CPSC 340: Machine Learning and Data Mining

Decision Trees

Fall 2018

Admin

- Assignment 1 is due Friday: start early.
- Waiting list people: you should be registered soon-ish.
  - Start on the assignment now.
  - Grad not wanting grad credit: you maybe able to register in 340?
- Course webpage: www.ugrad.cs.ubc.ca/~cs340
  - Sign for Piazza and an undergrad account.
- Tutorials and office hours start this week.
  - Office hours calendar: http://www.cs.ubc.ca/~mgelbart/calendar.html
- Auditing: message me on Piazza if you want to audit.
  - We're still waiting to see if everyone gets in.

Last Time: Data Representation and Exploration

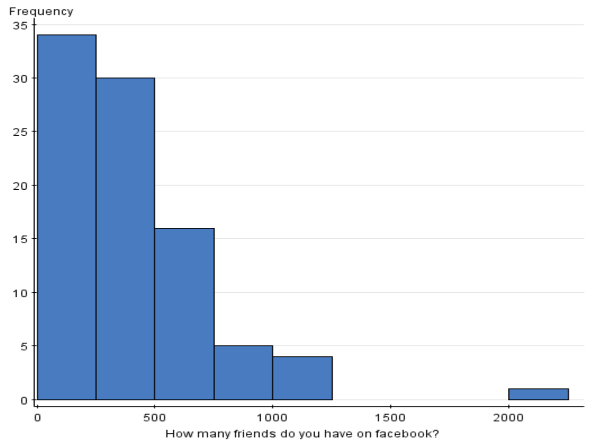
- We discussed example-feature representation:
  - Samples: another name we'll use for examples.

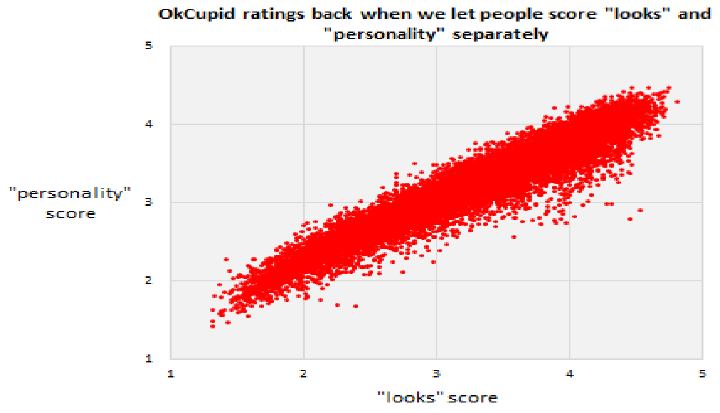
"Feature"

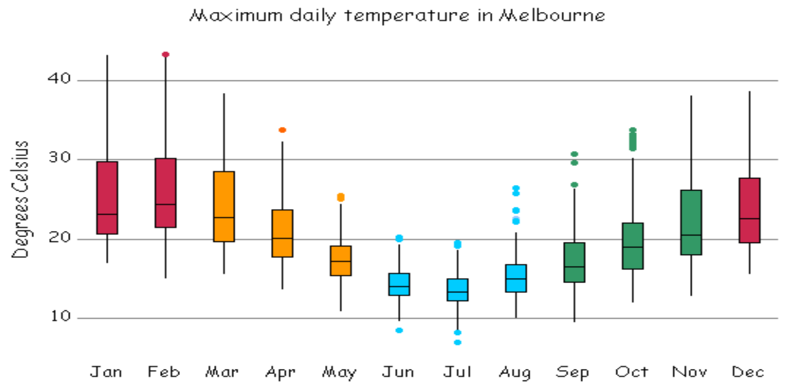
Age	Job?	City	Rating	Income
23	Yes	Van	A	22,000.00
23	Yes	Bur	BBB	21,000.00
22	No	Van	CC	0.00
25	Yes	Sur	AAA	57,000.00

"Example"

