

The UCLA logo consists of the letters "UCLA" in white, bold, sans-serif font, centered within a solid blue rectangular background.

Computer
Science



Reasoning about Missing Data in Machine Learning

Guy Van den Broeck

Outline

1. Missing data at prediction time
 - a. Reasoning about expectations
 - b. Applications: classification and explainability
 - c. Tractable circuits for expectation
 - d. Fairness of missing data
2. Missing data during learning

References and Acknowledgements

- ❑ Pasha Khosravi, Yitao Liang, YooJung Choi and Guy Van den Broeck. [What to Expect of Classifiers? Reasoning about Logistic Regression with Missing Features](#), *In IJCAI*, 2019.
- ❑ Pasha Khosravi, YooJung Choi, Yitao Liang, Antonio Vergari and Guy Van den Broeck. [On Tractable Computation of Expected Predictions](#), *In NeurIPS*, 2019.
- ❑ YooJung Choi, Golnoosh Farnadi, Behrouz Babaki and Guy Van den Broeck. [Learning Fair Naive Bayes Classifiers by Discovering and Eliminating Discrimination Patterns](#), *In AAI*, 2020.
- ❑ Guy Van den Broeck, Karthika Mohan, Arthur Choi, Adnan Darwiche and Judea Pearl. [Efficient Algorithms for Bayesian Network Parameter Learning from Incomplete Data](#), *In UAI*, 2015.

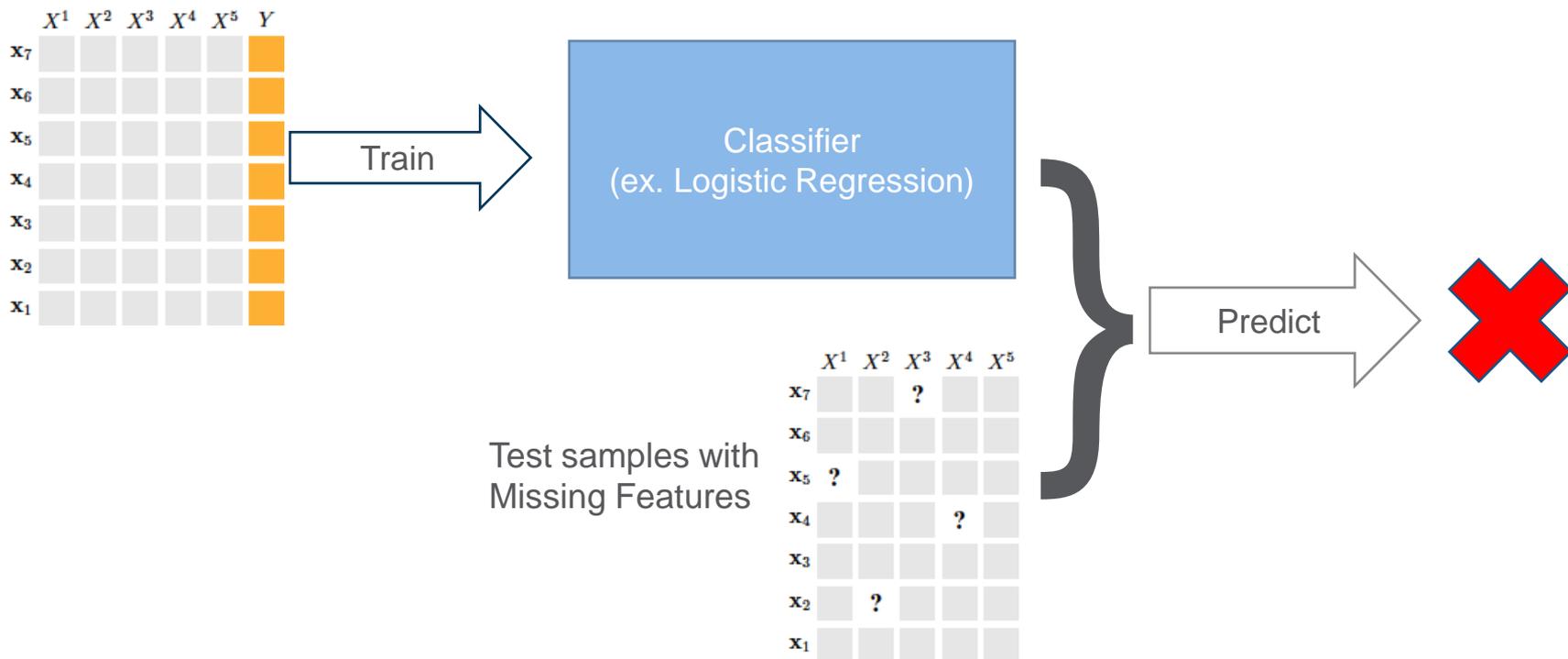
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Missing data at prediction time



Common Approaches

- Fill out the missing features, i.e. doing imputation.
- Makes unrealistic assumptions (mean, median, etc).
- More sophisticated methods such as MICE don't scale to bigger problems (and also have assumptions).
- We want a more principled way of dealing with missing data while staying efficient.

	X^1	X^2	X^3	X^4	X^5
x_8					
x_7					
x_6					
x_5					
x_4					
x_3					
x_2					
x_1					

Discriminative vs. Generative Models

Terminology:

- **Discriminative Model:** conditional probability distribution, $P(C | X)$.
For example, Logistic Regression.
- **Generative Model:** joint features and class probability distribution, $P(C, X)$.
For example, Naïve Bayes.

Suppose we only observe some features \mathbf{y} in X , and we are missing \mathbf{m} :

$$P(C|\mathbf{y}) = \sum_{\mathbf{m}} P(C, \mathbf{m}|\mathbf{y}) \propto \sum_{\mathbf{m}} P(C, \mathbf{m}, \mathbf{y})$$

We need a generative model!

