

Feature Selection

Feature Selection

- Give set of features, some features are more important than others
- We want to select some subset of features to be used by learning algorithms
- Exhaustive approach:
 - Train systems on all $D!$ possible combinations and choose the best one.
 - Pro: It's a globally optimal solution
 - Con: It's often not-feasible

D!

Greedy Feature Selection

D features

$\{F_1, F_2, \dots\}$

D-1 features

- Greedy heuristic:
 - Start from empty set of features $F = \emptyset$
 - For iteration t , for each remaining feature j
 - Run learning algorithm for features $F \cup j$
 - Select next best feature \hat{j}
 - $F = F \cup \{\hat{j}\}$
 - Continue until converge on locally optimal result
- You could also do backwards feature selection
 - Start with all features, remove worst, etc..

all features

$\{ \quad \quad \}$

- This would involve training/evaluating

$$\underline{D} + \underline{(D-1)} + \underline{(D-2)} + 1 = \sum_{i=1}^D i = \frac{D(D+1)}{2} \text{ systems}$$

D systems

- Better....

Separability Feature Selection

- What if we were rank features somehow out-of-the-gate and then greedily add them one by one
- This would just be D systems
- So how do we rank them?
- If we don't have class labels we could use something like least covariance
 - We want to use features that are unique.
- If we do have class labels maybe we can find a way to measure a feature's effect on class separability...

Feature Selection by L1

Feature Selection by L1

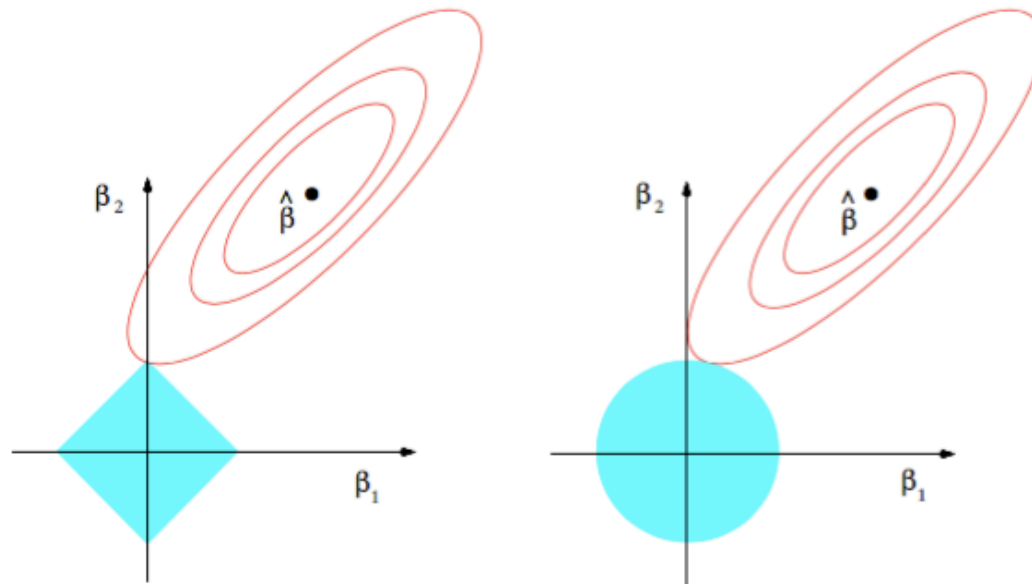


FIGURE 3.11. Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions $|\beta_1| + |\beta_2| \leq t$ and $\beta_1^2 + \beta_2^2 \leq t^2$, respectively, while the red ellipses are the contours of the least squares error function.

Boston Housing Dataset

```
from sklearn.linear_model import Lasso
from sklearn.preprocessing import StandardScaler
from sklearn.datasets import load_boston
```

```
boston = load_boston()
scaler = StandardScaler()
X = scaler.fit_transform(boston["data"])
Y = boston["target"]
names = boston["feature_names"]
```

```
lasso = Lasso(alpha=.3)
lasso.fit(X, Y)
```

```
print "Lasso model: ", pretty_print_linear(lasso.coef_, names, sort = True)
```

```
Lasso model: -3.707 * LSTAT + 2.992 * RM + -1.757 * PTRATIO + -1.081 * DIS + -0.7
* NOX + 0.631 * B + 0.54 * CHAS + -0.236 * CRIM + 0.081 * ZN + -0.0 * INDUS + -0.0
* AGE + 0.0 * RAD + -0.0 * TAX
```