- We discussed summary statistics and visualizing data.







http://www.statcrunch.com/5.0/viewresult.php?resid=1024581
http://cdn.okccdn.com/blog/humanexperiments/looks-v-personality.png
http://www.scc.ms.unimelb.edu.au/whatisstatistics/weather.html

Last Time: Supervised Learning

- We discussed supervised learning:

Egg	Milk	Fish	Wheat	Shellfish	Peanuts	…
0	0.7	0	0.3	0	0	
0.3	0.7	0	0.6	0	0.01	
0	0	0	0.8	0	0	
0.3	0.7	1.2	0	0.10	0.01	
0.3	0	1.2	0.3	0.10	0.01	

Sick?
1
1
0
1
1

- Input for an example (day of the week) is a set of features (quantities of food).
- Output is a desired class label (whether or not we got sick).
- Goal of supervised learning:
  – Use data to find a model that outputs the right label based on the features.
  – Model predicts whether foods will make you sick (even with new combinations).
  – This framework can be applied any problem where we have input/output examples.

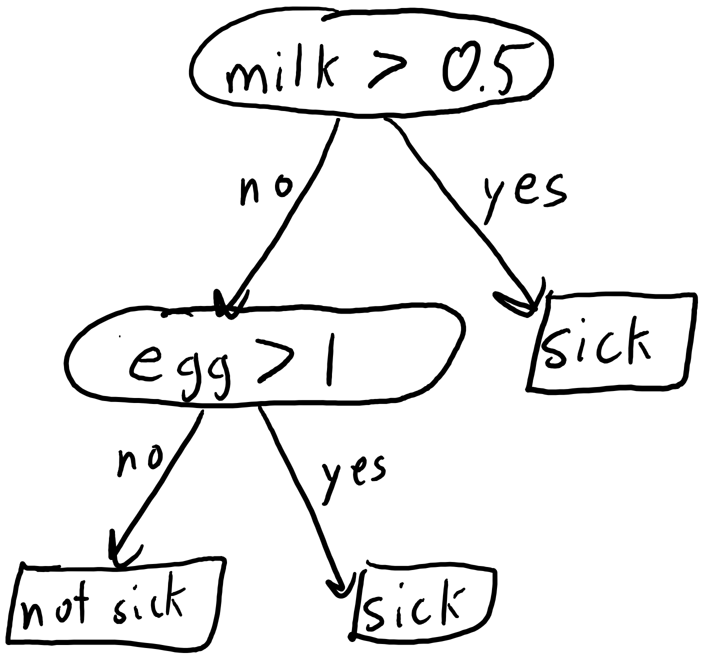
Decision Trees

- Decision trees are simple programs consisting of:
  - A nested sequence of "if-else" decisions based on the features (splitting rules).
  - A class label as a return value at the end of each sequence.

- Example decision tree:

```
if (milk > 0.5)
        {
                return 'sick'
        }
        else
        {
                if (egg > 1)
                        return 'sick'
                else
                        return 'not sick'
        }
```

Can draw sequences of decisions as a tree:



Supervised Learning as Writing A Program

- There are many possible decision trees.
  - We're going to search for one that is good at our supervised learning problem.

- So our input is data and the output will be a program.
  - This is called "training" the supervised learning model.
  - Different than usual input/output specification for writing a program.

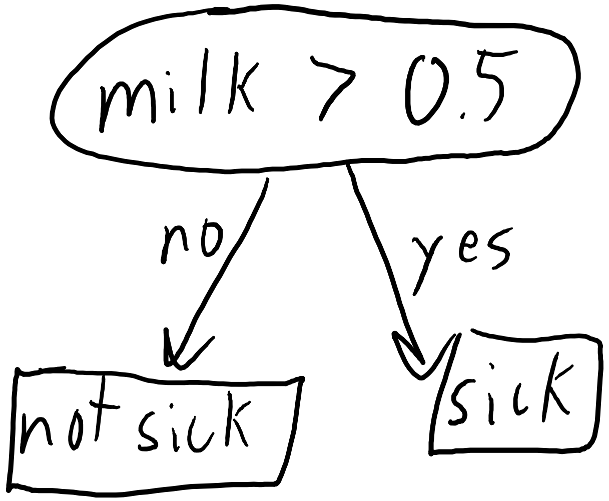
- Supervised learning is useful when you have lots of labeled data BUT:
  1. Problem is too complicated to write a program ourselves.
  2. Human expert can't explain why you assign certain labels.

