Discrete Optimization for some AI problems Lecture 1: IP models to learn rules

Sanjeeb Dash IBM Research Travel supported by ONR

12th Cargese-Porquerolles workshop, Sep 4-8, 2023

IP models to learn rules

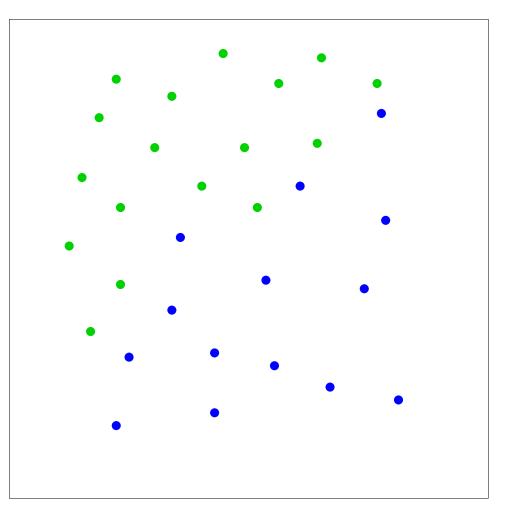
- ► ML models for Binary Classification
- Boolean (decision) rules
- ► Interpretable Machine Learning
- ► Integer Programming Formulation
- Column Generation Technique
- Cardinality constrained Multilinear set
 Polyhedral results
- Variants/applications of basic model
 Fairness/Model diagnostics
- ► Logistic Regression
- Knowledge graph completion

Supervised Binary Classification

- Features: X_1, \ldots, X_m
- Data: $\{(x_i; y_i) : i \in 1, 2, \dots, n\}$ where $x_i \in \mathbb{R}^m$.
- Label $y_i \in \{0, 1\}$
- Feature X_j is either numeric or categorical.
- Goal: Separate 0s from 1s or find function f such that $y_i \approx f(x_i)$.

Supervised Binary Classification

Blood	Choles-	Heart
Pressure	-terol	Disease
X_1	X_2	Y
100	75	0
120	175	1
80	250	1
110	150	0
90	190	1
•	•	

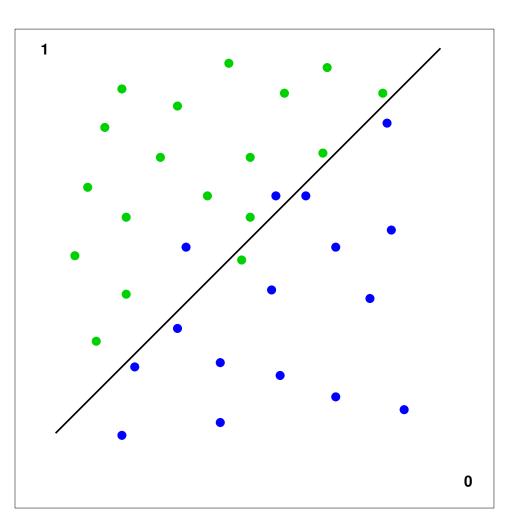


- Linear support vector machines
- Decision Trees
- Neural networks

Linear support vector machines

Find hyperplane that separates points labelled 1 from points labelled 0

Few nonzero coefficients \rightarrow more interpretable



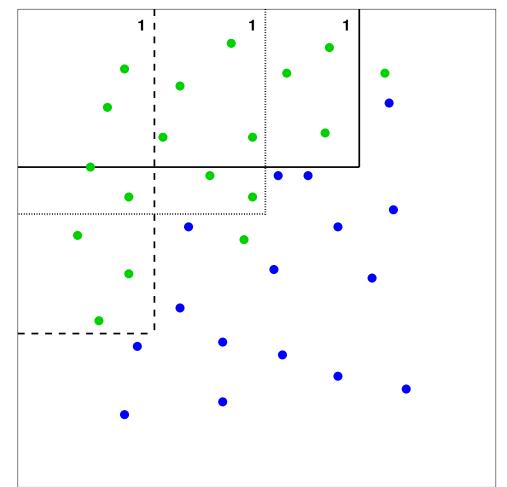
Vapnik, Chervonenkis '63 - SVM
Boser, Guyon, Vapnik '92 - Kernel "trick"

Learn boolean rule sets for binary classification

 $(X_1 \le 150 \text{ AND } X_2 \ge 170) \text{ OR}$ $(X_1 \le 100 \text{ AND } X_2 \ge 130) \text{ OR}$ $(X_1 \le 80 \text{ AND } X_2 \ge 70)$

