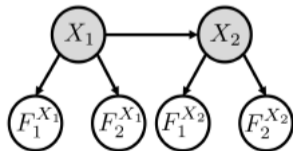
Correctly predicted → low credit-risk

- ▶ bad checking account status
- ▶ bad credit history
- ▶ credit history of 36 months
- ▶ no known property

Correctly predicted → high credit-risk

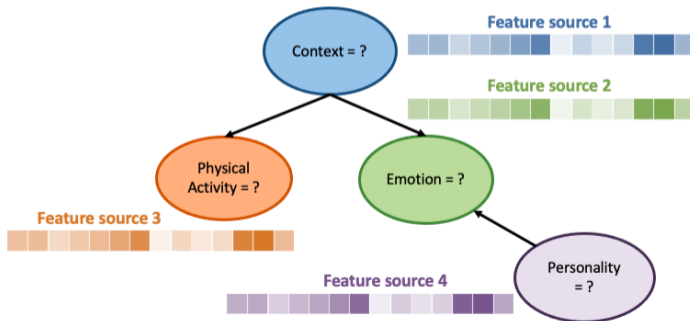
## Instance-wise Multidimensional Classification [ELZ21, EZ23]

- ▶ 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**

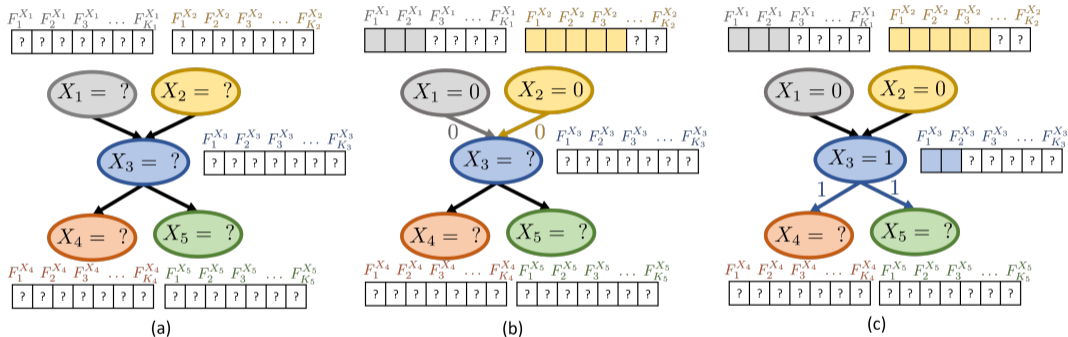
## Alternative Approach

- ▶ 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



**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	<b>0.5905</b>	0.3890	0.4668	0.5443	0.3905	0.3864	0.3578	0.4483
	MA	<b>0.7401</b>	0.6491	0.6500	<b>0.7101</b>	0.6952	0.6209	0.6755	0.7013
	AF	<b>5.8654</b>	16.0000	<b>8.6333</b>	16.0000	16.0000	16.0000	16.0000	16.0000
Voice	GA	<b>0.8753</b>	0.6897	0.8224	0.6824	0.2735	<b>0.8359</b>	0.7663	0.7220
	MA	<b>0.9364</b>	0.8243	0.8748	0.8343	0.5210	<b>0.9142</b>	0.8780	0.8514
	AF	2.5127	19.0000	<b>2.2719</b>	19.0000	19.0000	19.0000	19.0000	19.0000
Jura	GA	<b>0.4402</b>	0.3036	0.3481	0.4010	0.1588	0.2591	0.2562	0.2393
	MA	<b>0.6352</b>	0.5405	0.5845	0.6016	0.4764	0.4889	0.5307	0.4830
	AF	<b>7.0517</b>	9.0000	<b>8.2394</b>	9.0000	9.0000	9.0000	9.0000	9.0000
Song	GA	0.3299	0.2114	0.2509	0.2611	0.3082	<b>0.4229</b>	0.3471	<b>0.3548</b>
	MA	0.7134	<b>0.6012</b>	0.6709	0.6360	0.6802	<b>0.7565</b>	0.6728	0.6724
	AF	<b>16.3172</b>	98.0000	<b>16.6072</b>	98.0000	98.0000	98.0000	98.0000	98.0000
Flare	GA	0.8173	0.0277	0.7800	0.0463	<b>0.8204</b>	0.7802	0.8202	0.8202
	MA	0.9205	0.2194	0.8906	0.5736	<b>0.9226</b>	0.9035	0.9225	0.9225
	AF	<b>1.3040</b>	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	<b>0.7409</b>	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	<b>0.3203</b>
	MA	0.7783	0.7391	0.7641	0.7700	0.6885	0.7026	<b>0.7934</b>	0.7718
	AF	<b>8.5983</b>	72.0000	<b>15.3432</b>	72.0000	72.0000	72.0000	72.0000	72.0000
Child	GA	<b>0.5620</b>	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	<b>4.4293</b>	17.0000	<b>5.8147</b>	17.0000	17.0000	17.0000	17.0000	17.0000
Hepar2	GA	0.4200	0.0900	0.4170	0.0350	0.4180	0.4150	<b>0.4230</b>	0.4150
	MA	0.7807	0.4260	0.7757	0.4193	0.7813	0.7792	<b>0.7813</b>	0.7747
	AF	<b>12.6213</b>	67.0000	<b>31.9470</b>	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	<b>0.8420</b>	0.8399	<b>0.8420</b>	<b>0.8420</b>
	AF	<b>1.8575</b>	9.0000	8.4295	9.0000	9.0000	9.0000	9.0000	9.0000
Insurance	GA	<b>0.8270</b>	0.6920	0.8100	0.6150	0.4320	0.6062	0.7240	0.7310
	MA	<b>0.9050</b>	0.8350	0.9030	0.7840	0.5870	0.7841	0.8540	0.8520
	AF	<b>2.9115</b>	25.0000	5.4565	25.0000	25.0000	25.0000	25.0000	25.0000