     OR

  2. We don't have a human expert for the problem.

Learning A Decision Stump: "Search and Score"

- We'll start with "decision stumps":
  - Simple decision tree with 1 splitting rule based on thresholding 1 feature.



- How do we find the best "rule" (feature, threshold, and leaf labels)?
  1. Define a 'score' for the rule.
  2. Search for the rule with the best score.

Learning A Decision Stump: Accuracy Score

- Most intuitive score: classification accuracy.
  - "If we use this rule, how many examples do we label correctly?"
- Computing classification accuracy for (egg > 1):
  - Find most common labels if we use this rule:
    - When (egg > 1), we were "sick" 2 times out of 2.
    - When (egg ≤ 1), we were "not sick" 3 times out of 4.
  - Compute accuracy:
    - The accuracy ("score") of the rule (egg > 1) is 5 times out of 6.

Milk	Fish	Egg
0.7	0	1
0.7	0	2
0	0	0
0.7	1.2	0
0	1.2	2
0	0	0

Sick?
1
1
0
0
1
0

- This "score" evaluates quality of a rule.
  - We "learn" a decision stump by finding the rule with the best score.

Learning A Decision Stump: By Hand

- Let’s search for the decision stump maximizing classification score:

Milk	Fish	Egg
0.7	0	1
0.7	0	2
0	1.2	0
0.7	1.2	0
0	1.3	2
0	0	0

Sick?
1
1
0
0
1
0

First we check the “baseline” rule of doing nothing: this gets 3/6 accuracy.
If (milk > 0) predict “sick” (2/3) else predict “not sick” (2/3): 4/6 accuracy
If (fish > 0) predict “not sick” (2/3) else predict “sick” (2/3): 4/6 accuracy
If (fish > 1.2) predict “sick” (1/1) else predict “not sick” (3/5): 5/6 accuracy
If (egg > 0) predict “sick” (3/3) else predict “not sick” (3/3): 6/6 accuracy
If (egg > 1) predict “sick” (2/2) else predict “not sick” (3/4): 5/6 accuracy

- Highest-scoring rule: (egg > 0) with leaves “sick” and “not sick”.
- Notice we only need to test feature thresholds that happen in the data:
  - There is no point in testing the rule (egg > 3), it gets the “baseline” score.
  - There is no point in testing the rule (egg > 0.5), it gets the (egg > 0) score.
  - Also note that we don’t need to test “<“, since it would give equivalent rules.

Supervised Learning Notation (MEMORIZE THIS)

$$X = \begin{array}{c} \begin{array}{cccccc} \text{Egg} & \text{Milk} & \text{Fish} & \text{Wheat} & \text{Shellfish} & \text{Peanuts} \end{array} \\ \left.\left[\underbrace{\begin{array}{cccccc} 0 & 0.7 & 0 & 0.3 & 0 & 0 \\ 0.3 & 0.7 & 0 & 0.6 & 0 & 0.01 \\ 0 & 0 & 0 & 0.8 & 0 & 0 \\ 0.3 & 0.7 & 1.2 & 0 & 0.10 & 0.01 \\ 0.3 & 0 & 1.2 & 0.3 & 0.10 & 0.01 \end{array}}_{\text{'d'}}\right]\right\} \text{'n'} \end{array} \qquad y = \begin{array}{c} \text{Sick?} \\ \left.\left[\begin{array}{c} 1 \\ 1 \\ 0 \\ 1 \\ 1 \end{array}\right]\right\} \text{'n'} \end{array}$$

- Feature matrix 'X' has rows as examples, columns as features.
  - x_{ij} is feature 'j' for example 'i' (quantity of food 'j' on day 'i').
  - x_i is the list of all features for example 'i' (all the quantities on day 'i').
  - x^j is column 'j' of the matrix (the value of feature 'j' across all examples).
- Label vector 'y' contains the labels of the examples.
  - y_i is the label of example 'i' (1 for "sick", 0 for "not sick").