Generative vs Discriminative Models

Discriminative Models
(ex. Logistic Regression)

Generative Models
(ex. Naïve Bayes)

$$P(C | X)$$

$$P(C, X)$$

Missing
Features



Classification
Accuracy



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Generative Model Inference as Expectation

Let's revisit how generative models deal with missing data:

$$\begin{aligned} P(C|\mathbf{y}) &= \sum_{\mathbf{m}} P(C, \mathbf{m}|\mathbf{y}) \\ &= \sum_{\mathbf{m}} P(C|\mathbf{m}, \mathbf{y}) P(\mathbf{m}|\mathbf{y}) \\ &= \mathbb{E}_{\mathbf{m} \sim P(M|\mathbf{y})} P(C|\mathbf{m}, \mathbf{y}) \end{aligned}$$

It's an expectation of a classifier under the feature distribution

What to expect of classifiers?

What if we train both kinds of models:

1. Generative model for feature distribution $P(X)$.
2. Discriminative model for the classifier $F(X) = P(C | X)$.

“**Expected Prediction**” is a principled way to reason about outcome of classifier $F(X)$ under feature distribution $P(X)$.

$$E_{\mathcal{F}, P}(\mathbf{y}) = \mathbb{E}_{\mathbf{m} \sim P(\mathbf{M} | \mathbf{y})} [\mathcal{F}(\mathbf{y}\mathbf{m})]$$

Expected Predication Intuition

- **Imputation Techniques:** Replace the missing-ness uncertainty with one or multiple possible inputs, and evaluate the models.
- **Expected Prediction:** Considers all possible inputs and reason about expected behavior of the classifier.

$$E_{\mathcal{F},P}(\mathbf{y}) = \sum_{\mathbf{m}} P(\mathbf{m} \mid \mathbf{y}) \cdot \mathcal{F}(\mathbf{y}\mathbf{m}) = \mathbb{E}_{\mathbf{m} \sim P(\mathbf{M}|\mathbf{y})} [\mathcal{F}(\mathbf{y}\mathbf{m})]$$

Hardness of Taking Expectations

- How can we compute the expected prediction?
- In general, it is intractable for arbitrary pairs of discriminative and generative models.
- Even when
 - ✓ Classifier F is Logistic Regression and
 - ✓ Generative model P is Naïve Bayes,the task is NP-Hard.



Solution: Conformant learning

Given a classifier and a dataset, learn a generative model that

1. *Conforms* to the classifier: $F(X) = P(C | X)$.
2. Maximizes the likelihood of generative model: $P(X)$.

No missing features → Same quality of classification



Has missing features → No problem, do inference

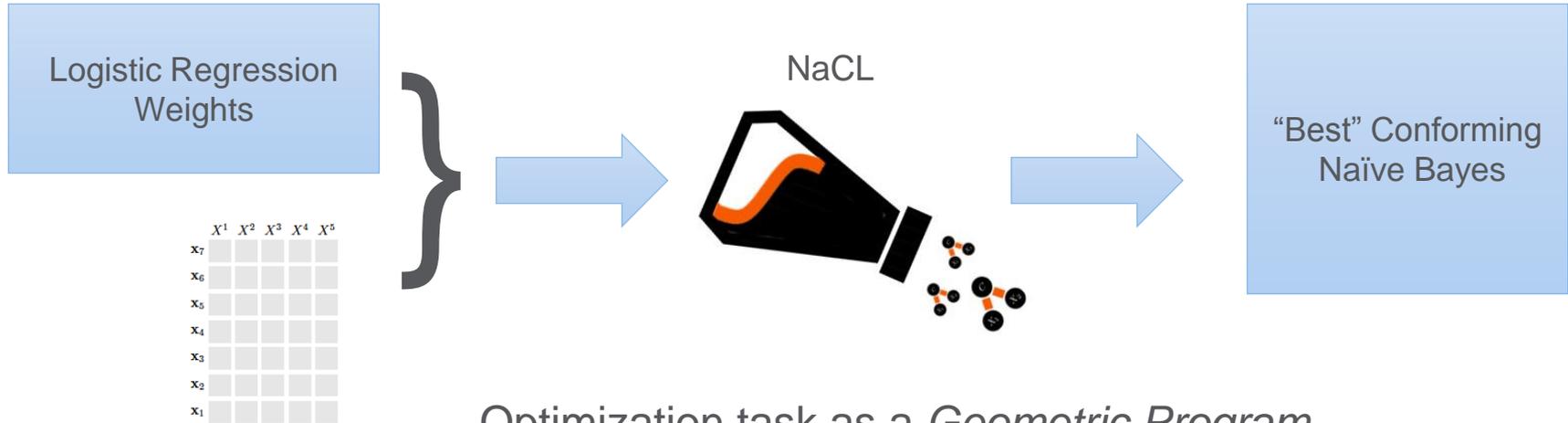


Example: Naïve Bayes (NB) vs. Logistic Regression (LR):

- Given NB there is one LR that it conforms to
- Given LR there are many NB that conform to it



Naïve Conformant Learning (NaCL)