Feature Selection by Information

Gain

$$y \ln g(\theta, x)$$

$$y \log \hat{y}$$

$$p_{uc} \log p_{ui}$$

loss

logistic regression

Cross-entropy

- Given probability of events v_1, \dots, v_n as $P(v_1), \dots, P(v_n)$ we can compute the entropy as

$$H(P(v_1), \dots, P(v_n)) = \sum_{i=1}^n (-P(v_i) \log_n P(v_i))$$

- Entropy measure the randomness of the data

- Example: Tossing a fair coin

- $v_1 = \text{heads}, v_2 = \text{tails},$

- $P(v_1) = 0.5, P(v_2) = 0.5$

- $H\left(\frac{1}{2}, \frac{1}{2}\right) = -\frac{1}{2} \log_2 \frac{1}{2} - \frac{1}{2} \log_2 \frac{1}{2} = 1$

1 ∈ entropy random

① → deterministic

Feature Selection via Information Gain

$$\begin{array}{cc} 1 & 1-0=1 \\ 0 & 1-1=0 \end{array}$$

- Let us assume we have a dataset with binary labels:

$$Y_i \in \{0,1\}$$

- And that all features are discrete.
- Let a chosen feature $j \in \{1, \dots, D\}$ have k possible values (thus a discretized feature).
- Then the dataset $X = \{X_i\}_{i=1}^N$ can be split into subsets $\{E_1, \dots, E_k\}$ according to each observation's value, $X_{i,j}$
- The intuition is to compute the original entropy of the system and then the average entropy on this split
 - We want to maximize this difference
 - This is our "gain"
- Or, we can say that we want to minimize the average entropy after the split.

Feature Selection via Information Gain

- Let $p = \#\{1\}$, be the number of samples with label one over the entire dataset
- Let $n = \#\{0\}$ be the number of samples with label zero over the entire dataset
- Finally let p_i, n_i be the number samples in subset E_i , with label one and zero, respectively.
- Let's define the average entropy with respect to A as:

$$\mathbb{E}(H(A)) = \sum_{i=1}^k \frac{p_i + n_i}{p + n} H\left(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i}\right)$$

Feature Selection via Information Gain

- We can now compute information Gain (IG), or reduction in entropy, that would occur if we split on this attribute/feature:

$$IG(A) = H\left(\frac{p}{p+n}, \frac{n}{p+n}\right) - \mathbb{E}(H(A))$$

Handwritten red annotations: A red oval circles the entropy term $H(\frac{p}{p+n}, \frac{n}{p+n})$. Another red oval circles the expected entropy term $\mathbb{E}(H(A))$. A red arrow points from the text "A feature" to the variable A in the equation.

- We should choose the attribute with the largest IG!
 - I.e. the one with the smallest average entropy.

Example

- For reference:
 - $H(P(v_1), \dots, P(v_n)) = \sum_{i=1}^n (-P(v_i) \log_2 P(v_i))$
 - $\mathbb{E}(H(A)) = \sum_{i=1}^k \frac{p_i + n_i}{p + n} H\left(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i}\right)$
- Class 1 Samples
 - $\{(1,1), (1,3), (2,2)\}$
- Class 0 Samples
 - $\{(1,2), (3,2), (2,2)\}$
- Let's figure out which feature provides the highest information gain!

Example

Class 1 Samples $\checkmark \quad \checkmark \quad \checkmark$
 $\{(1,1)(1,3), (2,2)\}$

Class 0 Samples
 $\{(1,2), (3,2), (2,2)\}$

$$\begin{array}{c}
 x \Rightarrow \\
 \begin{array}{cc}
 f_1 & f_2 \\
 \hline
 1 & 1 \\
 \rightarrow & 1 & 3 \\
 \rightarrow & 2 & 2 \\
 \rightarrow & 1 & 2 \\
 \rightarrow & 3 & 2 \\
 \rightarrow & 2 & 2
 \end{array}
 \end{array}$$

$$\begin{array}{c}
 y \Rightarrow \\
 \begin{array}{c}
 1 \\
 1 \\
 1 \\
 0 \\
 0 \\
 0
 \end{array}
 \end{array}$$