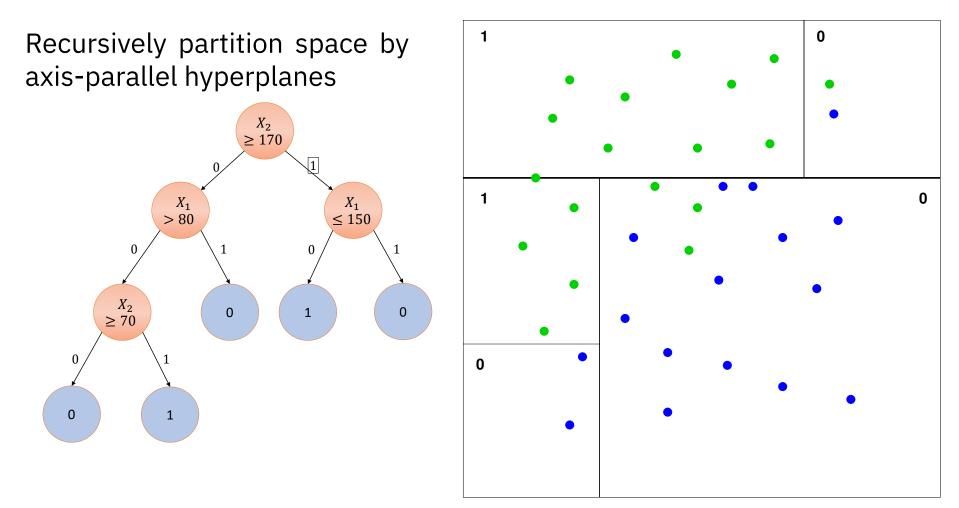
Boolean rule set \equiv Boolean formulae in Disjunctive normal form

A data point is classified as 1 if it satisfies at least one rule



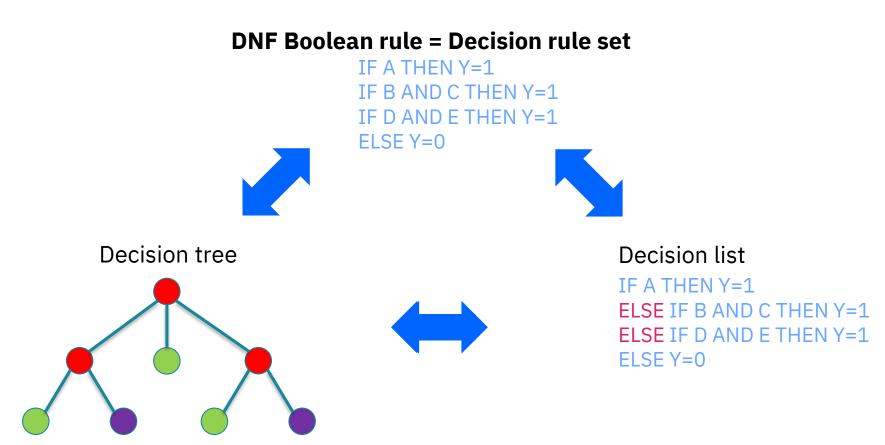
Dawes '79
 Cohen '95 - RIPPER
 Hongyu, Rudin, Seltzer '17 - Scalable Bayesian Rule Sets
 Boros, Hammer, Ibaraki, Kogan, Mayoraz, Muchnik '00 - L.A.D.

Decision trees



- Hunt, Marin, Stone '66
- ⊳ Quinlan '86 ID3, C4.5
- > Breiman, Friedman, Olshen, Stone '84 CART
- Bertsimas, Dunn '17 IP formulations for decision trees

Related classifiers



Rivest '87: Learning decision lists

Transforming one classifier to another one can lead to exponential blowup in "size"/"complexity".

Interpretable Machine Learning

Explainable AI (XAI), Interpretable AI/ML, or Transparent AI refer to models that can be easily understood by humans unlike "black box" models

Interpretable models Sparse linear models (e.g., SVM) Decision trees Decision rule sets Decision lists Noninterpretable models Dense linear models Neural Networks Random Forests

Interpretable models can be examined for:

Safety/Reliability, Fairness/Lack of Bias, Causality, Robustness

Doshi-Velez, Kim '17: "Towards a rigorous science of interpretable ML" Schmidt et. al. '17, Muggleton et. al. '18: Higher inspection time \rightarrow lower interpretability

Prior work on Boolean rule sets

- ► Using heuristics and/or multiple criteria
- Covering e.g. RIPPER (Cohen '95)
- Bottom-up combining
- Associative classification

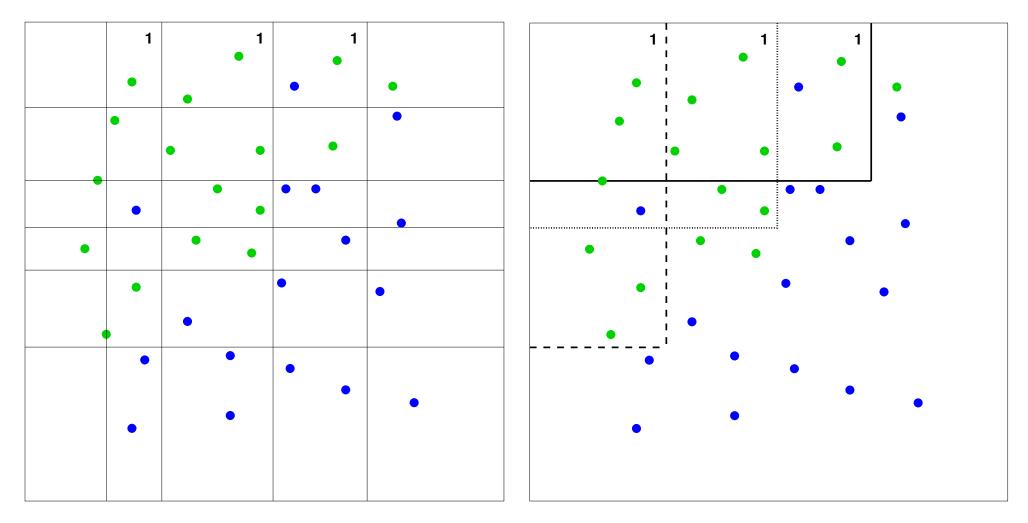
Interpretable Boolean rule sets: Few rules/few conditions per rule

