Project Proposals

- Due next Monday (13th Feb) 11.59pm ET
- 2 page proposal (more details on "Course Logistics" document on canvas) + References

- Today by 5pm ET, we will post:
 - Project topics and some concrete problems
 - Sample proposals and final reports from past iterations
 - LaTeX and Word templates which you will use to write the proposal

Office Hours and Paper Presentations

- Office hours switch this week
 - Suraj and Jiaqi today
 - Hima on Thursday
- Students signed up for presentations next week should see us in office hours this week
 - Full slide deck (ideally!)
 - An overview of what you plan to present

Rule Based Approaches

Agenda

Paper 1: Interpretable Rule Lists (Letham et. al.)

 Paper 2: Interpretable Rule Sets (Lakkaraju et. al.)

Discussion



Interpretable Classifiers Using Rules and Bayesian Analysis

Benjamin Letham, Cynthia Rudin, Tyler McCormick, David Madigan; 2015

Contributions

- Introducing a generative model called Bayesian Rule Lists (BRL)
 - Goal is to output a decision list (if then else-if)
- Novel prior structure to encourage sparsity
- Predictive accuracy on par with top algorithms

Decision List: Example

```
if male and adult then survival probability 21% (19%–23%) else if 3rd class then survival probability 44% (38%–51%) else if 1st class then survival probability 96% (92%–99%) else survival probability 88% (82%–94%)
```

This is "an" accurate and interpretable decision list – possibly one of many such lists

Introduction: BRL

- Produces a posterior distribution over permutations of if.. then.. Else-if.. rules from a large set of pre-mined rules
- Decision lists with high posterior probability tend to be both accurate and interpretable
 - Prior favors concise lists with small number of rules and fewer terms in left hand side

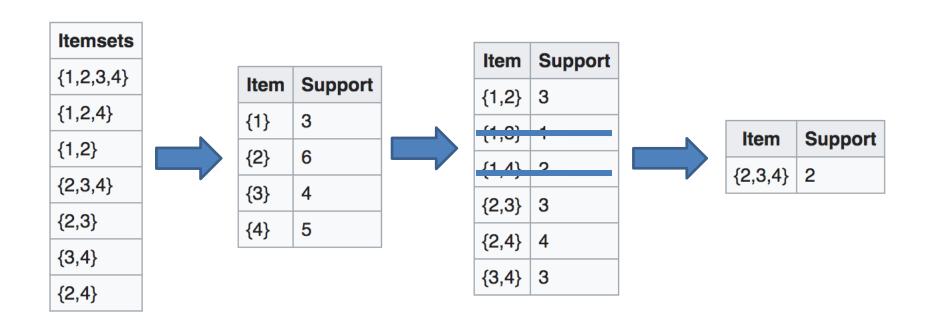
Introduction: BRL

- New type of balance between accuracy, interpretability, and computation
- What about using other similar models?
 - Decision trees (CART)
 - They employ greedy construction methods
 - Not particularly computationally demanding but affects quality of solution – both accuracy and interpretability

Pre-mined Rules

- A major source of practical feasibility: premined rules
 - Reduces model space
 - Complexity of problem depends on number of pre-mined rules
- As long as pre-mined set is expressive, accurate decision list can be found + smaller model space means better generalization (Vapnik, 1995)

Pre-mined Rules: Intuition



Minimum Support = 3

nis is Apriori algorithm. FP-growth is a single pass algorithm (more efficier

Preliminaries: Notation

■ Training dat $\{(x_i, y_i)\}_{i=1}^n$ $x_i \in \mathbb{R}^d$ $y_i \in \{1, \dots, L\}$