Supervised Learning Notation (MEMORIZE THIS)

$$X = \left.\underbrace{\begin{array}{cccccc} \textbf{Egg} & \textbf{Milk} & \textbf{Fish} & \textbf{Wheat} & \textbf{Shellfish} & \textbf{Peanuts} \\ \hline 0 & 0.7 & 0 & 0.3 & 0 & 0 \\ 0.3 & 0.7 & 0 & 0.6 & 0 & 0.01 \\ 0 & 0 & 0 & 0.8 & 0 & 0 \\ 0.3 & 0.7 & 1.2 & 0 & 0.10 & 0.01 \\ 0.3 & 0 & 1.2 & 0.3 & 0.10 & 0.01 \end{array}}_{'d'}\right\}'n' \qquad y = \left.\begin{array}{c} \textbf{Sick?} \\ \hline 1 \\ 1 \\ 0 \\ 1 \\ 1 \end{array}\right\}'n'$$

- Training phase:
  - Use ‘X’ and ‘y’ to find a ‘model’ (like a decision stump).
- Prediction phase:
  - Given an example x_i, use ‘model’ to predict a label ‘yhat$_i$’ (“sick” or “not sick”). $\hookrightarrow \hat{y}_i$
- Training error:
  - Fraction of times our prediction $\hat{y}_i$ does not equal the true y_i label.

Decision Stump Learning Pseudo-Code

Input: <u>feature matrix</u> X and <u>label vector</u> y

```
Compute error if using "baseline" rule: number of times $y_i$ does not equal most common value.
for each feature 'j' (column of 'X')
    for each threshold 't'
        set 'y-yes' to most common label of objects 'i' satisfying rule ($x_{ij} > t$)
        set 'y-no' to most common label of objects not satisfying rule.
        set '$\hat{y}$' to be our predictions for each object 'i' based on the rule.
        compute error 'E', number of objects where $\hat{y}_i \neq y_i$ ($\hat{y}_i$ = y-yes if satisfied,
                                                                        $\hat{y}_i$ = y-no if not satisfied)
        store the rule (j, t, y-yes, y-no) if it has the lowest error so far.
```

Output: an <u>optimal decision stump rule</u> (the "model")

Cost of Decision Stumps

- How much does this cost?
- Assume we have:
  - 'n' examples (days that we measured).
  - 'd' features (foods that we measured).
  - 'k' thresholds (>0, >1, >2, …) for each feature.
- Computing the score of one rule costs O(n):
  - We need to go through all 'n' examples to find most common labels.
  - We need to go through all 'n' examples again to compute the accuracy.
  - See notes on webpage for review of "O(n)" notation.
- We compute score for up to k*d rules ('k' thresholds for each of 'd' features):
  - So we need to do an O(n) operation k*d times, giving total cost of O(ndk).

Cost of Decision Stumps

- Is a cost of O(ndk) good?
- Size of the input data is O(nd):
  - If ‘k’ is small then the cost is roughly the same cost as loading the data.
    - We should be happy about this, you can learn on any dataset you can load!
  - If ‘k’ is large then this could be too slow for large datasets.

- Example: if all our features are binary then k=1, just test (feature > 0):
  - Cost of fitting decision stump is O(nd), so we can fit huge datasets.
- Example: if all our features are numerical with unique values then k=n.
  - Cost of fitting decision stump is O(n^2d).
    - We don’t like having n^2 because we want to fit datasets where ‘n’ is large!
  - Bonus slides: how to reduce the cost in this case down to O(nd log n).
    - Basic idea: sort features and track labels. Allows us to fit decision stumps to huge datasets.