- Accuracy-simplicity optimization
- Interpretable decision sets (IDS): Lakkaraju, Bach, Leskovec '16
- Bayesian rule sets (BRS): Wang, Rudin, Doshi-Velez, Liu, Klampfl, MacNeille '17
- Optimized ORs of ANDs: Wang Rudin '15
- Disjunctions of conjunctions: Hauser et. al. '10

These methods use rule mining to generate candidate clauses

- IP formulation with fixed # clauses, solved approximately using LP: Su, Wei, Varshney, Malioutov '16

Learn boolean rule sets for binary classification



- 1) Choose rectangle boundaries from fixed gridlines.
- 2) Penalty for misclassication 1 or # of times misclassified?

Binarization

	77			X_1	X_1	X_2	X_2	Y
X_1	X_2	Y		< 80	< 100	< 150	< 200	
100	75	0			1	<u> </u>	<u> </u>	
120	175	1		U	上	⊥	Ŧ	
				0	0	0	1	1
80	250	1		1	1		\cap	1
110	150	0	\rightarrow	<u></u>	<u>т</u>		0	
90	190	1		1	1	1	1	0
90	T90	⊥		0	1	0	1	1
:	•	:		0	-		-	
		<u> </u>		•				

Goal: Learn boolean functions (assume X_i is binary) in DNF form as classifiers

 $(X_1 \wedge X_3 \wedge X_4) \lor (X_2 \wedge X_5)$

Notation

Inputs to model

 $\overline{x_i \in \mathbb{R}^m, y_i \in \{0, 1\}}$ - data point *i* and it's label *C* - upper bound on complexity of chosen rule set

Model information

 \mathcal{K} - set of all possible rules $a_{ik} \in \{0, 1\}$ - $a_{ik} = 1$ iff data point *i* satisfies rule *k*. c_k - 'complexity' of rule k = 1 + number of conditions in rule

Variables

 $w_k \in \{0,1\}$ - binary variable which is 1 iff rule k is selected $\xi_i \ge 0$ - variable which is 1 iff chosen rules do not 'cover' data point i

- All features are assumed to be binary at this point
- $a_{ik} = x_{ik}$ if k is index of a rule containing a single binary feature
- $\sum_{i \in k} a_{ik} w_k \ge 1$ iff $\lor_{k:w_k=1}$ rule $_k(x_i) = 1$
- Here we assume rule_k is a function from $\mathbb{R}^m \to \{0, 1\}$.

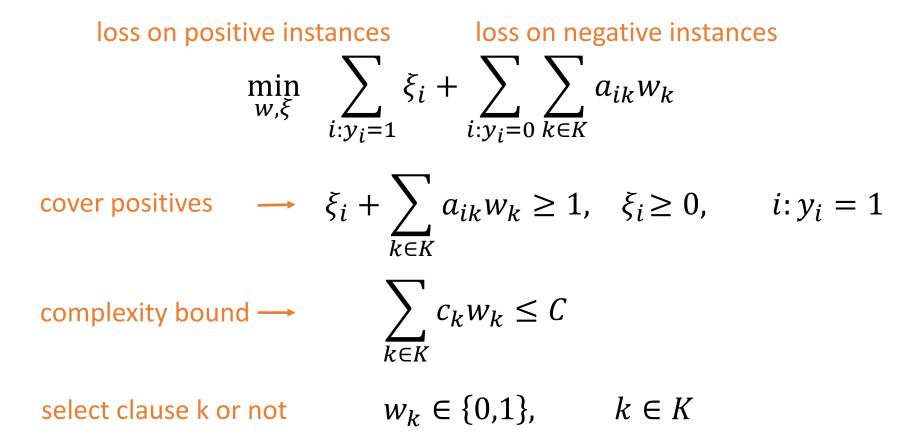
IP to select "best" subset of rules

Minimize 0-1 loss subject to complexity bound: loss on positive instances loss on negative instances $\min_{w,\xi} \sum_{i:v_i=1} \xi_i + \sum_{i:v_i=0} \xi_i$ cover positives $\longrightarrow \xi_i + \sum a_{ik} w_k \ge 1, \quad \xi_i \ge 0, \qquad i: y_i = 1$ cover negatives $\longrightarrow \xi_i \ge a_{ik} w_k, k \in K, \xi_i \ge 0, i: y_i = 0$ complexity bound $\longrightarrow \sum c_k w_k \leq C$ select clause k or not $w_k \in \{0,1\},\$ $k \in K$

MIP has exponentially many inequalities/variables and is hard to solve

"Master" IP with Hamming Loss objective

Minimize Hamming loss subject to complexity bound:

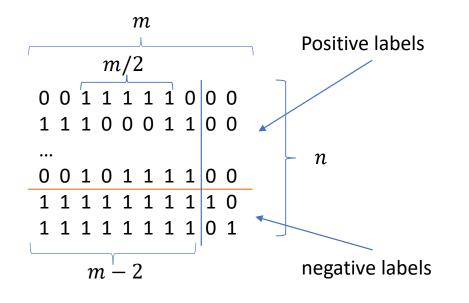


Dash, Günlük, Wei (NIPS 2018): Search over exponential list of clauses using column generation.

