Week 8, Lecture 15 - Decision Trees

Aaron Meyer

Outline

- Administrative Issues
- Decision Trees
- Applications
- Implementation

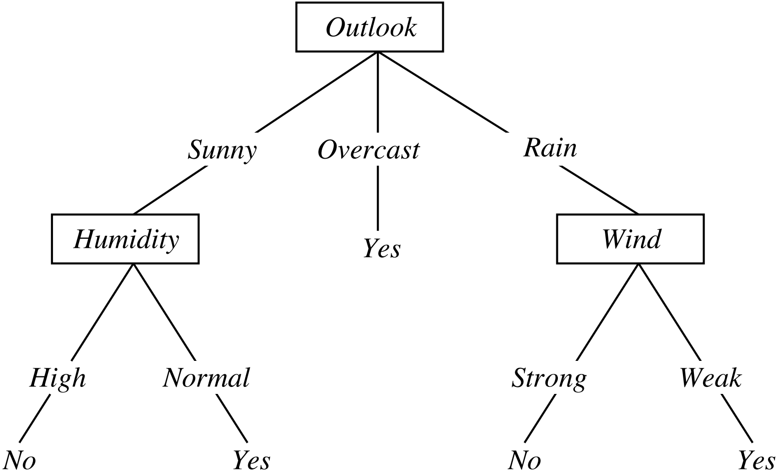
Classification

- With MLR and PLSR we talked about supervised regression
  - Continuous Y and continuous predictions
- With clustering, we get discrete predictions
  - But no Y output
- In the next two lectures, we're going to talk about methods that give discrete Y predictions
  - Decision trees (today)
  - Support vector machines (next lecture)

Decision Tree Representation

- Classification of instances by sorting them down the tree from the root to some leaf note
  - **node** $\approx$ test of some attribute
  - **branch** $\approx$ one of the possible values for the attribute
- Decision trees represent a **disjunction of conjunctions of constraints on the attribute values of instances**
- Equivalent to a set of if-then-rules
  - each branch represents one if-then-rule
    - **if-part:** conjunctions of attribute tests on the nodes
    - **then-part:** classification of the branch

Decision Tree Representation



- This decision tree is equivalent to:
  - if (Outlook = Sunny) $\wedge$ (Humidity = Normal) then Yes;
  - if (Outlook = Overcast) then Yes;
  - if (Outlook = Rain) $\wedge$ (Wind = Weak) then Yes;

Appropriate Problems

- Instances are represented by attribute-value pairs, e.g. (Temperature, Hot)
- Target function has discrete output values, e.g. *yes* or *no*
- **Disjunctive descriptions** may be required
- Training data may **contain errors**
- Training data may contain **missing attribute values**
  - Last three points make Decision Tree Learning more attractive than CANDIDATE-ELIMINATION

ID3

- Learns decision trees by constructing them **top-down**
- employs a **greedy search algorithm without backtracking** through the space of all possible decision trees
  - finds the shortest but not neccessarily the best decision tree
- **key idea:**
  - selection of the next attribute according to a statistical measure
  - all examples are considered at the same time (simultaneous covering)
  - recursive application with reduction of selectable attributes until each training example can be classified unambiguously

ID3 algorithm

`ID3(Examples, Target_attribute, Attributes)`

Create a `Root` for the tree

- If all examples are **positive**, Return single-node tree `Root`, with `label = +`
- If all examples are **negative**, Return single-node tree `Root`, with `label =` $-$
- If `Attributes` is empty, Return single-node tree `Root`, with `label =` most common value of `Target_attribute` in `Examples`

ID3 algorithm

`ID3(Examples, Target_attribute, Attributes)`

otherwise, Begin

- A $\leftarrow$ attribute in Attributes that best classifies Examples
  decision attribute for Root $\leftarrow$ A
- **For each possible value v_i of A**
  - Add new branch below Root with $A = v_i$
  - Let `Examples_vi` be the subset of Examples with v_i for A
  - If `Examples` is empty
    - Then add a leaf node with `label` = most common value of `Target_attribute` in `Examples`
    - Else add `ID3(Examples_vi, Target_Attribute, Attributes − {A})`
- Return `Root`

The best classifier

- **Central choice:** Which attribute classifies the examples best?
- ID3 uses the **information gain**
  - statistical measure that indicates how well a given attribute separates the training examples according to their target classification