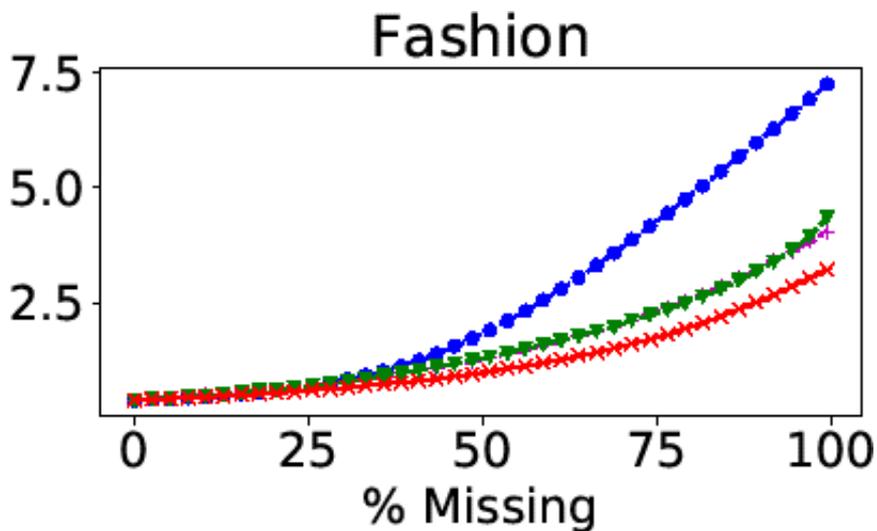
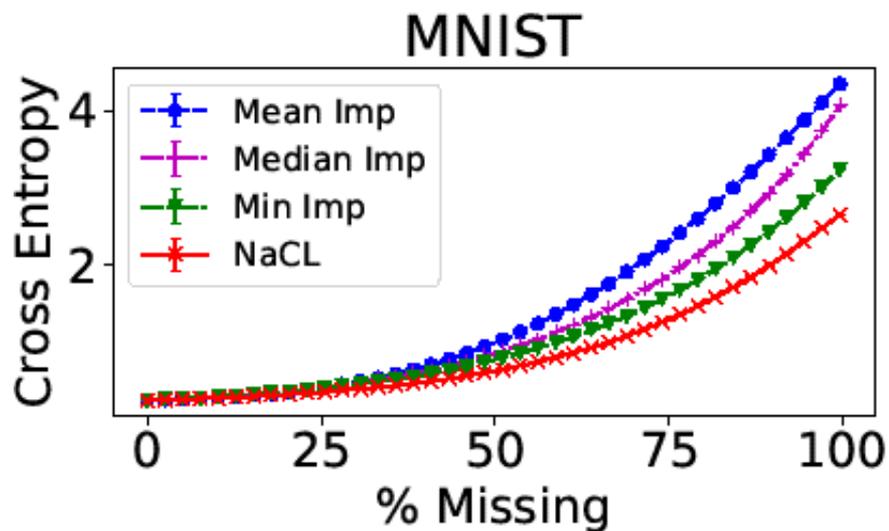
Optimization task as a *Geometric Program*

GitHub: github.com/UCLA-StarAI/NaCL

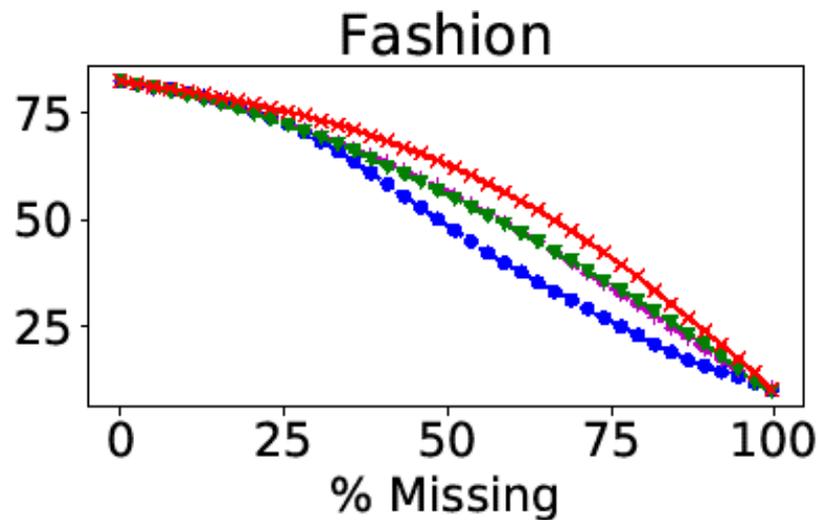
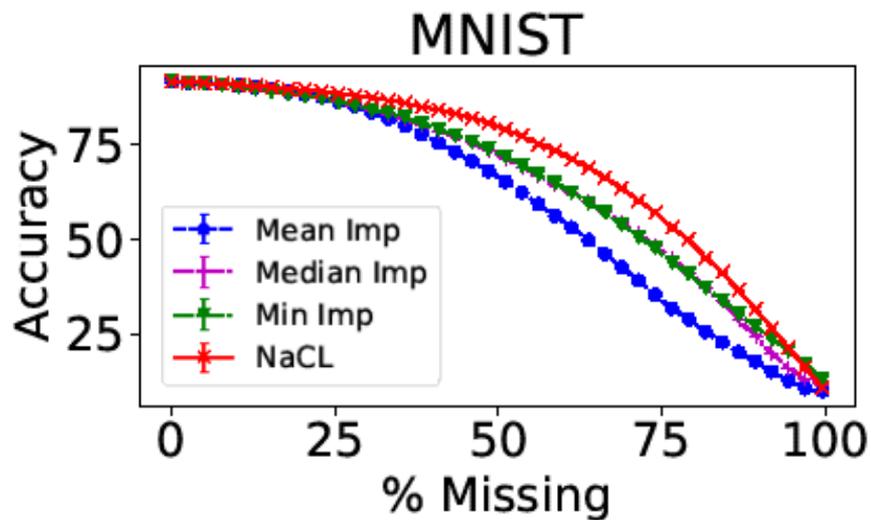
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Experiments: Fidelity to Original Classifier



Experiments: Classification Accuracy



Sufficient Explanations of Classification

Goal:

To explain an instance of classification

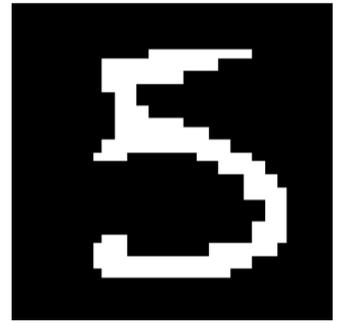
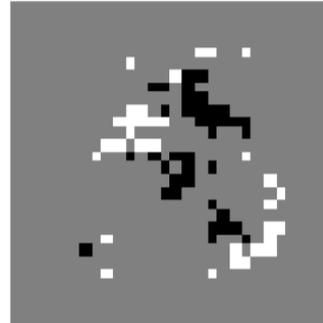
Support Features:

Making them missing

→ probability goes down

Sufficient Explanation:

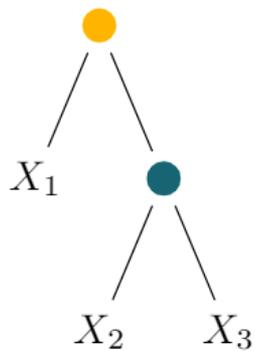
Smallest set of support features
that retains the expected classification



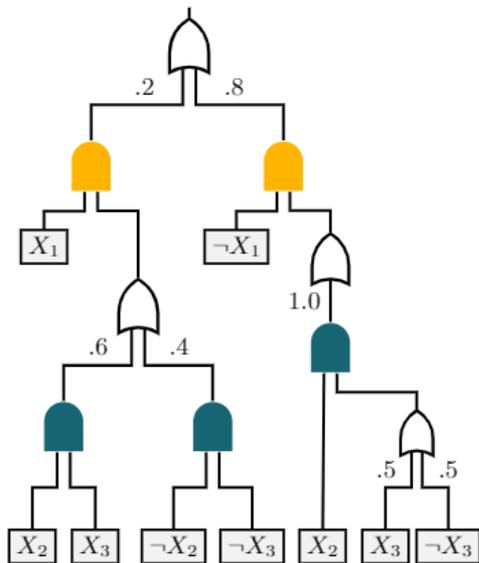
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What about better distributions and classifiers?

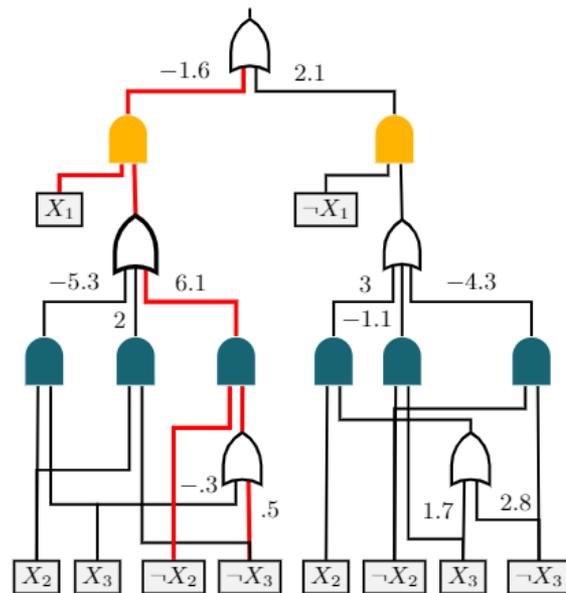


(a) A vtree



(b) A Probabilistic Circuit

Generative



(c) A Logistic/Regression Circuit

Discriminative

Hardness of Taking Expectations

If f is a regression circuit, and p is a generative circuit
with **different** vtree

Proved #P-Hard



If f is a classification circuit, and p is a generative circuit
with **different** vtree

Proved NP-Hard

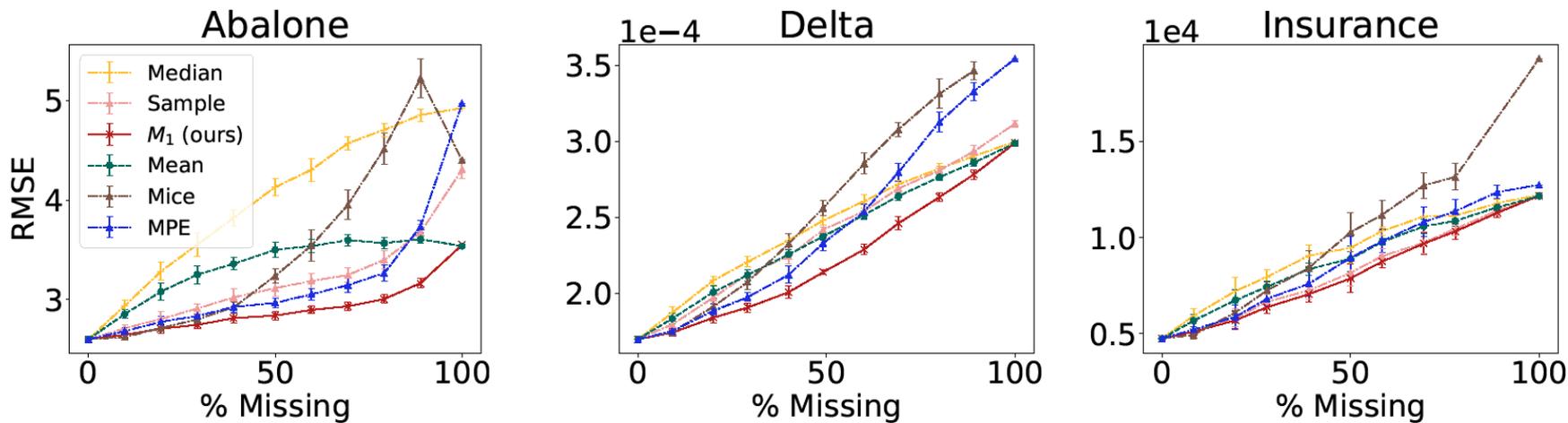


If f is a regression circuit, and p is a generative circuit
with the **same** vtree