Gap between 0-1 loss and Hamming Loss

Thm (Lawless, Dash, Günlük, Wei '22) The 0-1 loss of the Hamming IP solution can be 'arbitrarily' worse than that of the of 0-1 IP solution.

(No constant ratio between the two losses)



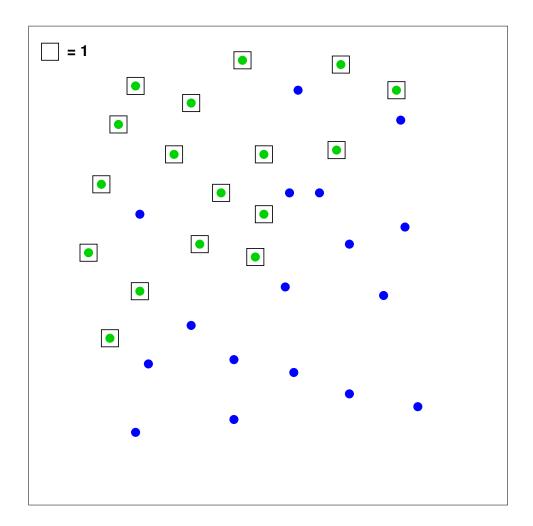
K = set of all rules that are conjunctions of m/2 features

Optimal rule set for 0-1 loss = disjunction of all rules which has 0-1 loss of 2/n

Optimal rule set for Hamming loss = empty disjunction which has 0-1 loss of (n-2)/n

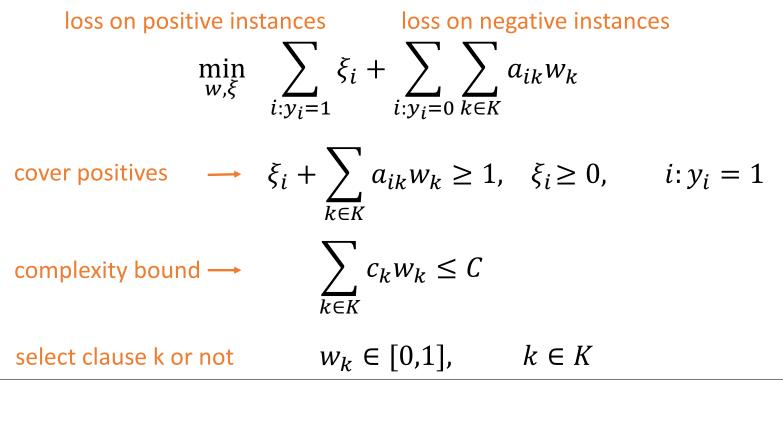
$$n = \binom{m-2}{m/2} + 2$$

Overfitting



"Master" LP with Hamming Loss objective

Minimize Hamming loss subject to complexity bound:



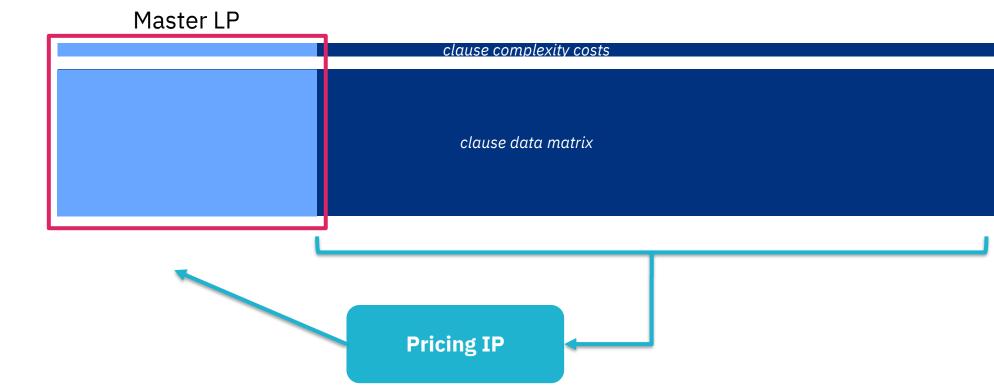
reduced cost of rule k

$$\sum_{i:y_i=0} a_{ik} - \sum_{i:y_i=1} \mu_i a_{ik} + \lambda c_k$$

Related work

- "Boosting" rule-based classifiers
- Demirez, Bennett, Shawe-Taylor '02: LP-Boost
- Goldberg, Eckstein '10: L₀-RBoost
- Eckstein, Kagawa, Goldberg '17, '19: Rule-enhanced penalized regression