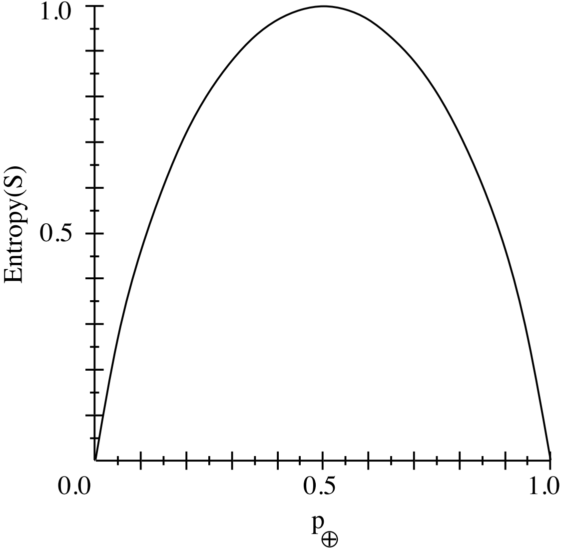
$$Gain(S,A) = \underbrace{Entropy(S)}_{\text{original entropy of S}} - \underbrace{\sum_{v \in values(A)} \frac{|S_v|}{|S|} \cdot Entropy(S_v)}_{\text{relative entropy of S}}$$

- Interpretation:
  - Denotes the reduction in entropy caused by partitioning S according to A
  - Alternative: number of saved yes/no questions (i.e., bits)
  - Attribute with $\max_A Gain(S,A)$ is selected!

Entropy

- Statistical measure from information theory that **characterizes (im-)purity** of an arbitrary collection of examples S
  - Definition: $H(S) \equiv \sum_{\forall i} -p_i \log_2 p_i$
- Interpretation
  - Specification of the minimum number of bits of information needed to encode the classification of an arbitrary member of S
  - Alternative: number of yes/no questions

Entropy



- Minimum of H(S)

Illustrative Example

Example days:

Day	*Sunny*	*Temp.*	*Humidity*	*Wind*	*PlayTennis*
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Illustrative Example

- entropy of S

$$S = \{D1, ..., D14\} = [9+, 5-]$$
$$H(S) = -\frac{9}{14} \cdot \log_2 \frac{9}{14} - \frac{5}{14} \cdot \log_2 \frac{5}{14} = 0.940$$

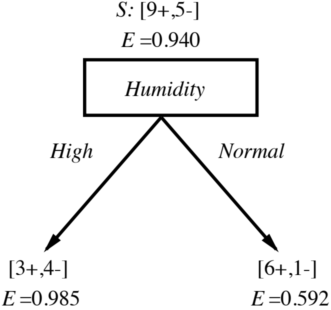
- information gain (e.g. $Wind$)

$$S_{Weak} = \{D1, D3, D4, D5, D8, D9, D10, D13\} = [6+, 2-]$$
$$S_{Strong} = \{D2, D6, D7, D11, D12, D4\} = [3+, 3-]$$

$$\begin{aligned} Gain(S, Wind) &= H(S) - \sum_{v \in Wind} \frac{|S_v|}{|S|} \cdot H(S_v) \\ &= H(S) - \frac{8}{14} \cdot H(S_{Weak}) - \frac{6}{14} \cdot H(S_{Strong}) \\ &= 0.940 - \frac{8}{14} \cdot 0.811 - \frac{6}{14} 1.000 \\ &= 0.048 \end{aligned}$$

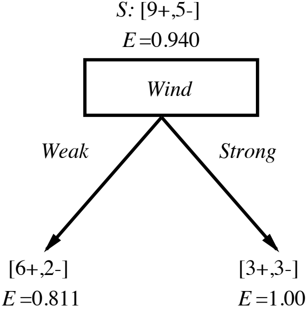
Illustrative Example

Which attribute is the best classifier?