Polytime algorithm



Regression Experiments



Approximate Expectations of Classification

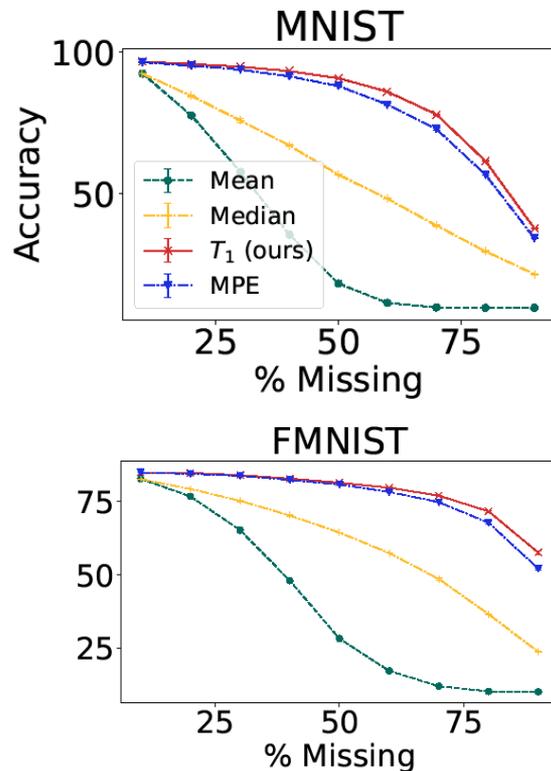
What to do for classification circuits?
(Even with same vtree, expectation was intractable.)

⇒ Approximate classification using Taylor series
of the underlying regression circuit.

$$\mathbb{E}_{\mathbf{x} \sim p_n(\mathbf{x})} [\gamma \circ g_m(\mathbf{x})] \approx \sum_{i=0}^d \frac{\gamma^{(i)}(\alpha)}{i!} M_i(g_m - \alpha, p_n)$$

⇒ Requires higher order moments
of regression circuit...

⇒ This is also efficient! 😊



Exploratory Classifier Analysis

Expected predictions enable reasoning about behavior of predictive models

We have learned an regression and a probabilistic circuit for
“Yearly health insurance costs of patients”

Q1: Difference of costs between smokers and non-smokers

$$M_1(f, p(\cdot | \textit{Smoker})) - M_1(f, p(\cdot | \textit{Non Smoker})) = 22,614$$

...or between female and male patients?

$$M_1(f, p(\cdot | \textit{Female})) - M_1(f, p(\cdot | \textit{Male})) = 974$$

Exploratory Classifier Analysis

Can also answer more complex queries like:

Q2: Average cost for female (F) smokers (S)
with one child (C) in the South East (SE)?

$$M_1(f, p(. | F, S, C, SE)) = 30,974$$

Q3: Standard Deviation of the cost for the same sub-population?

$$\sqrt{M_2(.) - (M_1(.))^2} = 11,229$$

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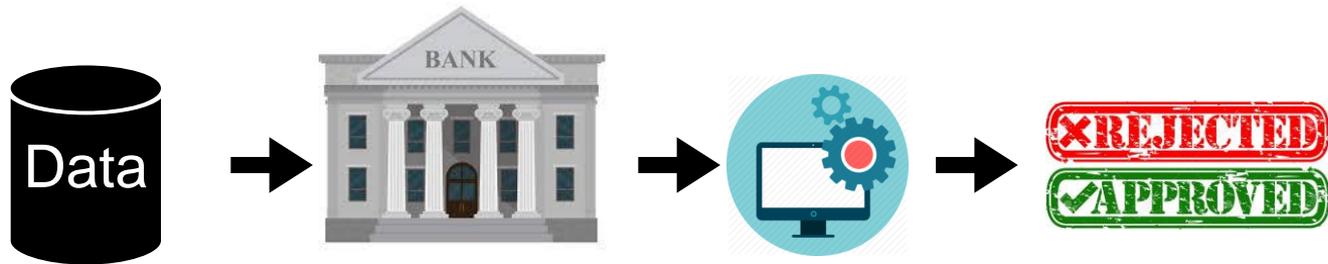
Algorithmic Fairness

Legally recognized
'protected classes'



Race (Civil Rights Act of 1964)
Color (Civil Rights Act of 1964)
Sex (Equal Pay Act of 1963; Civil Rights Act of 1964)
Religion (Civil Rights Act of 1964)
National origin (Civil Rights Act of 1964)
Citizenship (Immigration Reform and Control Act)
Age (Age Discrimination in Employment Act of 1967)
Pregnancy (Pregnancy Discrimination Act)
Familial status (Civil Rights Act of 1968)
Disability status (Rehabilitation Act of 1973; Americans with Disabilities Act of 1990)
Veteran status (Vietnam Era Veterans' Readjustment Assistance Act of 1974; Uniformed Services Employment and Reemployment Rights Act);
Genetic information (Genetic Information Nondiscrimination Act)

Individual Fairness

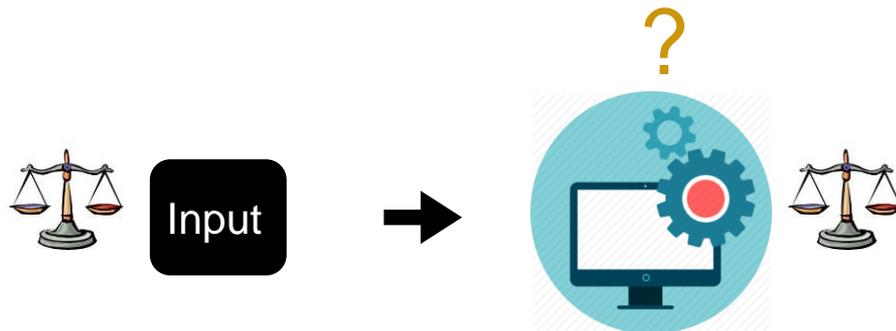


- Individual fairness:  = 
- Existing methods often define individuals as a **fixed set of observable features**
- Lack of discussion of certain features **not being observed at prediction time**



What about learning from fair data?