Column generation subproblem



- ► Almost the same as the Maximum monomial agreement problem
- Kearns, Shapire, Sellie '94
- Goldberg, Shan '07
- Eckstein, Goldberg '10, '12: branch-and-bound method

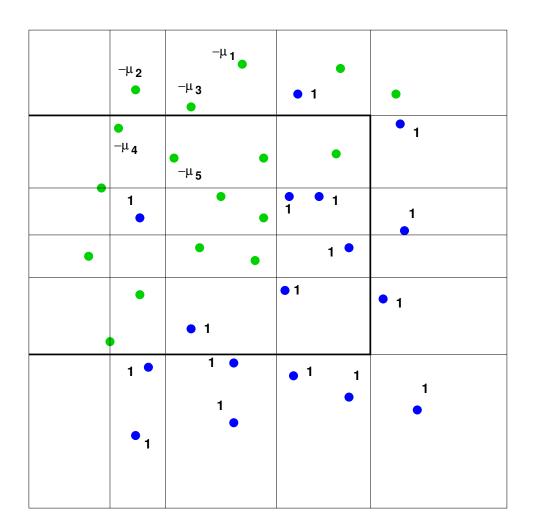
Column generation subproblem..

$\overline{\mathbf{v}}$	V			$\overline{X_1}$	X_1	X_2	X_2	Y
X_1	X_2	Υ Ω		< 80	≤ 100	< 150	< 200	
100	75	0				1		
120	175	1		0	- -		エ 1	
80	250	1		0	0		T O	
110	150		\rightarrow	1	1	0	0	1
		1	7	1	1	1	1	0
90	190	-		0	1	0	1	1
•	:	:		:	:	:	:	
				•	•	•	•	•

 \downarrow

X_1	X_1	X_2	X_2	$X_1 \le 80 \land$	$X_1 \le 100 \land$
≤ 80	≤ 100	≤ 150	≤ 200	$X_2 \le 150$	$X_2 \le 200$
0	1	1	1	0	1
0	0	0	1	0	0
1	1	0	0	0	0
1	1	1	1	1	1
0	1	0	1	0	1
	•		•	:	•

Pricing Problem



Pricing Problem

reduced cost of clause incl. complexity penalty

$$\min_{z,a} \sum_{i:y_i=0}^{d} a_i - \sum_{i:y_i=1}^{d} \mu_i a_i + \lambda \left(1 + \sum_{j=1}^{d} z_j\right)$$

clause acts as conjunction of features

$$a_i = \prod_{j:x_{ij}=0} (1 - z_j) \qquad \forall i$$

at most U features

$$1 \leq \sum_{j=1}^{d} z_j \leq U, \qquad z_j \in \{0,1\}, j = 1, \dots, d$$

whether to select feature j

Pricing IP

reduced cost of clause incl. complexity penalty

$$\begin{split} \min_{z,a} & \sum_{i:y_i=0} a_i - \sum_{i:y_i=1} \mu_i a_i + \lambda \left(1 + \sum_{j=1}^d z_j \right) \\ \text{clause} & a_i + z_j \leq 1, \qquad i: y_i = 1, \qquad j: x_{ij} = 0 \\ \text{acts as} & \text{conjunction} & a_i + \sum_{j:x_{ij}=0} z_j \geq 1, \qquad a_i \geq 0, \qquad i: y_i = 0 \\ \text{at most U} & 1 \leq \sum_{j=1}^d z_j \leq U, \qquad z_j \in \{0,1\}, j = 1, \dots, d \end{split}$$

at

whether to select feature j

23

Solving the pricing IP

IP

 \triangleright Pricing IP is hard to solve, as it has a poor LP relaxation bound, e.g., for the ILPD data set with U=5:

# Binary Features	# data points	Opt. Obj Value	LP Bound
155	520	-9 (after 10 min)	-98

Limit clause size, time limit

Sample data points for large data sets

Clause generation heuristic

For k = 1, 2, ...
1) Extend previously generated k - 1-literal clauses to k-literals, choose the best
2) Use bounds to eliminate some of the generated clauses.

Numerical Evaluation

- ► Main competitors
- Bayesian Rule Sets (BRS): Wang et al. '17]
- Alternating Minimization: (AM) Su, Wei, Varshney, Malioutov '16
- Block Coordinate Descent: (BCD) Su, Wei, Varshney, Malioutov '16
- IDS: Lakkaraju et al. '17 [code was too slow]