Gain (S, Humidity)

= .940 - (7/14).985 - (7/14).592
= .151



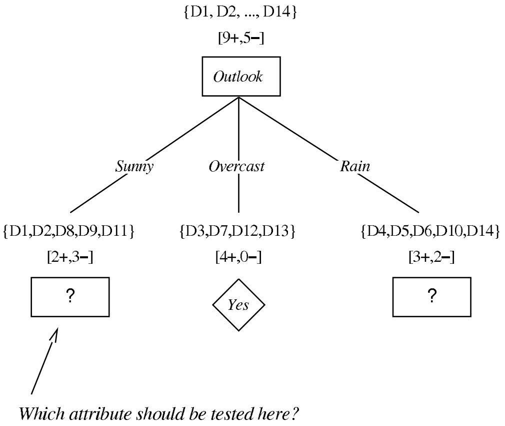
Gain (S, Wind)

= .940 - (8/14).811 - (6/14)1.0
= .048

Illustrative Example

- Informations gains for the four attributes:
  - *Gain(S, Outlook)* $=$ *0.246*
  - *Gain(S, Humidity)* $=$ *0.151*
  - *Gain(S, Wind)* $=$ *0.048*
  - *Gain(S, Temperature)* $=$ *0.029*
- *Outlook* is selected as best classifier and is therefore root of the tree
- Now branches are created below the root for each possible value
  - Because every example for which *Outlook* $=$ *Overcast* is positive, this node becomes a leaf node with the classification *Yes*
  - The other descendants are still ambiguous (e.g. $H(S) \neq 0$)
  - Hence, the decision tree has to be further elaborated below these nodes

Illustrative Example



$S_{sunny} = \{D1,D2,D8,D9,D11\}$

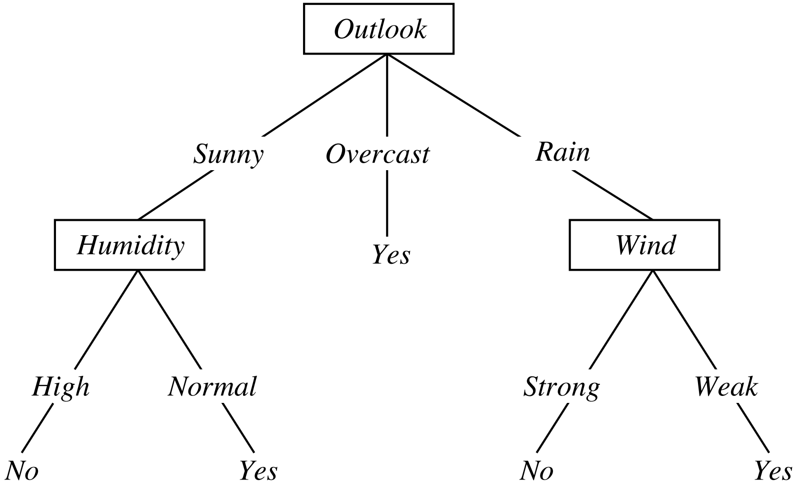
$Gain\ (S_{sunny}\ ,\ Humidity) = .970 - (3/5)\ 0.0 - (2/5)\ 0.0 = .970$

$Gain\ (S_{sunny}\ ,\ Temperature) = .970 - (2/5)\ 0.0 - (2/5)\ 1.0 - (1/5)\ 0.0 = .570$

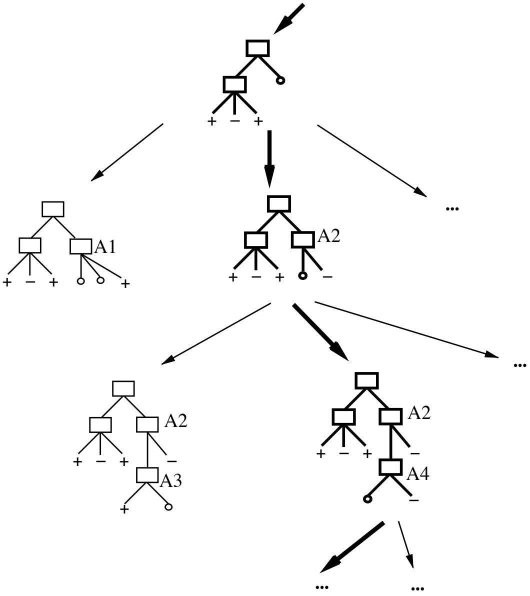
$Gain\ (S_{sunny}\ ,\ Wind) = .970 - (2/5)\ 1.0 - (3/5)\ .918 = .019$