$$E_{f_1} \begin{bmatrix} 1 & 1 & \cdot & 1 \\ 1 & 3 & \cdot & 1 \\ 1 & 2 & \cdot & 0 \end{bmatrix} \rightarrow \left(-\frac{1}{3} \log \frac{1}{3} - \frac{2}{3} \log \frac{2}{3} \right)$$

$$E_{f_2} \begin{bmatrix} 2 & 2 & \cdot & 1 \\ 2 & 2 & \cdot & 0 \end{bmatrix} \rightarrow 1$$

$$E_{f_3} \begin{bmatrix} 3 & 2 & \cdot & 0 \end{bmatrix} \rightarrow 0$$

$$\begin{array}{c}
 E_{f_1} \\
 \frac{3}{6} \left(-\frac{1}{3} \log \frac{1}{3} - \frac{2}{3} \log \frac{2}{3} \right) + \frac{3}{6} \left(1 \right) + \frac{1}{6} \left(0 \right) \Rightarrow \text{total entropy of } f_1
 \end{array}$$

Example

- $H(P(v_1), \dots, P(v_n)) = \sum_{i=1}^n (-P(v_i) \log_2 P(v_i))$

- $\mathbb{E}(H(A)) = \sum_{i=1}^k \frac{p_i + n_i}{p + n} H\left(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i}\right)$

- Positive Samples

- $\{(1,1), (1,3), (2,2)\}$

- Negative Samples

- $\{(1,2), (3,2), (2,2)\}$

- Feature 1

- $p_1=2, n_1=1$

- $p_2=1, n_2=1$

- $p_3=0, n_3=1$

- $\mathbb{E}(H(1)) =$

$$\begin{aligned} & (2+1)/(3+3) * (-2/3 * \log_2(2/3) + -1/3 * \log_2(1/3)) \\ & + (1+1)/(3+3) * (-1/2 * \log_2(1/2) + -1/2 * \log_2(1/2)) \\ & + (0+1)/(3+3) * (0 \log_2(0) - 1 \log_2(1)) = 0.7925 \end{aligned}$$

- $IG(1) = (-3/6 \log(3/6) - 3/6 \log(3/6)) - 0.7925 = 0.2075$

$$1 - 0.7925 = 0.2075$$

Example

- Positive Samples
 - $\{(1,1)(1,3),(2,2)\}$
- Negative Samples
 - $\{(1,2),(3,2),(2,2)\}$
- Feature 2
 - $p_1=1, n_1=0$
 - $p_2=1, n_2=3$
 - $p_3=1, n_3=0$
 - $\mathbb{E}(H(2))=$

$$\frac{(1+0)}{(3+3)} * (-1/1 * \log_2(1/1) + -0 * \log_2(0))$$

$$+ \frac{(1+3)}{(3+3)} * (-1/4 * \log(1/4) + -3/4 \log(3/4))$$

$$+ \frac{(1+0)}{(3+3)} * (-1/1 \log(1/2) - 0/1 \log(0/1)) = 0.5409$$
 - $IG(2) = (-3/6 \log(3/6) - 3/6 \log(3/6)) - 0.5409 = 0.4591$
- Recall $IG(1)=0.2075$
- So we should prioritized feature 2!

More than 2 classes?

- Think about how you can change the equations for work for more than two class...

$$H(P(v_1), \dots, P(v_n)) = \sum_{i=1}^n (-P(v_i) \log_n P(v_i))$$

$$\mathbb{E}(H(A)) = \sum_{i=1}^k \frac{p_i + n_i}{p + n} H(P(v_1), \dots, P(v_n))$$

$$IG(A) = H\left(\frac{p}{p+n}, \frac{n}{p+n}\right) - \mathbb{E}(H(A))$$

IG for real-valued features

$$\left. \begin{matrix} 0.1 \\ 0.3 \\ 0.8 \\ 0.2 \\ 0.4 \end{matrix} \right\} \mu \quad \sigma \quad \frac{x - \mu}{\sigma}$$

zero
if $x_{ik} \geq 0$

$x_i < 0$
 $y_i = 1$
 $y_i = 0$

- The examples we showed work for categorical and/or enumerated features
- This could be expanded to work on real-valued features
- Two approaches:
 1. Break up the range of possible values into enumerated/discrete regions
 2. Assume some distribution (say Gaussian)
 1. Separate the data by class
 2. Find the parameters for ~~Gaussians~~ for each feature within in subset.
 3. For each sample compute the probability of class k given j^{th} attribute value $X_{i,j}$, $P(j = X_{i,j} | Y_i = C_k)$ and use these to compute the entropy.