## Joint Feature Acquisition & Classifier Selection [EYC23b, EYC23a]

- ▶ 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

$$D_S^* = \underset{1 \leq j \leq N}{\text{argmax}} [\mathbf{\Omega}_j^T \phi_S].$$

- ▶ Optimum classifier selection strategy

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

- ▶ Optimum feature acquisition strategy via dynamic programming

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

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

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



# Intuition

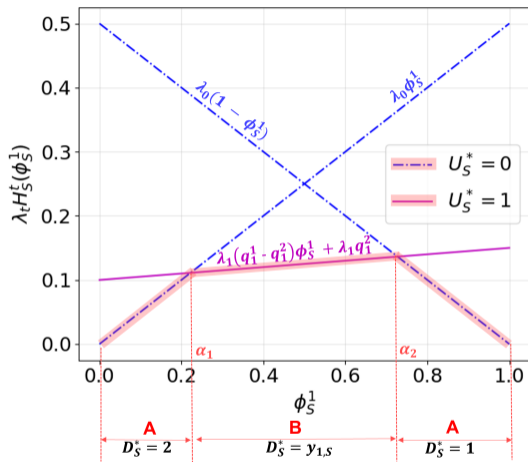
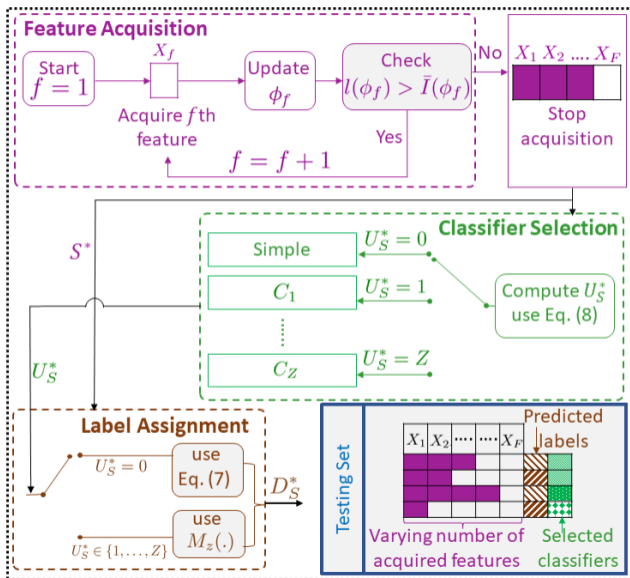


Figure 7: Illustration of classifier selection and label assignment processes in the case of two label values (i.e.,  $N = 2$ ), a simple classifier (region A), and a single powerful classifier (region B).

# SFCS Algorithm

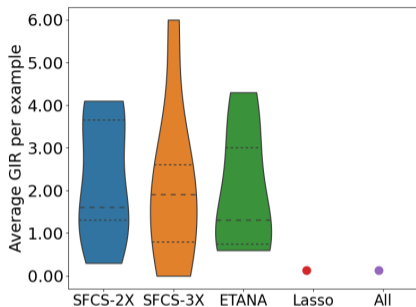


## Some Results

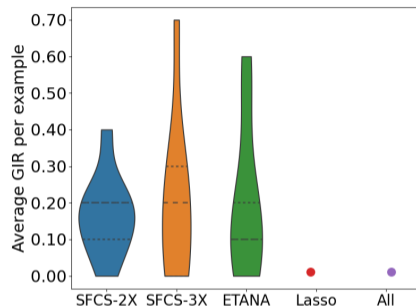
Method	Monks Problem		Diabetes		EEG Eye State		MagicTelescope		Student		German Credit	
	Acc	Feat	Acc	Feat	Acc	Feat	Acc	Feat	Acc	Feat	Acc	Feat
SFCS-SVM	0.536	5.722	<b>0.753</b>	6.056	0.536	<b>3.315</b>	0.794	6.316	0.864	4.656	0.732	12.081
SFCS-DT	0.795	5.722	0.753	6.056	0.485	<b>3.315</b>	0.807	6.316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