Illustrative Example

Resulting decision tree



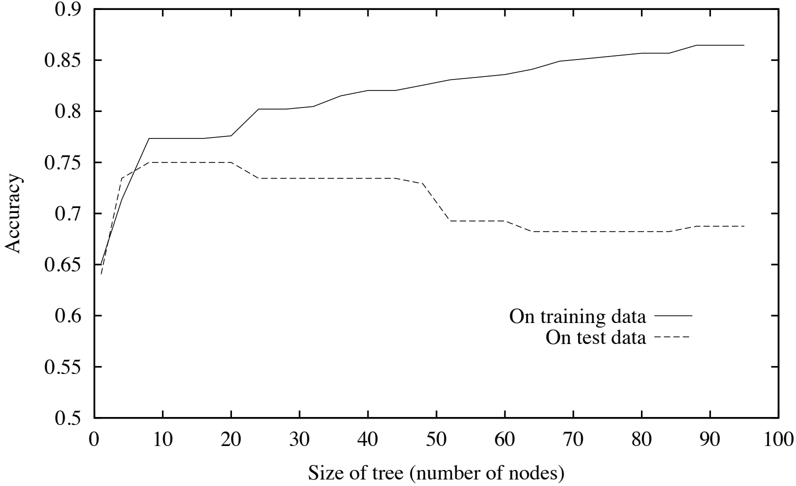
Hypothesis Space Search



Inductive Bias

- As mentioned above, ID3 searches
  - Complete space of possible, but not completely
  - Preference Bias
- Inductive bias: Shorter trees are prefered to longer trees. Trees that place high information gain attributes close to the root are also prefered.
- Why prefer shorter hypotheses?
  - Occam's Razor: Prefer the simplest hypothesis that fits the data!
  - see Minimum Description Length Principle (Bayesian Learning)
  - e.g., if there are two decision trees, one with 500 nodes and another with 5 nodes, the second one should be prefered
  - better chance to avoid overfitting

Overfitting



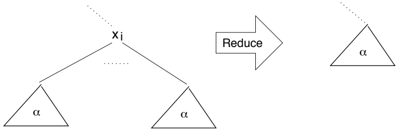
Given a hypothesis space H, a hypothesis $h \in H$ is said to overfit the training data if there exists some alternative hypothesis $h' \in H$, such that h has smaller error than h' over the training, but h' has

Overfitting

- Reasons for overfitting:
  - Noise in the data
  - Number of training examples is to small too produce a representative sample of the target function
- How to avoid overfitting:
  - Stop the tree grow earlier, before it reaches the point where it perfectly classifies the training data
  - Allow overfitting and then **post-prune** the tree (more successful in practice!)
- How to determine the perfect tree size:
  - Separate validation set to evaluate utility of post-pruning
  - Apply statistical test to estimate whether expanding (or pruning) produces an improvement

Reduced Error Pruning

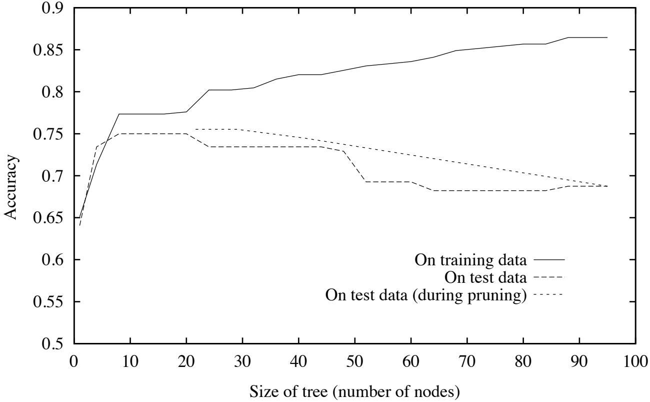
- Each of the decision nodes is considered to be candidate for pruning



- Pruning a decision node consists of removing the subtree rootet at the node, making it a leaf node and assigning the most common classification of the training examples affiliated with that node
- Nodes are removed only if the resulting tree performs not worse than the original tree over the validation set
- Pruning starts wit the node whose removal most increases accuracy and continues until further pruning is harmful

Reduced Error Pruning

Effect of reduced error pruning:



Any node added to coincidental regularities in the training set is likely to be pruned.