Model learned from repaired data can still be unfair!



Number of discrimination patterns:

Dataset	$\lambda = 0.5$	$\lambda = 0.9$	$\lambda = 0.95$	$\lambda = 0.99$	$\lambda = 1.0$
COMPAS	11,512	7,862	8,872	8,926	0
Adult	>1e6	1,078	1,123	1,087	0
German	>1e6	1	9	0	0

Independent

Individual Fairness with Partial Observations

- **Degree of discrimination:** $\Delta(x, y) = P(d|xy) - P(d|y)$



Decision given
partial evidence

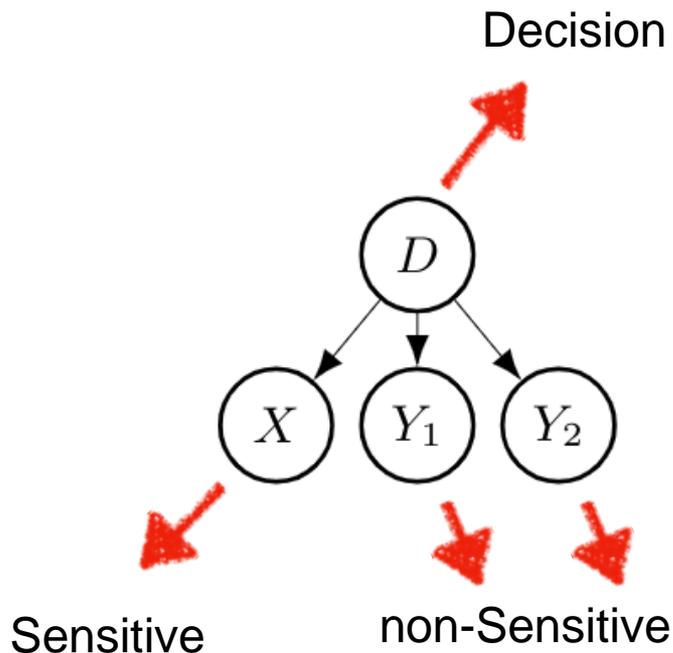


Decision without
sensitive attributes

“What if the applicant had not disclosed their gender?”

- **δ -fairness:** $\Delta(x, y) \leq \delta, \forall x, y$
- A violation of δ -fairness is a **discrimination pattern** x, y .

Discovering and Eliminating Discrimination



1. **Verify** whether a Naive Bayes **classifier** is δ -fair by mining the classifier for discrimination patterns
2. **Parameter learning** algorithm for Naive Bayes classifier to **eliminate discrimination** patterns

Technique: Signomial Programming

$$\operatorname{argmax} P(C, X_1, X_2, \dots, X_m, Y_1, Y_2, \dots, Y_n)$$

*Max Likelihood
Naive Bayes*

s. t.

$$P(C|X_1, Y_1) - P(C|Y_1) \leq \delta$$

...

$$P(C|X_m, Y_1) - P(C|Y_1) \leq \delta$$

...

$$P(C|X_1, Y_n) - P(C|Y_n) \leq \delta$$

...

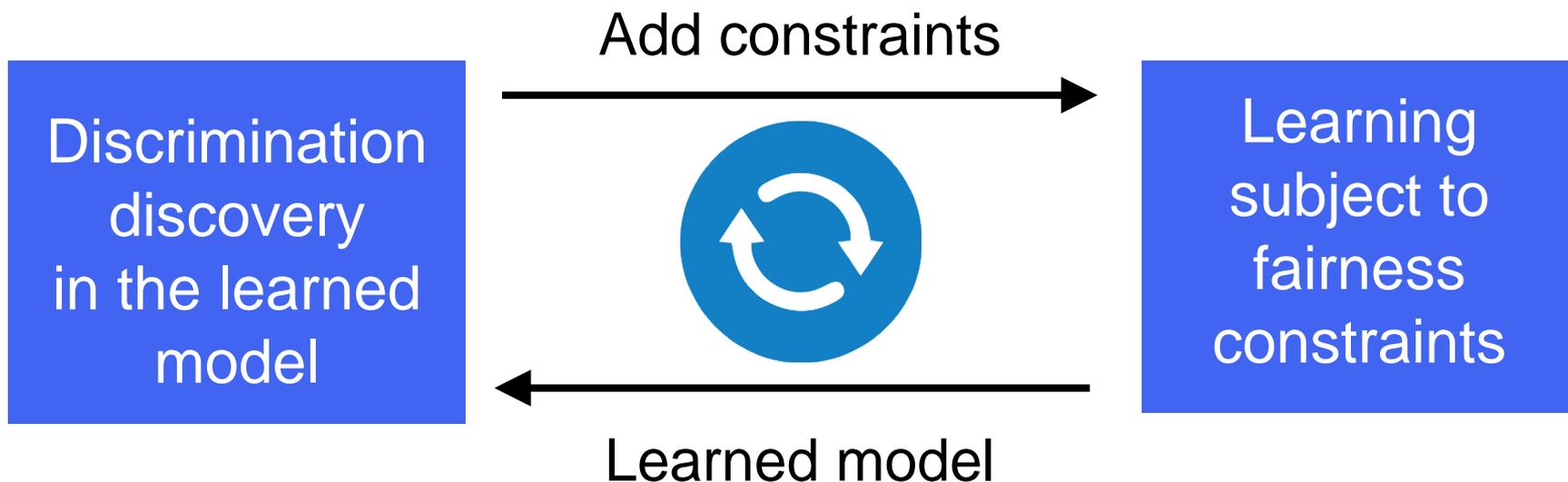
$$P(C|X_1, X_2, Y_1) - P(C|Y_1) \leq \delta$$

...