$$\mathbf{x} = (x_1, \dots, x_n) \quad \mathbf{y} = (y_1, \dots, y_n)$$

Two labels: stroke or no stroke

Bayesian Decision Lists

```
if a_1 then y \sim \text{Multinomial}(\boldsymbol{\theta}_1), \boldsymbol{\theta}_1 \sim \text{Dirichlet}(\boldsymbol{\alpha} + \mathbf{N}_1)
else if a_2 then y \sim \text{Multinomial}(\boldsymbol{\theta}_2), \boldsymbol{\theta}_2 \sim \text{Dirichlet}(\boldsymbol{\alpha} + \mathbf{N}_2)
:
else if a_m then y \sim \text{Multinomial}(\boldsymbol{\theta}_m), \boldsymbol{\theta}_m \sim \text{Dirichlet}(\boldsymbol{\alpha} + \mathbf{N}_m)
else y \sim \text{Multinomial}(\boldsymbol{\theta}_0), \boldsymbol{\theta}_0 \sim \text{Dirichlet}(\boldsymbol{\alpha} + \mathbf{N}_0).
```

where
$$N_j = (N_{j,1}, ..., N_{j,L})$$

Preliminaries: Multinomial

Sampling from a multinomial:

Throw a dice 20 times:

```
>>> np.random.multinomial(20, [1/6.]*6, size=1)
array([[4, 1, 7, 5, 2, 1]])
```

Parameters are probability values

Preliminaries: Dirichlet

- Dirichlet: sampling over a probability simplex
 - E.g., (0.6, 0.4) is a sample from a Dirichlet distribution;

- K-dimensional Dirichlet has k parameters
 - any nocitive number
 - $oldsymbol{\Theta} \sim \mathsf{Dirichlet}(lpha_1, lpha_2, \dots, lpha_m)$

$$P(\theta_1, \theta_2, \dots, \theta_m) = \frac{\Gamma(\sum_k \alpha_k)}{\prod_k \Gamma(\alpha_k)} \prod_{k=1}^m \theta_k^{\alpha_k - 1}$$

Preliminaries: Dirichlet Prior

 Conjugate prior for multinomial distribution

 Conjugate prior: posterior in the same family as prior

$$(p_1,\ldots,p_k) \sim \text{Dirichlet}(\alpha_1,\ldots,\alpha_k)$$

Prior:

$$(p_1,\ldots,p_k)\Big|(x_1,\ldots,x_k)\sim \text{Dirichlet}(\alpha_1+x_1,\ldots,\alpha_k+x_k).$$

Posterior:

Bayesian Association Rules

$$a o y\sim ext{Multinomial}(oldsymbol{ heta}). \qquad oldsymbol{ heta}|oldsymbol{lpha}\sim ext{Dirichlet}(oldsymbol{lpha}). \ oldsymbol{ heta}|\mathbf{x},\mathbf{y},oldsymbol{lpha}\sim ext{Dirichlet}(oldsymbol{lpha}+N). \ N=(N_{\cdot,1},\ldots,N_{\cdot,L})$$

Generative Model

- Sample a decision list length $m \sim p(m|\lambda)$.
- Sample the default rule parameter $\theta_0 \sim \text{Dirichlet}(\alpha)$.
- For decision list rule j = 1, ..., m: Sample the cardinality of antecedent a_j in d as $c_j \sim p(c_j | c_{< j}, \mathcal{A}, \eta)$. Sample a_j of cardinality c_j from $p(a_j | a_{< j}, c_j, \mathcal{A})$. Sample rule consequent parameter $\theta_j \sim \text{Dirichlet}(\alpha)$.
- For observation i = 1, ..., n: Find the antecedent a_j in d that is the first that applies to x_i . If no antecedents in d apply, set j = 0. Sample $y_i \sim \text{Multinomial}(\theta_j)$.

Our goal is to sample from the posterior distribution over antecedent lists

$$p(d|\mathbf{x}, \mathbf{y}, \mathcal{A}, \boldsymbol{\alpha}, \lambda, \eta) \propto p(\mathbf{y}|\mathbf{x}, d, \boldsymbol{\alpha})p(d|\mathcal{A}, \lambda, \eta).$$

is 4 complete collection of pre-mined antecedents

Prior Probabilities

$$p(d|\mathcal{A}, \lambda, \eta) = p(m|\mathcal{A}, \lambda) \prod_{j=1}^{m} p(c_j|c_{< j}, \mathcal{A}, \eta) p(a_j|a_{< j}, c_j, \mathcal{A}).$$

Truncated Poisson:

$$p(m|\mathcal{A},\lambda) = \frac{(\lambda^m/m!)}{\sum_{j=0}^{|\mathcal{A}|} (\lambda^j/j!)}, \qquad m = 0, \dots, |\mathcal{A}|.$$

Ensures that sampled values are within bounds!