Rule Post-Pruning

- Rule post-pruning involves the following steps:
    1. Infer the decision tree from the training set (Overfitting allowed!)
    2. Convert the tree into a set of rules
    3. Prune each rule by removing any preconditions that result in improving its estimated accuracy
    4. Sort the pruned rules by their estimated accuracy
- One method to estimate rule accuracy is to use a separate validation set
- Pruning rules is more precise than pruning the tree itself

Alternative Measures

- Natural bias in information gain favors attributes with many values over those with few values
- e.g. attribute `Date`
  - Very large number of values (e.g. March 21, 2005)
  - Inserted in the above example, it would have the highest information gain, because it perfectly separates the training data
  - But the classification of unseen examples would be impossible
- Alternative measure: `GainRatio`
  - $GainRatio(S, A) = \frac{Gain(S,A)}{SplitInformation(S,A)}$
  - $SplitInformation(S, A) \equiv -\sum_{i=1}^{n} \frac{S_i}{S} \log_2 \frac{S_i}{S}$
  - `SplitInformation(S,A)` is sensitive to how broadly and uniformly A splits S (entropy of S with respect to the values of A)
  - *GainRatio* penalizes attributes such as `Date`

Summary

- Practical and intuitively understandable method for concept learning
- Able to learn disjunctive, discrete-valued concepts
- Noise in the data is allowed
- ID3 is a simultaneous covering algorithm based on information gain that performs a greedy top-down search through the space of possible decision trees
- Inductive Bias: Short trees are prefered (Occam's razor)
- Overfitting is an important issue and can be reduced by pruning

Applications - Medical Diagnosis / Prediction

Predicting cesarean delivery with decision tree models

Cynthia J. Sims, MD,[a] Leslie Meyn, BS,[a] Rich Caruana, PhD,[b, c] R. Bharat Rao, PhD,[d] Tom Mitchell, PhD,[b] and Marijane Krohn, PhD[a]

Pittsburgh, Pennsylvania, Los Angeles, California, and Princeton, New Jersey

OBJECTIVE: The purpose of this study was to determine whether decision tree–based methods can be used to predict cesarean delivery.
STUDY DESIGN: This was a historical cohort study of women delivered of live-born singleton neonates in 1995 through 1997 (22,157). The frequency of cesarean delivery was 17%; 78 variables were used for analysis. Decision tree rule-based methods and logistic regression models were each applied to the same 50% of the sample to develop the predictive training models and these models were tested on the remaining 50%.
RESULTS: Decision tree receiver operating characteristic curve areas were as follows: nulliparous, 0.82; parous, 0.93. Logistic receiver operating characteristic curve areas were as follows: nulliparous, 0.86; parous, 0.93. Decision tree methods and logistic regression methods used similar predictive variables; however, logistic methods required more variables and yielded less intelligible models. Among the 6 decision tree building methods tested, the strict minimum message length criterion yielded decision trees that were small yet accurate. Risk factor variables were identified in 676 nulliparous cesarean deliveries (69%) and 419 parous cesarean deliveries (47.6%).
CONCLUSION: Decision tree models can be used to predict cesarean delivery. Models built with strict minimum message length decision trees have the following attributes: Their performance is comparable to that of logistic regression; they are small enough to be intelligible to physicians; they reveal causal dependencies among variables not detected by logistic regression; they can handle missing values more easily than can logistic methods; they predict cesarean deliveries that lack a categorized risk factor variable. (Am J Obstet Gynecol 2000;183:1198-206.)

Key words: Decision trees, machine learning, predicting cesarean delivery, statistical models

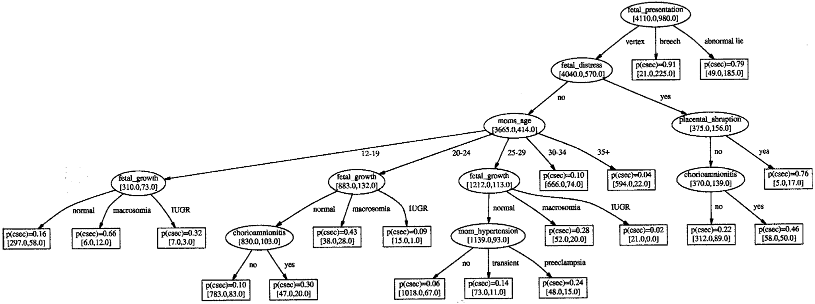
Applications - Medical Diagnosis / Prediction

Table I. Relationships between maternal and fetal characteristics and cesarean delivery