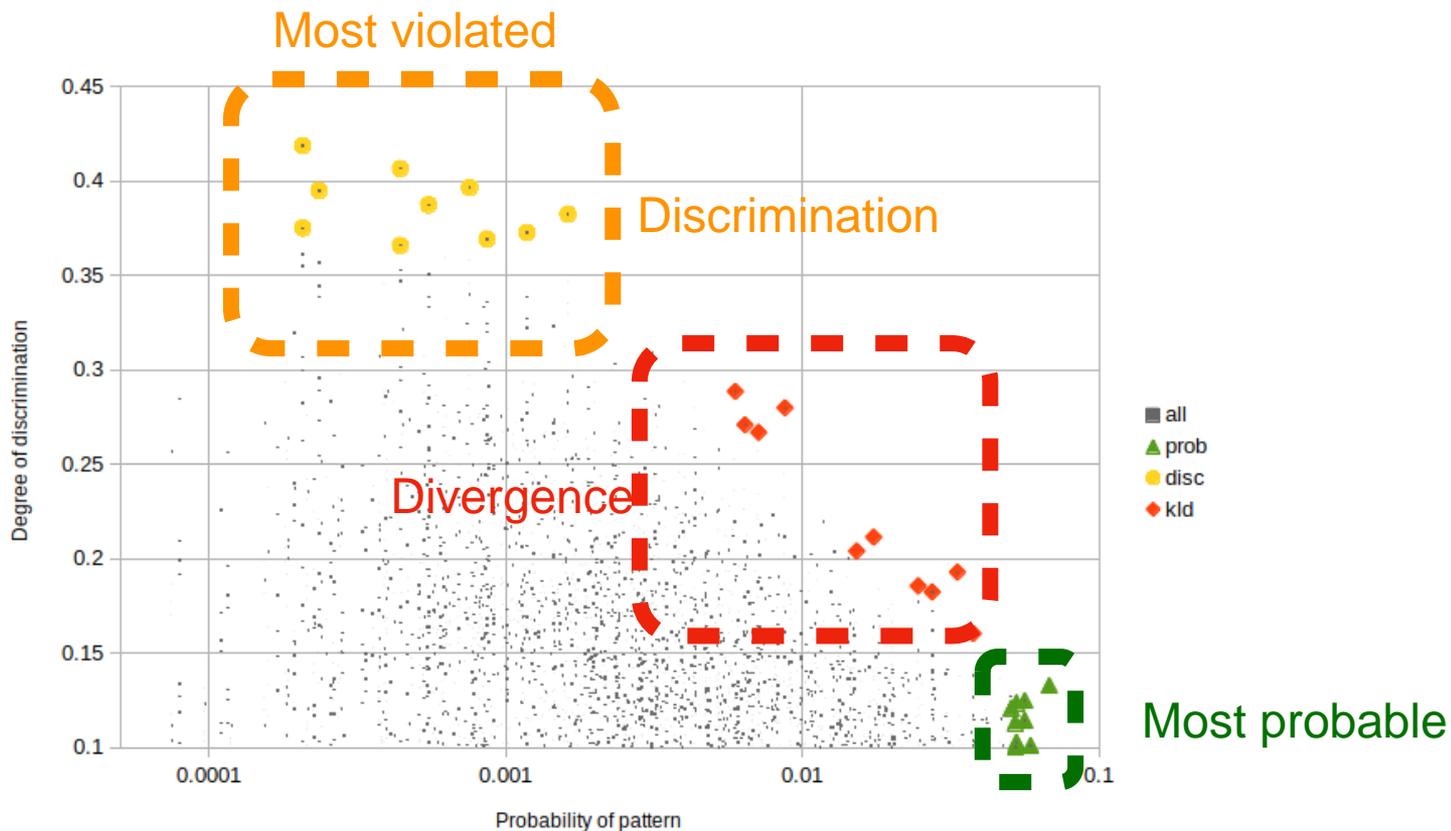
$$P(C|X_1, X_2, \dots, X_m, Y_1, Y_2, \dots, Y_n) - P(C|Y_1, Y_2, \dots, Y_n) \leq \delta$$

**δ -fair
constraints**

Cutting Plane Approach



Which constraints to add?



Quality of Learned Models?

Almost as good (likelihood) as
unconstrained unfair model

Dataset	Unconstrained	δ -Fair	Independent
COMPAS	-207,055	-207,395	-208,639
Adult	-226,375	-228,763	-232,180
German	-12,630	-12,635	-12,649

Higher accuracy than
other fairness approaches,
while recognizing discrimination
patterns involving missing data

dataset	Unconstrained	2NB	Repaired	δ -fair
COMPAS	0.880	0.875	0.878	0.879
Adult	0.811	0.759	0.325	0.827
German	0.690	0.679	0.688	0.696

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Current learning approaches

	Likelihood Optimization
Inference-Free	✗
Consistent for MCAR	✓
Consistent for MAR	✓
Consistent for MNAR	✗
Maximum Likelihood	✓

Current learning approaches

	Likelihood Optimization	Expectation Maximization
Inference-Free	✗	✗
Consistent for MCAR	✓	✓/✗
Consistent for MAR	✓	✓/✗
Consistent for MNAR	✗	✗
Maximum Likelihood	✓	✓/✗
Closed Form	n/a	✗
Passes over the data	n/a	?