(pause)

Decision Tree Learning

- Decision stumps have only 1 rule based on only 1 feature.
  - Very limited class of models: usually not very accurate for most tasks.

- Decision trees allow sequences of splits based on multiple features.
  - Very general class of models: can get very high accuracy.
  - However, it's computationally infeasible to find the best decision tree.

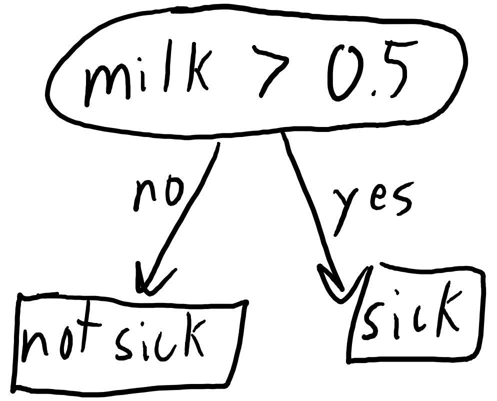
- Most common decision tree learning algorithm in practice:
  - Greedy recursive splitting.

Example of Greedy Recursive Splitting

- Start with the full dataset:

Egg	Milk	…	Sick?
0	0.7		1
1	0.7		1
0	0		0
1	0.6		1
1	0		0
2	0.6		1
0	1		1
2	0		1
0	0.3		0
1	0.6		0
2	0		1

Find the decision stump with the best score:



Split into two smaller datasets based on stump:

Egg	Milk	…	Sick?
0	0		0
1	0		0
2	0		1
0	0.3		0
2	0		1

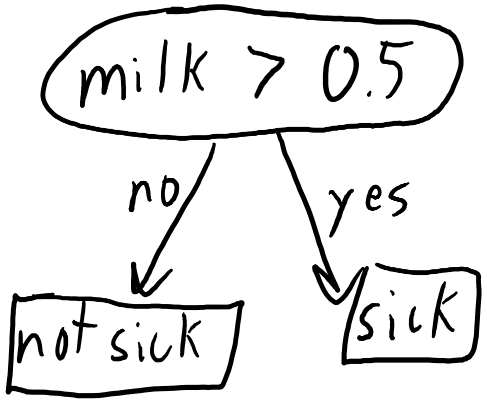
milk ≤ 0.5

Egg	Milk	…	Sick?
0	0.7		1
1	0.7		1
1	0.6		1
2	0.6		1
0	1		1
1	0.6		0

> 0.5

Greedy Recursive Splitting

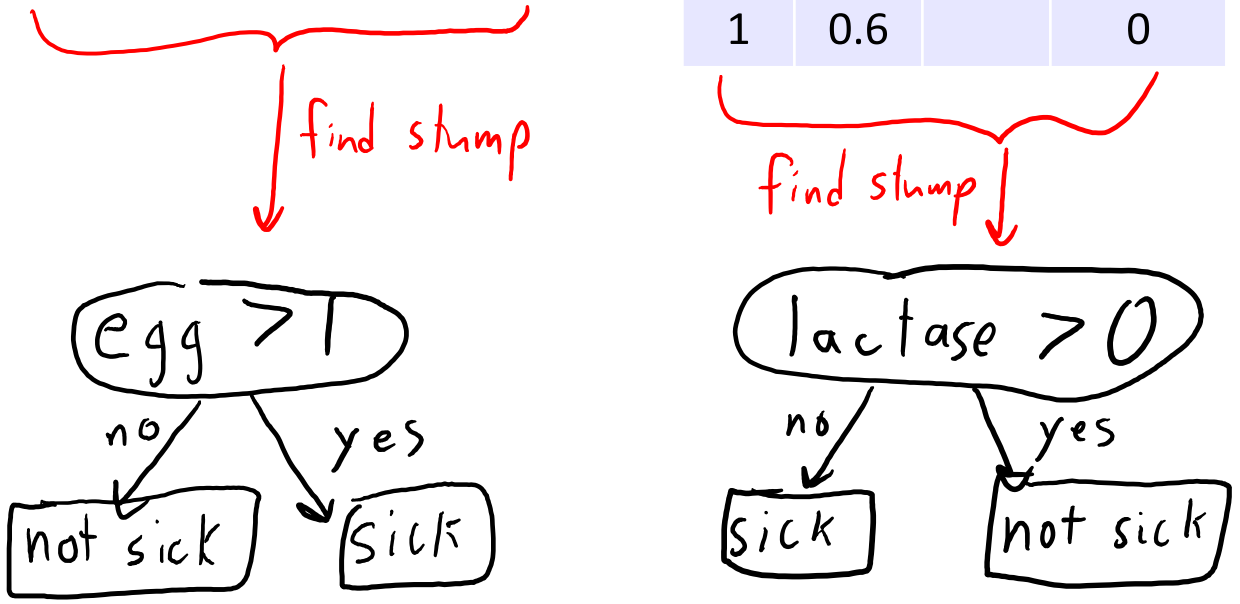
We now have a decision stump and two datasets:



Egg	Milk	…	Sick?
0	0		0
1	0		0
2	0		1
0	0.3		0
2	0		1

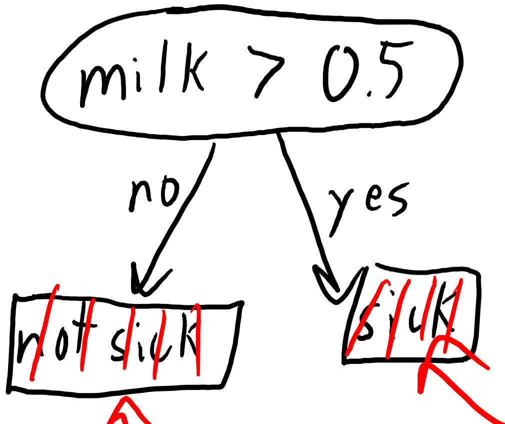
Egg	Milk	…	Sick?
0	0.7		1
1	0.7		1
1	0.6		1
2	0.6		1
0	1		1
1	0.6		0

Fit a decision stump to each leaf's data.



Greedy Recursive Splitting

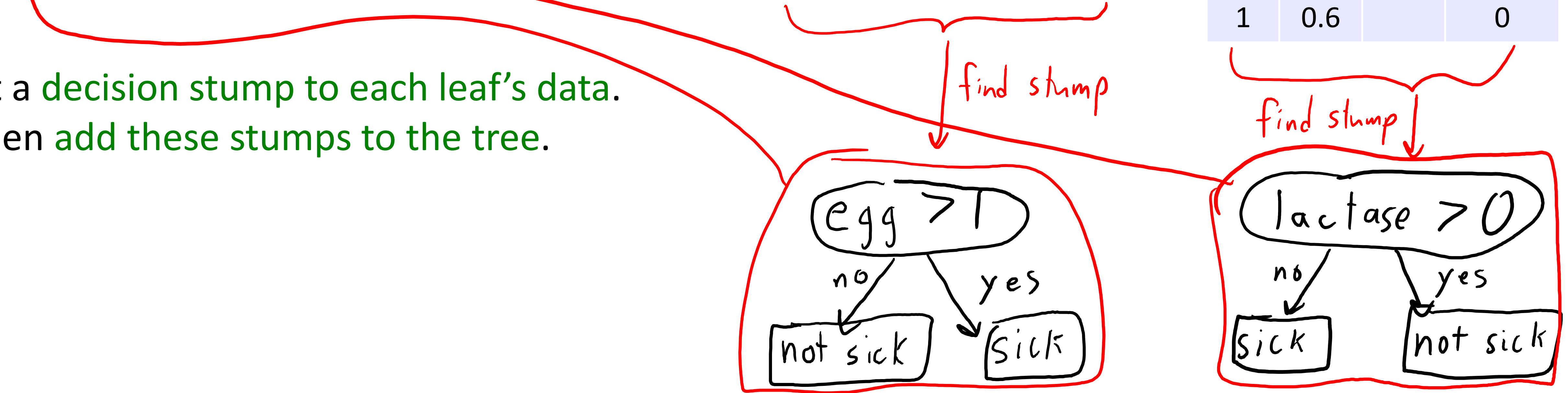
We now have a decision stump and two datasets:



Egg	Milk	...	Sick?
0	0		0
1	0		0
2	0		1
0	0.3		0
2	0		1

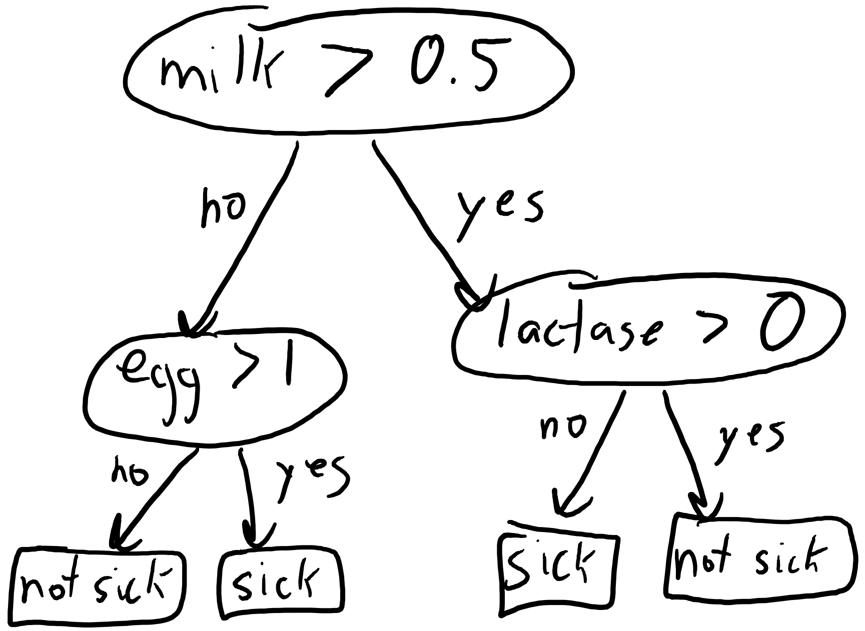
Egg	Milk	...	Sick?
0	0.7		1
1	0.7		1
1	0.6		1
2	0.6		1
0	1		1
1	0.6		0

Fit a decision stump to each leaf's data.
Then add these stumps to the tree.



Greedy Recursive Splitting

This gives a "depth 2" decision tree:



It splits the two datasets into four datasets:

milk ≤ 0.5 data

Egg	Milk	...	Sick?
0	0		0
1	0		0
2	0		1
0	0.3		0
2	0		1

milk > 0.5 data

Egg	Milk	...	Sick?
0	0.7		1
1	0.7		1
1	0.6		1
2	0.6		1
0	1		1
1	0.6		0

milk ≤ 0.5, egg ≤ 1

Egg	Milk	...	Sick?
0	0		0
1	0		0
0	0.3		0

Much more accurate!