Also, ensures expected value is close $t\lambda$ when there are a large number of pre-mined rules

Prior Probabilities

Another Truncated Poisson,

$$p(c_j|c_{< j}, \mathcal{A}, \eta) = \frac{(\eta^{c_j}/c_j!)}{\sum_{k \in R_{j-1}(c_{< j}, \mathcal{A})} (\eta^k/k!)}, \qquad c_j \in R_{j-1}(c_{< j}, \mathcal{A}).$$

 $p(a_j|a_{< j},c_j,\mathcal{A})$ is sampled uniformly from available antecedents with appropriate cardinality.

Likelihood

 Likelihood is the product of multinomial probability mass functions for the observed label counts at each rule

$$p(\mathbf{y}|\mathbf{x}, d, \boldsymbol{\theta}) = \prod_{j:\sum_{l} N_{j,l} > 0} \mathrm{Multinomial}(\mathbf{N}_{j}|\theta_{j}),$$
 $\theta_{j} \sim \mathrm{Dirichlet}(\boldsymbol{\alpha}).$

Marginalize over θ_j , integrate out the intermediate parar θ_j er

Markov Chain Monte Carlo

- Generate a chain of random samples until convergence
- Each random sample is a stepping stone for the next one (chain)
- New samples do not depend on any samples before the previous one (Markov)

Markov Chain Monte Carlo

- How to go to (optimal) d* from current dt
- Move an antecedent to a different position in the list

 Add an antecedent that is not currently in the list

Remove an antecedent from the list

Metropolis Hastings

- Start with a random decision list
- Choose a move based on "proposal distribution" Q
- After you choose your move, you compute an acceptance probability A
- Generate a random number u
- If u <= A, then accept; otherwise reject</p>

Metropolis Hastings

- 1. Initialize $x^{(t)}$ for t = 0
- 2. Draw a sample x' from $Q(x' \mid x^{(t)})$
- 3. Accept the move with probability $A(x' \mid x^{(t)}) = \min(1, \alpha)$ where $\alpha = P(x')/P(x_t)$. If accepted, let $x^{(t+1)} = x'$. Otherwise, let $x^{(t+1)} = x^{(t)}$.
- 4. Repeat steps 2-3 to draw samples

Proposal Probabilities

- Move chosen uniformly
- Which antecedents and their new position is also chosen uniformly

$$Q(d^*|d^t, \mathcal{A}) = \begin{cases} \frac{1}{(|d^t|)(|d^t| - 1)}, & \text{if move proposal,} \\ \frac{1}{(|\mathcal{A}| - |d^t|)(|d^t| + 1)}, & \text{if add proposal,} \\ \frac{1}{|d^t|}, & \text{if remove proposal.} \end{cases}$$

Estimating label of a new observation

$$p(\tilde{y} = l | \tilde{x}, d, \mathbf{x}, \mathbf{y}, \alpha) = \frac{\alpha_l + N_{j(d, \tilde{x}), l}}{\sum_{k=1}^{L} (\alpha_k + N_{j(d, \tilde{x}), k})}.$$

Match the antecedent by looking at feature values of new observation

Tic-Tac-Toe

	BRL	C5.0	CART	ℓ_1 -LR	SVM	RF	BCART
Mean accuracy Standard deviation	1.00 0.00	0.94 0.01	$0.90 \\ 0.04$	$0.98 \\ 0.01$	0.99 0.01	0.99 0.01	0.71 0.04

5 fold cross validation; accuracy computed across 5 folds

Stroke Prediction

- N = 12,586, 14% had stroke
- 6000 times larger than data for CHADS2 score
- Pre-mining: support 10% and max cardinality 2
- 5 fold evaluation