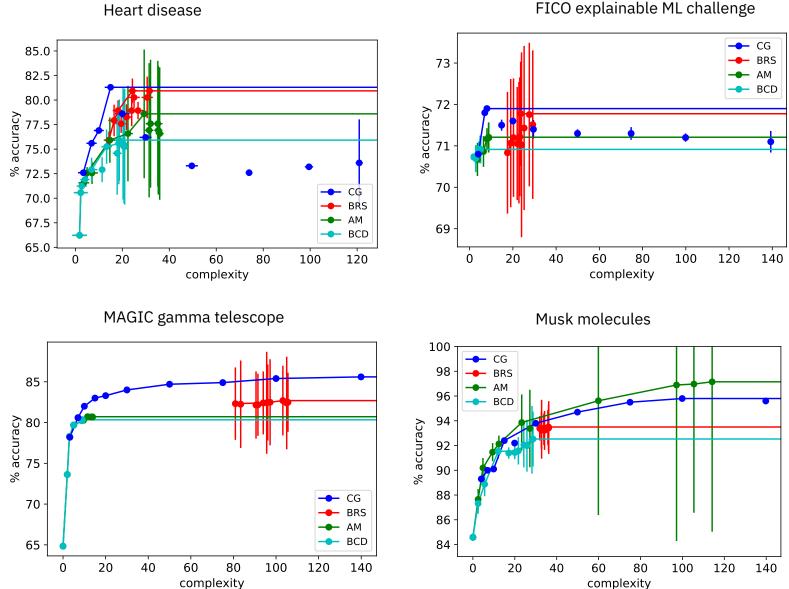
Complexity: # clauses + total # conditions

> Accuracy: 10-fold Cross Validation

▷ Binarization

- Sample decile thresholds for numerical features
- \triangleright Time limits for our code: \leq 5 min overall
- Master LP solves fast with CPLEX Barrier
- After column generation, we fix columns and solve IP with CPLEX

Complexity versus Accuracy



FICO explainable ML challenge

Comparison with other methods

Complexity = # clauses + total # conditions

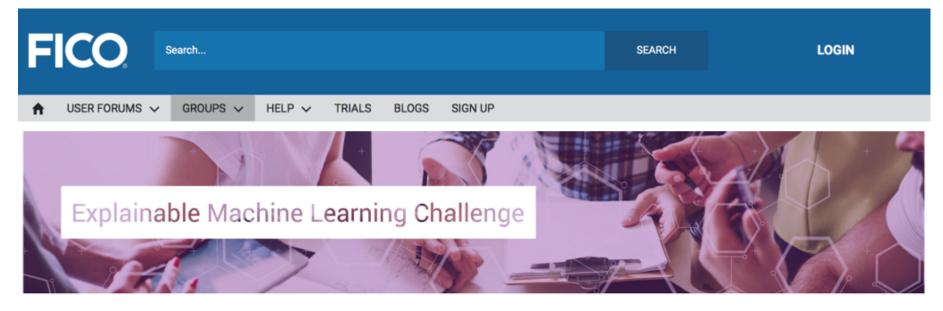
dataset	CG	BRS	AM	BCD	RIPPER	CART	RF
adult	83.5	81.7	83.0	82.4	83.6	83.1	84.7
bank	90.0	87.4	90.0	89.7	89.9	89.1	88.7
gas	98.0	92.2	97.6	97.0	99.0	95.4	99.7
magic	85.3	82.5	80.7	80.3	84.5	82.8	86.6
mushroom	100.0	99.7	99.9	99.9	100.0	96.2	99.9
musk	95.6	93.3	96.9	92.1	95.9	90.1	86.2
FICO	71.7	71.2	71.2	70.9	71.8	70.9	73.1

accuracy

complexity

size

adult	88.0	39.1	15.0	13.2	133.3	95.9	29,304
bank	9.9	13.2	6.8	2.1	56.4	3.0	37,609
gas	123.9	22.4	62.4	27.8	145.3	104.7	12,518
magic	93.0	97.2	11.5	9.0	177.3	125.5	17,117
mushroom	17.8	17.5	15.4	14.6	17.0	9.3	8,124
musk	123.9	33.9	101.3	24.4	143.4	17.0	5,937
FICO	13.3	23.2	8.7	4.8	88.1	155.0	9,871



Submissions will be accepted from April 18- August 31, 2018.

OVERVIEW DATASET DETAILS CHALLENGE RULES EXAMPLE EXPLANATIONS CHALLENGE FORUM ENTER YOUR SUBMISSION FAQ

Introduction

Complex machine learning models have recently achieved great predictive successes for many applications. While these models excel at capturing complex, non-linear relationships between variables, it is often the case that neither the trained model nor its individual predictions are readily explainable. In settings where regulators or consumers demand explanations, understanding the structure and predictions of these models will pave the way for their wide adoption in practice. Explainability will also help data scientists understand their datasets and the models' predictions, uncover and correct for biases, and ultimately create better models.

Motivation: Why the financial services industry?

Advanced machine learning methods are quickly finding applications throughout the financial services industry, transforming the handling of large and complex datasets, but there is a huge gap between our ability to construct effective predictive models and our ability to understand and control these models. In order to drive forward research in this area, FICO and a number of academic partners have collaborated to design a challenge based on a real financial dataset. The challenge is not necessarily focused on accuracy, rather, it is focused on evaluating the explanations generated by the participants.