Current learning approaches

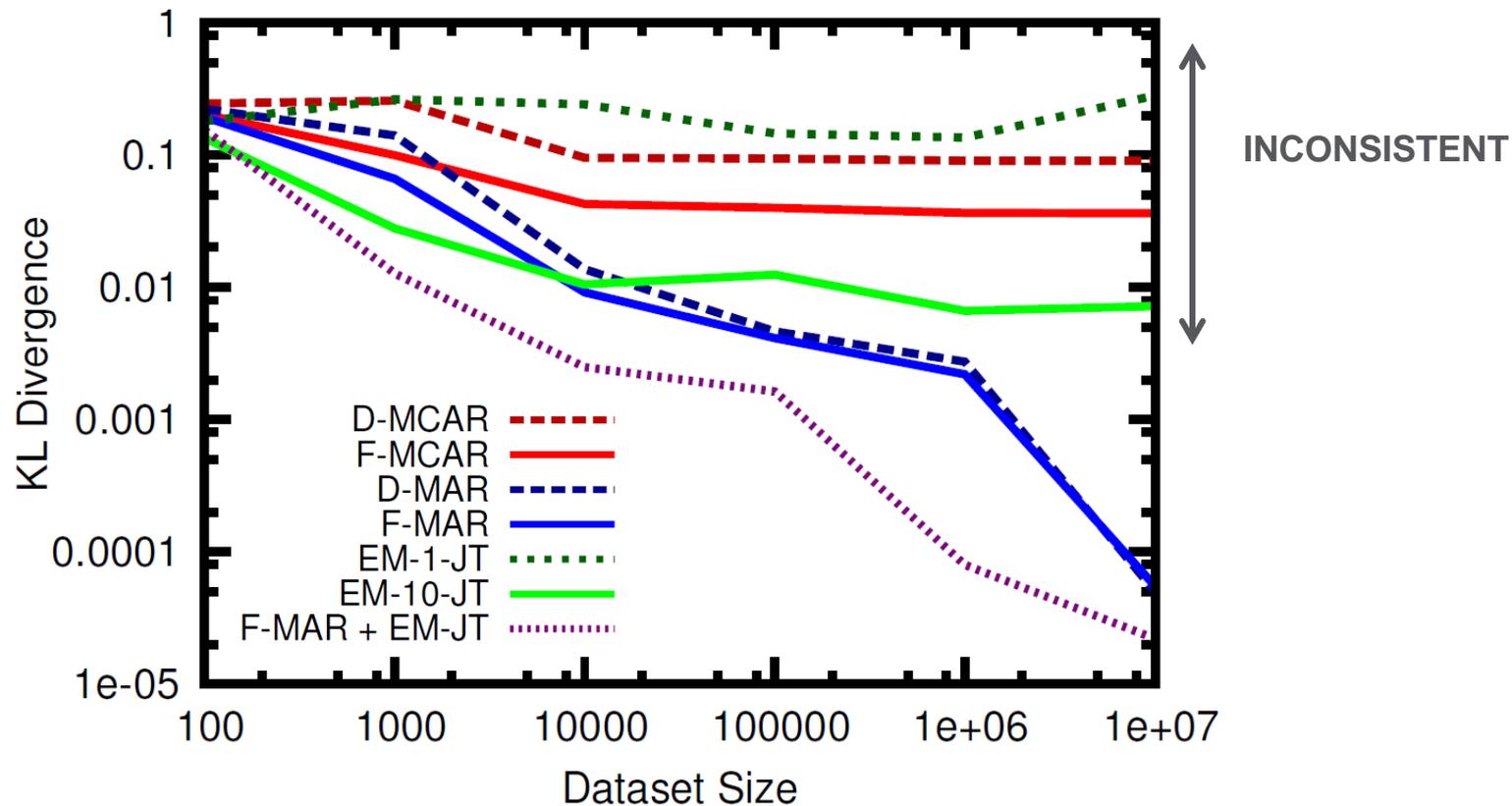
	Likelihood Optimization	Expectation Maximization
Inference-Free	✗	✗
Consistent for MCAR	✓	✓ / ✗
Consistent for MAR	✓	✓ / ✗
Consistent for MNAR	✗	✗
Maximum Likelihood	✓	✓ / ✗
Closed Form	n/a	✗
Passes over the data	n/a	?

Conventional wisdom: downsides are inevitable!

Deletion Algorithms for Missing Data Learning

	Likelihood Optimization	Expectation Maximization	Deletion [our work]
Inference-Free	✗	✗	✓
Consistent for MCAR	✓	✓/✗	✓
Consistent for MAR	✓	✓/✗	✓
Consistent for MNAR	✗	✗	✓/✗
Maximum Likelihood	✓	✓/✗	✗
Closed Form	n/a	✗	✓
Passes over the data	n/a	?	1

Benefits bear out in practice!



Conclusions

- Missing data is a central problem in machine learning
- We can do better than classical tools from statistics
- By doing reasoning about the data distribution!
 - In a generative model that conforms to the classifier
 - Expectations using tractable circuits as new ML models
 - Using causal missingness mechanisms
- Important in addressing problems of robustness, fairness, and explainability

References and Acknowledgements

- Pasha Khosravi, Yitao Liang, YooJung Choi and Guy Van den Broeck. What to Expect of Classifiers? Reasoning about Logistic Regression with Missing Features, *In IJCAI*, 2019.
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Thank You