Stroke Prediction

```
if hemiplegia and age > 60 then stroke risk 58.9\% (53.8\%–63.8\%) else if cerebrovascular disorder then stroke risk 47.8\% (44.8\%–50.7\%) else if transient ischaemic attack then stroke risk 23.8\% (19.5\%–28.4\%) else if occlusion and stenosis of carotid artery without infarction then stroke risk 15.8\% (12.2\%–19.6\%) else if altered state of consciousness and age > 60 then stroke risk 16.0\% (12.2\%–20.2\%) else if age \leq 70 then stroke risk 4.6\% (3.9\%–5.4\%) else stroke risk 8.7\% (7.9\%–9.6\%)
```

Stroke Prediction - AUC

	AUC	Training time (mins)
BRL-point	0.756 (0.007)	21.48 (6.78)
CHADS_2	$0.721\ \dot{(0.014)}$	no training
CHA_2DS_2 -VASc	$0.677\ (0.007)$	no training
CART	0.704 (0.010)	$12.62 \ (0.09)$
C5.0	$0.704 \ (0.011)$	2.56(0.27)
ℓ_1 logistic regression	0.767 (0.010)	0.05(0.00)
SVM	$0.753 \ (0.014)$	302.89 (8.28)
Random forests	0.774(0.013)	698.56 (59.66)



Interpretable Decision Sets

Hima Lakkaraju, Stephen Bach, Jure Leskovec; 2016

Contributions

- A framework called Interpretable Decision Sets (IDS) for classification
- Novel objective function + proof of submodularity
- Optimization procedure with optimality guarantees
- Detailed metrics for evaluating interpretability + user studies

Motivation

- Traditional classification models optimize for predictive accuracy
- Very little understanding of the model itself and its predictions
- Model being "readable" is not enough
- Humans should be able to reason about predictions and readily explain the functionality of the model

Decision Sets

```
If Respiratory-Illness=Yes and Smoker=Yes and Age≥ 50 then Lung Cancer
```

If Risk-LungCancer=Yes and Blood-Pressure≥ 0.3 then Lung Cancer

If Risk-Depression=Yes and Past-Depression=Yes then Depression

If BMI≥ 0.3 and Insurance=None and Blood-Pressure≥ 0.2 then Depression

If Smoker=Yes and BMI \geq 0.2 and Age \geq 60 then Diabetes

If Risk-Diabetes=Yes and BMI≥ 0.4 and Prob-Infections≥ 0.2 then Diabetes

If Doctor-Visits ≥ 0.4 and Childhood-Obesity=Yes then Diabetes

Criteria for Interpretability

- Parsimony: Fewer rules with fewer conditions
 - Cognitive limits of human understanding
- Distinctness: Minimal overlap of rules w.r.t the data points they cover
 - No redundant and contradicting explanations of data points
- Class Coverage: Explain all the classes in the data
 - Rules explaining minority classes are important

Problem Formulation

Input:

- Set of data points: $\mathcal{D} = \{(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)\}$
- Set of class labels: $\mathcal C$
- Set of frequent patterns obtained using Apriori algorithm: $S = \{ s_1, s_2, s_3, ..., s_M \}$

Ex: \underline{s}_i = Gender = Female and Age > 35 and Smoker = True

Output: An interpretable decision set $\mathcal{R} \subseteq \mathcal{S} \times \mathcal{C}$

Desiderata

- We need to optimize for the following criteria
 - Recall
 - Precision
 - Distinctness
 - Parsimony
 - Class Coverage
- Recall and Precision _ Accurate predications
- Distinctness, Parsimony, and Class Coverage
 Interpretability

- Parsimony
 - Fewer rules: $f_1(\mathcal{R}) = |\mathcal{S}| \text{size}(\mathcal{R})$

Number of conditions in the rule

Number of rules

Fewer predicates:

$$f_2(\mathcal{R}) = L_{\text{max}} \cdot |\mathcal{S}| - \sum_{r} \text{length}(r)$$

Maximum no. of conditions in any given Input pattern

Total number of input patterns

- Distinctness
 - Intra-class overlap:

$$f_3(\mathcal{R}) = N \cdot |S|^2 - \sum_{\substack{r_i, r_j \in \mathcal{R} \\ i \leq j \\ c_i = c_j}} \operatorname{overlap}(r_i, r_j)$$