Initial entropy: $H\left(\frac{p}{p+n}, \frac{n}{p+n}\right)$

Average Entropy after Split:

$$\mathbb{E} = \frac{1}{N} \sum_{i=1}^N H\left(P(j = X_{i,j} | Y_i = 0), P(x_j = X_{i,j} | Y_i = 1)\right)$$

- Don't worry, we'll explore the use of standard distributions more soon!

Choosing an Attribute

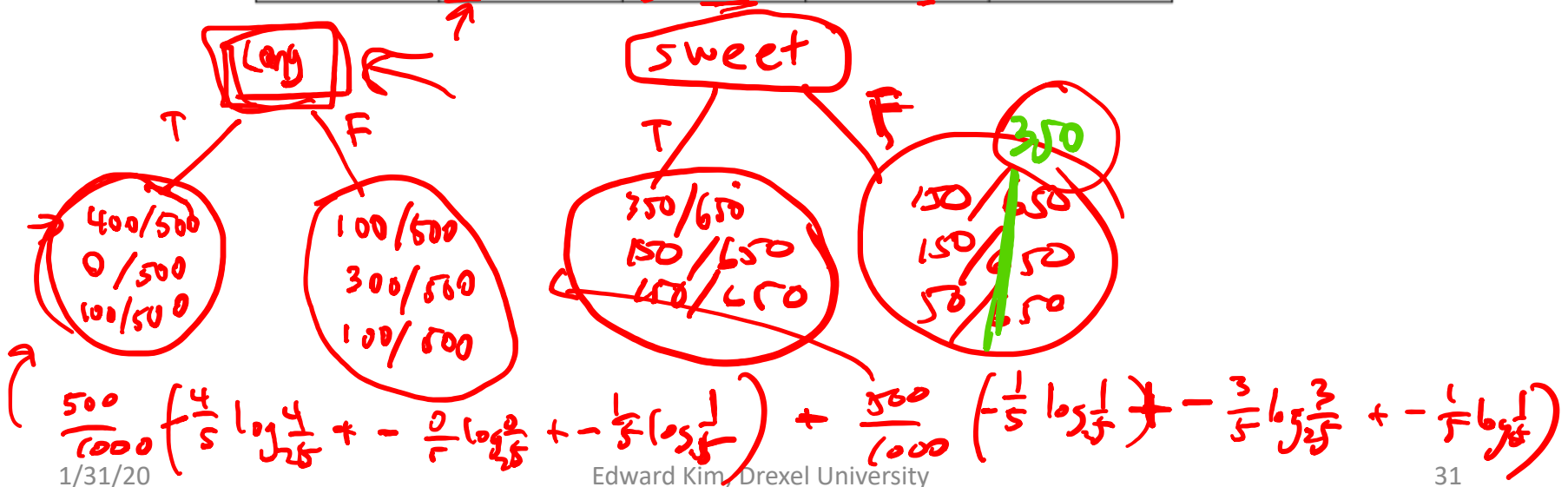
- While there's many ideas on how to choose the next attribute, let's use something we already talked about!
- Information gain/entropy!
- Recall the formula for entropy:

$$H(P(v_1), \dots, P(v_n)) = \sum_{i=1}^n -P(v_i) \log_n P(v_i)$$

Choosing an Attribute

- Idea: A good attribute splits the examples into subsets that contain (ideally) observations from just one class.

Fruit	Long	Sweet	Yellow	Total
Banana	400	350	450	500
Orange	0	150	300	300
Other	100	150	50	200
Total	500	650	800	1000



Example

Fruit	Long	Sweet	Yellow	Total
Banana	400	350	450	500
Orange	0	150	300	300
Other	100	150	50	200
Total	500	650	800	1000

- Building a tree completely using information gain is called the ID3 decision tree algorithm
- Let's build this ID3 DT all the way out!
- To do this we'll need a little more information

Banana			
Long	Sweet	Yellow	Count
F	F	F	50
F	F	T	50
F	T	F	0
F	T	T	0
T	F	F	0
T	F	T	50
T	T	F	0
T	T	T	350

Orange			
Long	Sweet	Yellow	Count
F	F	F	0
F	F	T	150
F	T	F	0
F	T	T	150
T	F	F	0
T	F	T	0
T	T	F	0
T	T	T	0