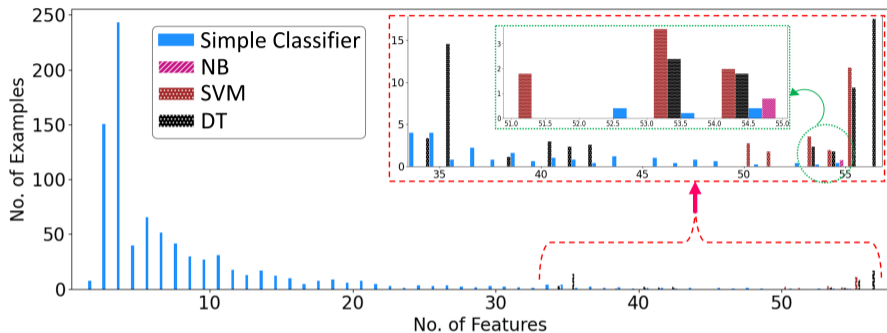


Figure 9: Distribution of number of acquired features during testing for the Spambase dataset using SFCS-3X (NB, SVM, DT).

- ▶ 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]

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## Algorithm 1 SeqSel

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```
1: Input: Variables  $\mathbf{A}, \mathbf{S}, \mathbf{X}, Y$ 
2:  $\mathbf{C}_1 \leftarrow \phi$ 
3: for  $X \in \mathbf{X}$  do
4:   if  $\exists A \subseteq \mathbf{A}$  such that  $(X \perp \mathbf{S} | A)$  then
5:      $\mathbf{C}_1 \leftarrow \mathbf{C}_1 \cup \{X\}$ 
6:  $\mathbf{C}_2 \leftarrow \phi$ 
7:  $\mathbf{X} \leftarrow \mathbf{X} \setminus \mathbf{C}_1$ 
8: for  $X \in \mathbf{X}$  do
9:   if  $(X \perp Y | \mathbf{A} \cup \mathbf{C}_1)$  then
10:     $\mathbf{C}_2 \leftarrow \mathbf{C}_2 \cup \{X\}$ 
11: return  $\mathbf{C}_1 \cup \mathbf{C}_2$ 
```

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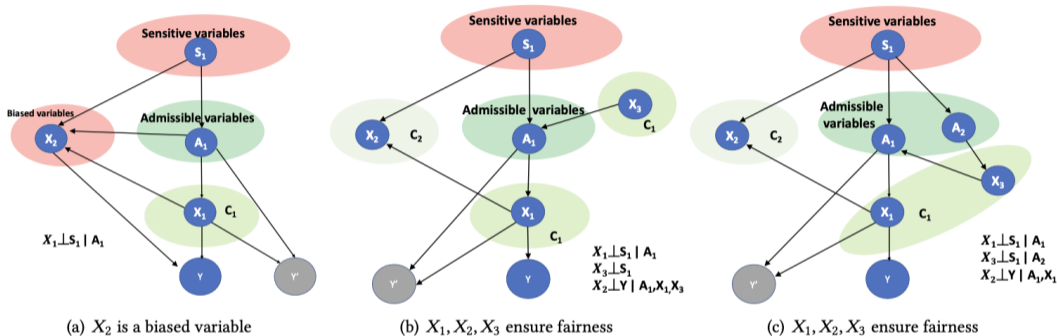
- ▶ Find variables  $X_i$  independent of  $\mathbf{S}$  by performing conditional independence test
- ▶ Variables whose paths from  $\mathbf{S}$  are blocked by  $\mathbf{A}$  do not provide any new information about  $\mathbf{S}$ 
  - ▶ Check if  $X_i$  is conditionally independent of  $\mathbf{S}$  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  $\alpha$  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]

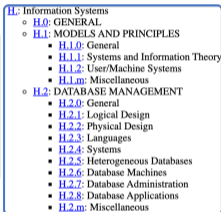


- ▶ Given  $\mathbf{A}$ ,  $D = \mathbf{A} \cup \mathbf{T}$  is **causally fair** if the Bayes optimal predictor  $Y'$ , trained on  $D$  satisfies causal fairness with respect to sensitive attributes  $\mathbf{S}$
- ▶ Goal: identify largest subset  $\mathbf{T}$  such that  $Y'$ , trained using these 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 [ZHZ<sup>+</sup>19]



Species identification



Text categorization

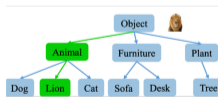
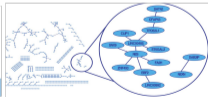


Image classification



Gene function prediction

- ▶ 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 [ZHZ<sup>+</sup>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  $\lambda$