 Number of points that satisfy both the rules

Inter-class overlap:

$$f_4(\mathcal{R}) = N \cdot |S|^2 - \sum_{\substack{r_i, r_j \in \mathcal{R} \\ i \leq j \\ c_i \neq c_i}} \text{overlap}(r_i, r_j)$$

Class Coverage

$$f_5(\mathcal{R}) = \sum_{c' \in \mathcal{C}} 1 \ \big(\exists r = (s, c) \in \mathcal{R} \text{ such that } c = c' \big)$$
Check if there exists some rule corresponding to a given class c

- Precision
 - Minimize "incorrect" covers:

$$f_6(\mathcal{R}) = N \cdot |\mathcal{S}| - \sum_{r \in \mathcal{R}} |\text{incorrect-cover}(r)|$$
 Given a rule $r = (s,c)$, the no. of data points which satisfy s but do not belong to class c .

- Recall
 - Encourage at least one "correct" cover per data point:

$$f_7(\mathcal{R}) = \sum_{(\mathbf{x},y) \in \mathcal{D}} 1 \left(|\{r|(\mathbf{x},y) \in \text{correct-cover}(r)\}| \geq 1 \right)$$
 Given a rule $r = (s,c)$, the no. of data points which satisfy s and belong to class c .

Complete objective is

$$\underset{\mathcal{R}}{\operatorname{argmax}} \sum_{i=1}^{7} \lambda_{i} f_{i}(\mathcal{R})$$

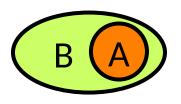
- The intra-class and inter-class overlap terms are non-monotone
- The parsimony, overlap, and precision terms are non-normal
- All the component terms are submodular

Submodularity

Diminishing returns characterization

$$F(A \land d) - F(A) \ge F(B \land d) - F(B)$$
Gain of adding **d** to a small set

Gain of adding **d** to a large set



A non-negative linear combination of submodular functions is submodular

Complete objective is

$$\underset{\mathcal{R} \subseteq \mathcal{S} \times \mathcal{C}}{\operatorname{argmax}} \sum_{i=1}^{7} \lambda_{i} f_{i}(\mathcal{R})$$

The complete objective is non-negative, non-normal, non-monotone, submodular

non-normai

All the component terms are submodular

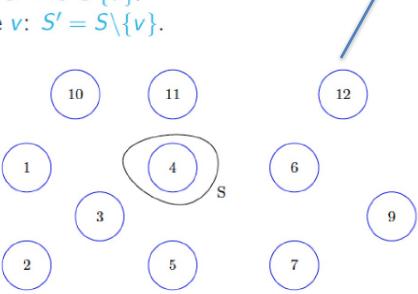
Optimizing the Objective

 Maximizing a non-monotone submodular function is NP-hard

- Smooth local search [SLS] algorithm provides a 2/5 approximation [Feige, Mirrokni, Vondrak FOCS 07; SIAM Comp. J. 11]
 - Will be at least 2/5 of the optimal solution

Local Operation:

- $\blacktriangle Add v: S' = S \cup \{v\}.$
- ▶ Remove v: $S' = S \setminus \{v\}$.



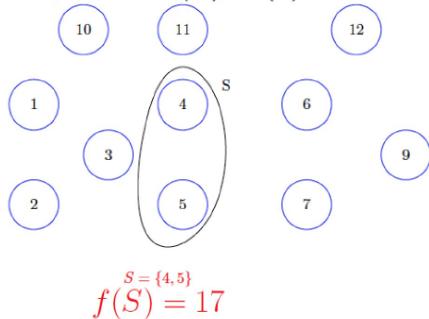
Each node here corresponds to a candidate rule = (pattern, class) tuple

$$f(S) = 10$$

Local Operation:

- ightharpoonup Add v: $S' = S \cup \{v\}$.
- ▶ Remove v: $S' = S \setminus \{v\}$.

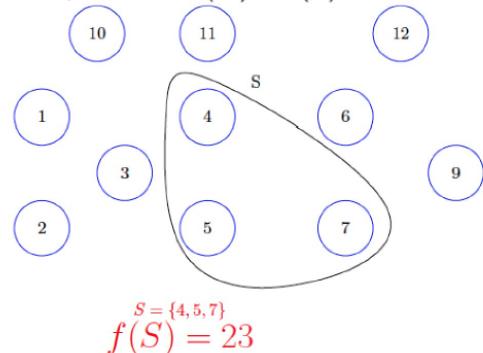
Improving local operation if f(S') > f(S).