Other			
Long	Sweet	Yellow	Count
F	F	F	0
F	F	T	0
F	T	F	50
F	T	T	50
T	F	F	50
T	F	T	0
T	T	F	50
T	T	T	0

ID3 Example

Banana			
Long	Sweet	Yellow	Count

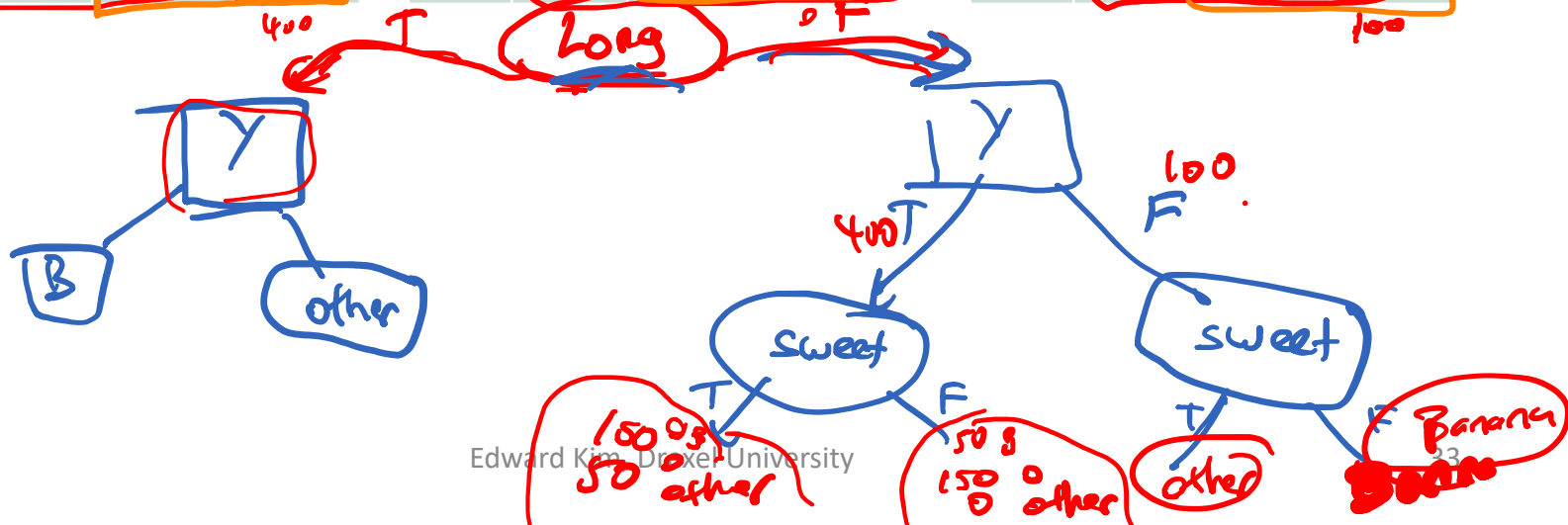
F	F	F	50
F	F	T	50
F	T	F	0
F	T	T	0
T	F	F	0
T	F	T	50
T	T	F	0
T	T	T	350

Orange			
Long	Sweet	Yellow	Count

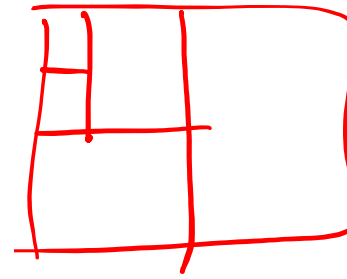
F	F	F	0
F	F	T	150
F	T	F	0
F	T	T	150
T	F	F	0
T	F	T	0
T	T	F	0
T	T	T	0