Every year, credit scoring methodologies provide millions of scores that evaluate the risk in billions of dollars in loans; in fact, the FICO Score is used in more

FICO 2018 XML Challenge

Predict repayment risk (good/bad) from credit history: roughly 10,000 data points, 23 numerical features, 0/1 labels

► Winning entry:

 $\begin{array}{l} (\text{NumSatTrades} \geq 23 \hspace{0.1cm} \text{AND} \hspace{0.1cm} \text{ExtRiskEstimate} \geq 71 \hspace{0.1cm} \text{AND} \hspace{0.1cm} \text{NetFracRevolBurden} \leq 64) \\ \\ \text{OR} \\ (\text{NumSatTrades} \leq 22 \hspace{0.1cm} \text{AND} \hspace{0.1cm} \text{ExtRiskEstimate} \geq 76 \hspace{0.1cm} \text{AND} \hspace{0.1cm} \text{NetFracRevolBurden} \leq 79) \end{array}$

Pricing Problem

reduced cost of clause incl. complexity penalty

$$\min_{z,a} \sum_{i:y_i=0}^{d} a_i - \sum_{i:y_i=1}^{d} \mu_i a_i + \lambda \left(1 + \sum_{j=1}^{d} z_j\right)$$

clause acts as conjunction of features

$$a_i = \prod_{j:x_{ij}=0} (1 - z_j) \qquad \forall i$$

at most U features

$$1 \leq \sum_{j=1}^{d} z_j \leq U, \qquad z_j \in \{0,1\}, j = 1, \dots, d$$

whether to select feature j

Multilinear optimization

Let S_1, \ldots, S_m be subsets of $\{1, \ldots, n\}$. The pricing problem is \equiv

$$\begin{array}{ll} \min & \sum_{i=1}^{m} c_i \delta_i + \sum_{i=1}^{n} f_i z_i \\ \text{s.t.} & \delta_i = \prod_{j \in S_i} z_j, \quad i = 1, \dots, m \\ & l \leq \sum_{j=1}^{n} z_j \leq u, \ z_j \in \{0, 1\}, \ \delta_i \in \{0, 1\} \end{array}$$

An integer linear programming formulation of this problem is given by the "standard linearization inequalities":

$$0 \le \delta_i \le z_j \le 1$$
$$\delta_i \ge \sum_{j \in S_i} z_j - (|S_i| - 1)$$

Multilinear sets

The **multilinear set**:

$$X = \{(z, \delta) \in \{0, 1\}^n \times \{0, 1\}^m : \delta_i = \prod_{j \in S_i} z_j, \quad i = 1, \dots, m\}$$

Del Pia, Khajavirad '16, '18, Del Pia, Khajavirad, Sahinidis '18 Crama, Rodriguez-Heck '17

The cardinality constrained multilinear set:

$$X^{l,u} = \{(z,\delta) \in X : \ l \ \le \sum_{j=1}^n z_j \le \ u\}$$

Mehrotra '97, Fischer, Fischer, McCormick '18

Pricing problem \equiv optimizing a linear function over $X^{l,u} \equiv$ optimizing a linear function over conv $(X^{l,u})$.

Binary polynomial optimization

Fortet '60: Binary polynomial optimization \equiv binary MIP

- Unconstrained binary polynomial optimization \equiv optimizing a linear function over the multilinear set X

Let $\beta, \gamma_i \in \mathbb{R}$, $\alpha_{ij} \in \mathbb{Z}_+$, $S_i \subseteq \{1, \ldots, n\}$

$$f(x) = \beta + \sum_{i=1}^m \gamma_i \prod_{j \in S_i} x_j^{\alpha_{ij}} =$$

$$\beta + \sum_{i=1}^{m} \gamma_i \prod_{j \in S_i} x_j \text{ if } x \in 0, 1^n.$$

Convex hull of $X^{l,u}$

$$X = \{(z, \delta) \in \{0, 1\}^n \times \{0, 1\}^m : \delta_i = \prod_{j \in S_i} z_j, \quad i = 1, \dots, m\}$$
$$X^{l,u} = \{(z, \delta) \in X : l \leq \sum_{j=1}^n z_j \leq u\}$$

> Fischer, Fischer, McCormick '18: Polyhedral characterization of $X^{l,u}$ when l = 0 and nested S_i

Nested S_i : $S_1 \subset S_2 \subset \cdots \subset S_m \subset \{1, \ldots, n\}$

▷ Dash, Günlük, Chen '21: Polyhedral characterization of $X^{l,u}$ for any $0 \le l < u \le n$ for nested S_i .

▷ Dash, Günlük, Chen '23: Polyhedral characterization of $X^{l,u}$ for any $0 \le l < u \le n$ when m = 2.

Notation

I - index set of data points $P \subseteq I$ - set of data points with label 1 $N \subseteq I$ - set of data points with label 0 neg_k = number of data points in N to which a rule assigns value 1

Assume P and N are partitioned into P_1, P_2 and N_1, N_2 . Interpretation is (P_1, N_1) correspond to one group, (P_2, N_2) to another. neg_k^l = number of data points in N_l to which a rule assigns value 1

Fairness

Achieve classification parity across multiple groups Assume we wish to add constraints to 0-1 loss MIP

Equality of opportunity Difference in rate of loss for positive instances of group 1 and 2 is bounded

$$\frac{1}{|P_1|} \sum_{i \in P_1} \xi_i - \frac{1}{|P_2|} \sum_{i \in P_2} \xi_i \le \varepsilon$$
$$\frac{1}{|P_2|} \sum_{i \in P_2} \xi_i - \frac{1}{|P_2|} \sum_{i \in P_1} \xi_i \le \varepsilon$$