Local Operation:

- ▶ Add v: $S' = S \cup \{v\}$.
- ▶ Remove v: $S' = S \setminus \{v\}$.

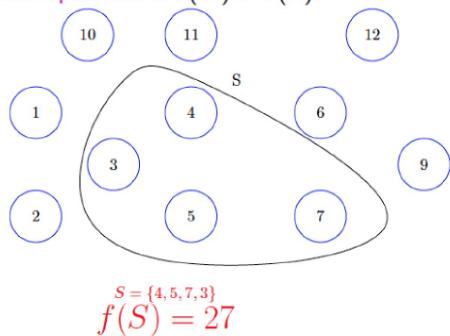
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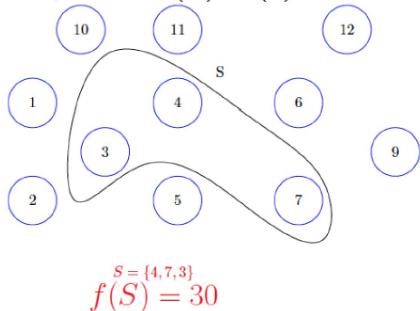
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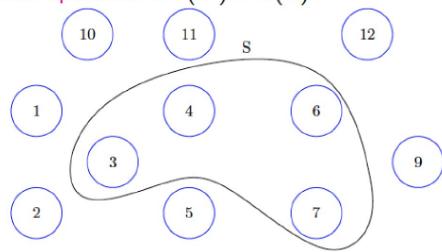
Improving local operation if f(S') > f(S).



Local Operation:

- ▶ Add v: $S' = S \cup \{v\}$.
- ▶ Remove v: $S' = S \setminus \{v\}$.

Improving local operation if f(S') > f(S).



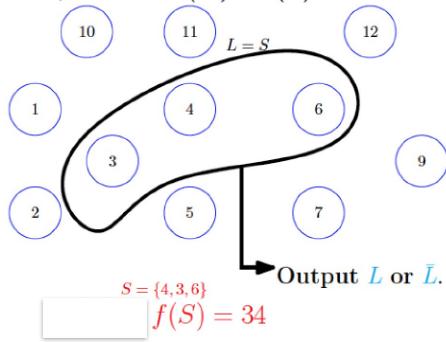
$$S = \{4,7,3,6\}$$

 $f(S) = 33$

Local Operation:

- ▶ Add v: $S' = S \cup \{v\}$.
- ▶ Remove v: $S' = S \setminus \{v\}$.

Improving local operation if f(S') > f(S).



S and S' correspond to the intermediate solution sets

Local Search

- ~1/3 approximation
 - At least 1/3 of optimal solution

- we use a slightly different version of this algorithm
 - Smooth local search
 - 2/5 approximation

Smooth Local Search

```
Algorithm 1 Smooth Local Search (SLS)
                                        1: Input: Objective f, domain X = \mathcal{S} \times \mathcal{C}, parameters \delta and \delta'
         Initialization 3: A = \emptyset
4: OPT = f(\Phi_X(X, 0))
5: for each element x \in X do
                                        6: Estimate \mathbb{E}[f(\Phi_X(A,\delta) \cup x)] - \mathbb{E}[f(\Phi_X(A,\delta) \setminus x)] within an
      Marginal gain \frac{1}{|X|^2} OPT
                                        7: Call this estimate \tilde{\omega}_{A,\delta}(x)
                                        8: end for
                                     9: for each element x \in X \setminus A such that \tilde{\omega}_{A,\delta}(x) > \frac{2}{|X|^2} OPT do
                                  \begin{array}{ccc} & 10: & A = A \cup x \\ & 11: & \text{Goto Line 5} \end{array}
If marginal gain >
      threshold.
    Add element
                                     12: end for
                              13: for each element x \in A such that \tilde{\omega}_{A,\delta}(x) < \frac{-2}{|X|^2} OPT do 14: A = A \setminus x 15: Goto Line 5
If marginal gain <
      threshold,
    Add element
                                       16: end for
                                       17: return \Phi_X(A, \delta')
```