Other			
Long	Sweet	Yellow	Count

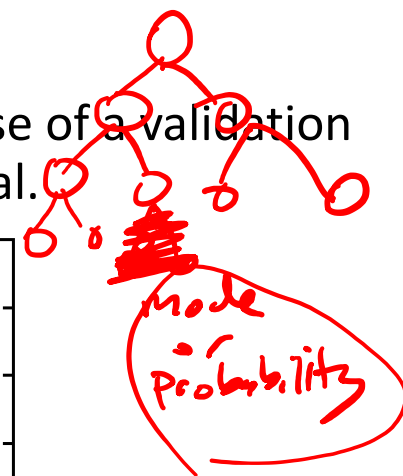
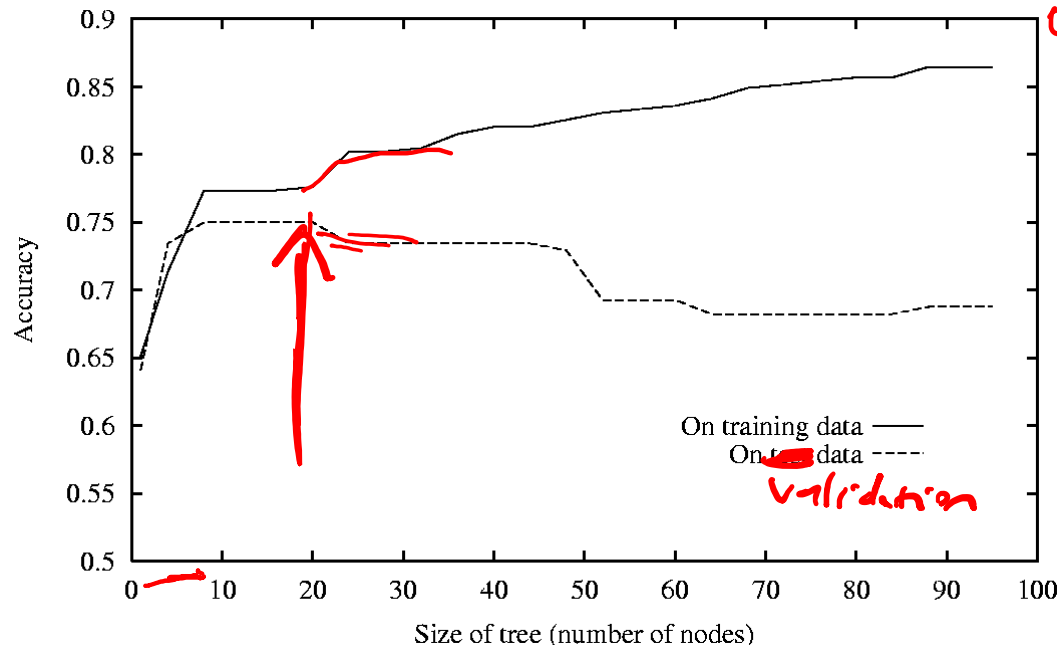
F	F	F	0
F	F	T	0
F	T	F	50
F	T	T	50
T	F	F	50
T	F	T	0
T	T	F	50
T	T	T	0



Overfitting



- What's the problem with fitting our data as closely as possible?
 - We may overfit the data!
- Since this is an iterative (or recursive) algorithm, the use of a validation set to decide between different versions is quite natural.



Reduced Error Approaches

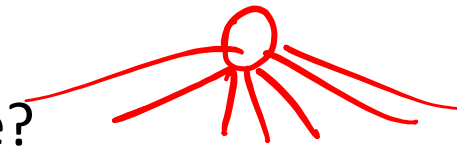
- How can we use the validation set?
- Evaluate it during the growing process.
 - At each *incomplete* branch, just assign the **mode** label of the data going down it.
- Find the level of growth that maximizes the accuracy of the validation set (or conversely minimizes the error).
- Then report test accuracy for that version.
- Reduced Error Growing
 - When you look to split a node based on training data, evaluating after using *validation set*
 - If things get worse, stop
- Reduced Error Pruning
 - Evaluate impact on *validation* set of pruning each possible node (plus those below it)
 - Greedily remove the one that most improve *validation* set accuracy
 - Continue until none help

Other Ideas

- There are other ideas....
- Pruning
 - Try removing each of the splits that happen before leaf nodes and evaluate the validation set on each of them.
 - As long as one of them improves the validation evaluation, remove the one that improves things the most
 - Keep doing this until no removal improves validation evaluation.
- Or maybe we could somehow use statistics to halt the growing process
 - If the information gain provided by a split is above some threshold, split, otherwise don't

Continuous Valued Inputs

- What if we have features that have continuous values?
 - One branch for each value?
 - Bad idea!!!! (impossible?)
- If we know the range of our values and we set how many branches the node should make then
 - Divide range evenly?
 - Somehow do it more intelligently?



$$x_i > 0 \quad y_i = 1$$
$$x_i < 0 \quad y_i = 0$$