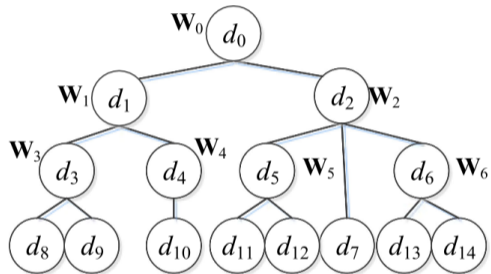
- ▶ Structural sparsity with  $\ell_{2,1}$ -norm

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

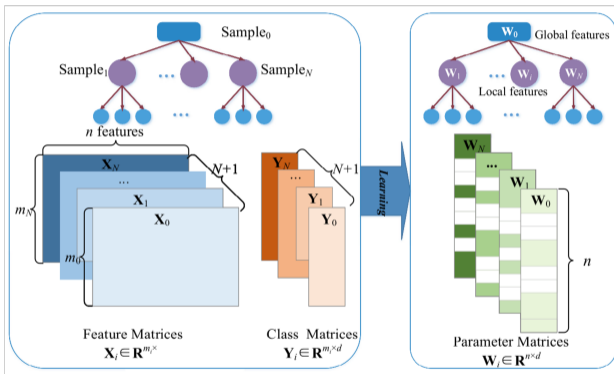
- ▶ Closed form solution obtained for least squares loss

- ▶ 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 [ZHZ<sup>+</sup>19]



## Algorithm 1. Hierarchical Feature Selection (Hier-FS)

**Input:** Input data  $X_i \in \mathbb{R}^{m_i \times n}$  and labels  $Y \in \{0, 1\}^{m_i \times d}$ , 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  $\lambda$ , and the maximal iteration number is  $T$ .

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

- 1: Set  $t = 0$  and initialize  $W_i \in \mathbb{R}^{n \times d}$  randomly;
- 2:  $W = [W_0, W_1, \dots, W_N]$ ;
- 3: **while**  $t < T$  **do**
- 4:   **for**  $i = 0 : N$  **do**
- 5:     Compute the diagonal matrix  $D_i^{(t)}$  according to  $d_{jj}^{(t)} = \frac{1}{2\|w_j^{(t)}\|_2}$ ;
- 6:   **end for**  
    // Update the root node and internal nodes.
- 7:   **for**  $i = 0 : N$  **do**
- 8:     Update  $W_i$  by  $W_i^{(t+1)} = (X_i^T X_i + \lambda D_i^{(t)})^{-1} X_i^T Y_i$ ;
- 9:   **end for**
- 10: Update  $W^{(t+1)} = [W_0, W_1, \dots, W_N]$ ;
- 11:  $t = t + 1$ ;
- 12: **end while**
- 13: **return**  $W$ ;

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

## Feature Selection for Hierarchical Classification [ZHZ<sup>+</sup>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

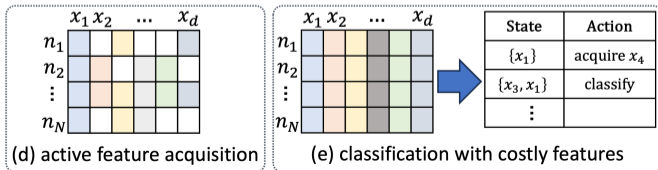
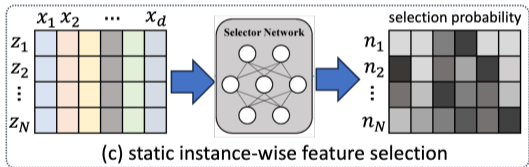
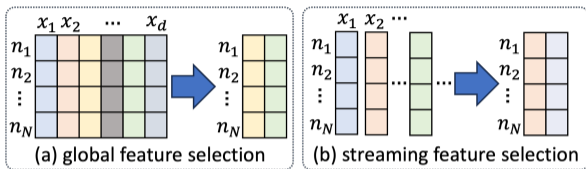
## Summary and Conclusion

# 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



## 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<sup>+</sup>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-wise Feature Acquisition”, Minitutorial at SIAM International Conference on Data Mining (SDM), Houston, TX, April 2024.

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- ▶ We thank you, the audience, for your attention
- ▶ We welcome your feedback and suggestions



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