Evaluation: Datasets

Dataset	# of datapoints	Features	Classes
Bail Outcomes	86K	Gender, age, current offense details, past criminal record	No Risk, Failure to Appear, New Criminal Activity
Student Performance	21K	Gender, age, grades, `absence rates & tardiness behavior through grades 6 to 8, suspension/withdrawal history	Graduated on Time, Delayed Graduation, Dropped out
Medical Diagnosis	150K	Current ailments, age, BMI, gender, smoking habits, medical history, family history	Asthma, Diabetes, Depression, Lung Cancer, Rare Blood Cancer

Evaluating Predictive Performance

Method	AUC Bail Data	AUC Student Data	AUC Medical Data
Our Approach	69.78	75.12	61.19
Bayesian Decision Lists (Letham et. al.)	67.18	72.54	59.18
Classification Based on Association (Liu et. al.)	70.68	76.02	63.03
CN2	71.02	76.36	64.78
Decision Trees	70.08	75.31	63.28
Gradient Boosted Trees	71.23	77.18	64.21
Random Forests	70.87	77.12	63.92

Evaluating Goodness of Rules

Results on Medical Diagnosis Data

Method	Fraction of Overlap	Fraction of Data Points Uncovered	Avg. Rule Width	Num. Rules	Fraction of Classes Covered
Our Approach	0.09	0.13	3.17	12	1.0
Bayesian Decision Lists (Letham et. al.)	0.00	0.18	8.46	11	0.67
Classification Based on Association (Liu et. al.)	0.00	0.14	8.60	32	1.00
CN2	0.12	0.14	9.78	38	1.00

Ablation Study

Results on Medical Diagnosis Data

	AUC	Frac. Overlap	Frac. Uncov.	Rule Length	Num. Rules	Frac. Classes
Full IDS	61.19	0.09	0.13	3.17	12	1.00
No Prec.	51.26	0.09	0.19	3.19	12	1.00
No Recall	53.38	0.10	0.14	3.18	11	1.00
No Overlap	61.02	0.16	0.14	3.54	11	1.00
No Conc.	63.64	0.04	0.13	6.88	14	1.00
No Class	59.28	0.01	0.15	3.09	10	0.83

Evaluating Interpretability: User Study

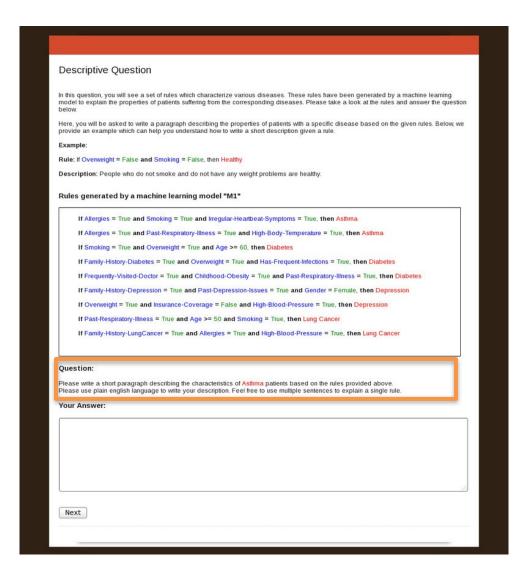
- Compared our interpretable decision sets to Bayesian Decision Lists (Letham et. al.)
- Each user is randomly assigned one of the two models

10 objective and 2 descriptive questions per user

Interface for Objective Questions



Interface for Descriptive Questions



User Study Results

Task	Metrics	Our Approach	Bayesian Decision Lists
Descriptive	Human Accuracy	0.81	0.17
	Avg. Time Spent (secs.)	113.4	396.86
	Avg. # of Words	31.11	120.57
Objective	Human Accuracy	0.97	0.82
	Avg. Time Spent (secs.)	28.18	36.34

Objective Questions: 17% more accurate, 22% faster; Descriptive Questions: 74% fewer words, 71% faster.