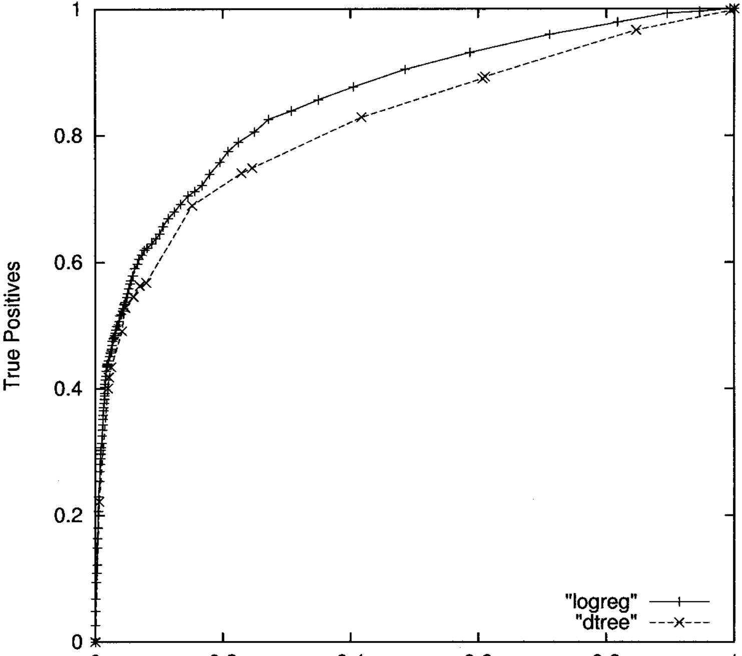
Variable	*Total*	*Cesarean delivery* No.	*Cesarean delivery* %	*Statistical significance**
African American race				$P < .001$
No	18,592	3221	17.3	
Yes	3,502	505	14.4	
Missing	63	9	14.3	
Age				$P < .001$
12-19 y	1,797	165	9.2	
20-24 y	3,222	460	14.3	
25-29 y	5,949	886	14.9	
30-34 y	7,062	1295	18.3	
≥35 y	4,127	929	22.5	
Married				$P < .001$
Yes	14,641	2631	18.0	
No	7,516	1104	14.7	
Insurance type				$P < .001$
Third-party	16,847	2988	17.7	
Public	5,310	747	14.1	
Previous cesarean delivery†				$P < .001$
No	9,521	568	6.0	
Yes	2,439	1204	49.4	
Cigarette use in pregnancy				$P = .747$
No	19,329	3251	16.8	
Yes	2,819	481	17.1	
Missing	9	3	33.3	
Diabetes				$P < .001$
None	21,464	3508	16.3	
Gestational	552	157	28.4	
Insulin-dependent	137	67	48.9	
Missing	4	3	75.0	
Hypertension				$P < .001$
None	20,222	3217	15.9	
Transient	1,168	234	20.0	
Preeclampsia or eclampsia	767	284	37.0	
Preterm delivery (<37 wk)				$P < .001$
No	19,790	3071	15.5	
Yes	2,365	664	28.1	
Missing	2	0	0	
Fetal presentation				$P < .001$
Vertex	20,550	2455	11.9	
Breech	855	740	86.5	
Abnormal lie	752	540	71.8	
Fetal growth by *International Classification of Diseases, Ninth Revision* code				$P < .001$
Intrauterine growth restriction	551	131	23.8	
Normal	20,167	3092	15.3	
Macrosomia	1,439	512	35.6	

*Missing cases were not included in calculations of *P* values.
†Among women who had at least one previous delivery.

Applications - Medical Diagnosis / Prediction



Applications - Medical Diagnosis / Prediction



Applications - Medical Diagnosis / Prediction

Table III. Variables used in decision tree and logistic regression nulliparous

	Nulliparous	
Variable	*Decision tree*	*Logistic*
African American race		Used
Grouped age	Used	Used
History of cesarean delivery		
Maternal admission weight		Used
Diabetes		Used
Structural heart disease		Used
Hypertension	Used	Used
Other pulmonary condition		
Placenta previa		Used
Uterine abnormality		Used
Herpes simplex virus infection		Used
Preterm labor		Used
Fetal growth	Used	Used
Preterm delivery		Used
Abruptio placentae	Used	Used
Chorioamnionitis	Used	Used
Type of membrane rupture		Used
Fetal presentation	Used	Used
Fetal distress	Used	Used
Umbilical cord prolapse		
Meconium-stained amniotic fluid		

Practical Notes

- Building and applying decision trees is extremely fast.
- Results are very interpretable.
- With boosting, DTs often win at prediction with large data and many variables.
  - But this comes at the expense of interpreting the model.
- Bootstrap difficult to apply to DTs, due to structure.

Implementation

Further Reading

- Computer Age Statistical Inference, Chapter 8
- sklearn.tree