Equalized odds Former condition + Difference in rate of loss for negative Instances of group 1 and 2 is bounded

$$\frac{1}{|N_1|} \sum_{i \in N_1} \xi_i - \frac{1}{|N_2|} \sum_{i \in N_2} \xi_i \le \varepsilon$$
$$\frac{1}{|N_2|} \sum_{i \in N_2} \xi_i - \frac{1}{|N_1|} \sum_{i \in N_1} \xi_i \le \varepsilon$$

Add more constraints to ensure ξ variables are correctly constrained

Fairness

Achieve classification parity across multiple groups Lawless, Dash, Gunluk, Wei '21: add constraints to Hamming loss MIP

Equality of opportunity Difference in rate of loss for positive instances of group 1 and 2 is bounded

Equalized odds Former condition + Difference in rate of loss for negative Instances of group 1 and 2 is bounded

$$\frac{1}{|P_1|} \sum_{i \in P_1} \xi_i - \frac{1}{|P_2|} \sum_{i \in P_2} \xi_i \le \varepsilon \qquad \qquad \frac{1}{|N_1|} \sum_k \operatorname{neg}_k^1 w_k - \frac{1}{|N_2|} \sum_k \operatorname{neg}_k^2 w_k \le \varepsilon$$
$$\frac{1}{|P_2|} \sum_{i \in P_2} \xi_i - \frac{1}{|P_2|} \sum_{i \in P_1} \xi_i \le \varepsilon \qquad \qquad \frac{1}{|N_2|} \sum_k \operatorname{neg}_k^2 w_k - \frac{1}{|N_1|} \sum_k \operatorname{neg}_k^1 w_k \le \varepsilon$$

Add more constraints to ensure ξ variables are correctly constrained

Heavy sets

Let \mathcal{R} be a set of *simple* regions $S \subset \mathbb{R}^N$ Let $|S| = |\{i \mid x_i \in S\}|$, and c_i be weight of datapoint x_i Malioutov, Dash, Wei '23 - sparse AND-rule regions

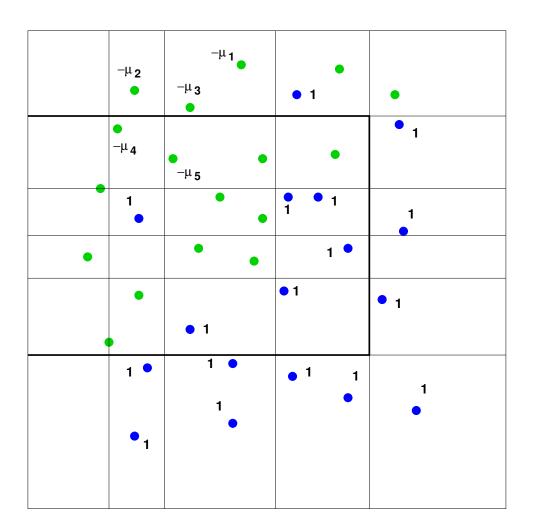
(1) Find heaviest-weight simple region from \mathcal{R} subject to region-size constraints

$$S^* = \arg \max_{S \in \mathcal{R}} \sum_{x_i \in S} c_i$$
, such that $|S| \le K$,

(2) Max average-of-weights with upper and lower bounds on region size:

$$S^* = \arg \max_{S \in \mathcal{R}} \frac{1}{|S|} \sum_{x_i \in S} c_i , \quad K_{\min} \le |S| \le K_{\max}.$$

Simple regions



Model changes (Let m_A, m_B be two models) $c_i = |m_B(x_i) - m_A(x_i)|^2$ High-error regions $c_i = |m_A(x_i) - y_i|^p$, p = 1, 2 for regression High-variance regions. $c_i = m_A(x_i)^2$, using the max-avg formulation

Heavy sets max-sum IP

Let $I = \{1, \ldots, n\}$ be index set of datapoints $a \in \{0, 1\}^I$ is a vector of binary variables $a_i = 1$ iff datapoint *i* is in chosen region J - index set of region boundaries

$$\begin{array}{ll} \max \sum_{i \in I} c_i a_i \\ \text{s.t. } a_i + z_j \leq 1, & \forall i \in I, j \in J : x_{ij} = 0 \\ a_i + \sum_{j:x_{ij} = 0} z_j \geq 1 & \forall i \in I \\ 1 \leq \sum_{j \in J} z_j & & \forall i \in I \\ a_i \in \{0, 1\} & & \forall i \in I \\ z_j \in \{0, 1\} & & \forall j \in J \end{array}$$

Heavy sets max-average IP

 β is average wt, w_{\max} maximum wt, $\beta_i=\beta a_i$

 $\max \beta$ $\beta_i \leq \beta$ $\forall i$ $\forall i$ $\beta_i \leq w_{\max}a_i$ $\beta + w_{\max}a_i \le \beta_i + w_{\max}$ $\forall i$ $\beta_i \ge 0$ $\forall i$ $\beta \ge 0$ $\sum w_i a_i = \sum \beta_i$ $\overline{i \in I}$ $\overline{i \in I}$ $\sum a_i \ge \sigma |I|$ $i \in I$ max-sum Constraints

41

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