milk < 0.5, egg > 1

Egg	Milk	...	Sick?
2	0		1
2	0		1

milk > 0.5, lactase ≤ 0

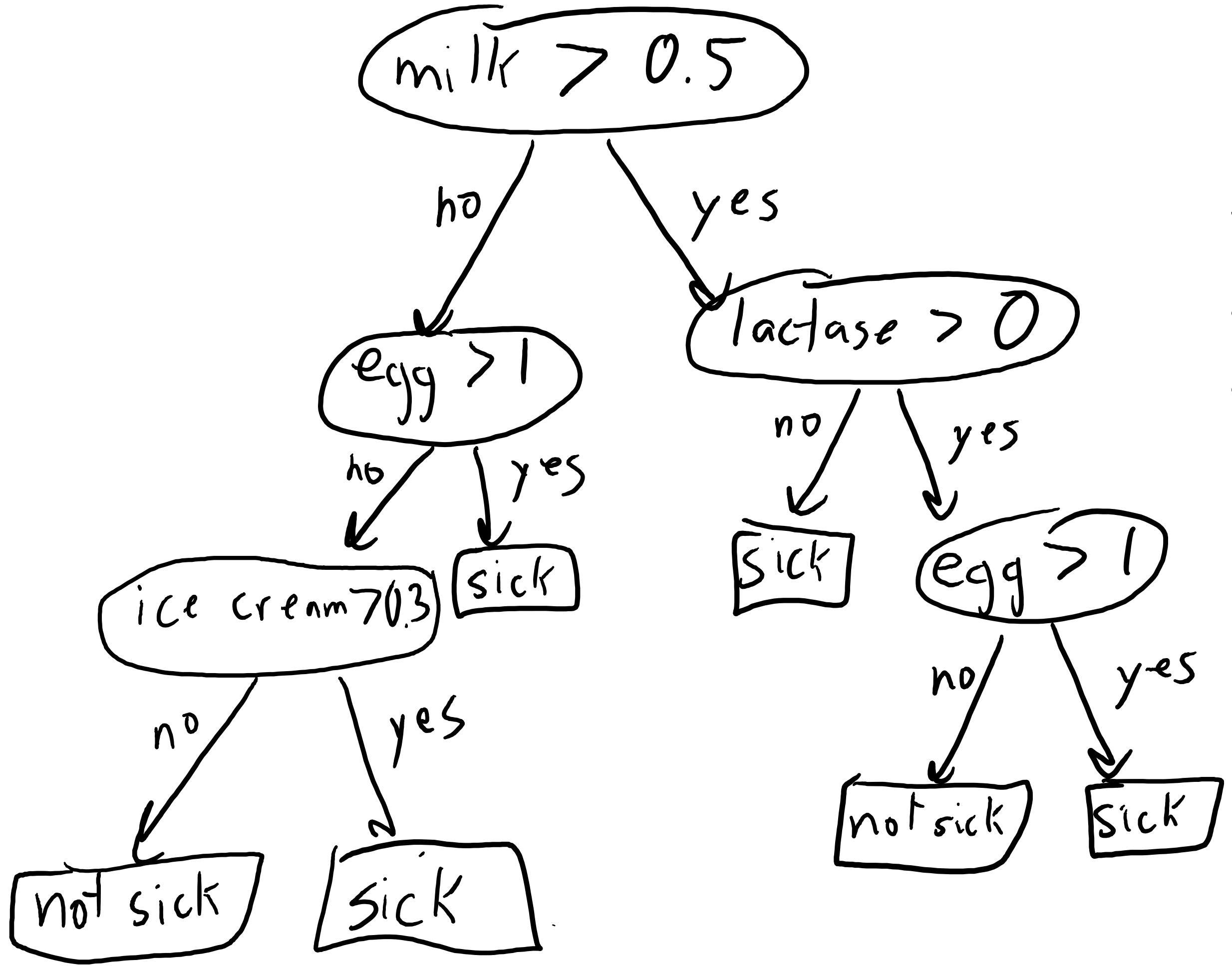
Egg	Milk	...	Sick?
0	0.7		1
1	0.7		1
1	0.6		1
2	0.6		1

milk > 0.5, lactase > 0

Egg	Milk	...	Sick?
1	0.6		0

Greedy Recursive Splitting

We could try to split the four leaves to make a "depth 3" decision tree:



We might continue splitting until:

- The leaves each have only one label.
- We reach a user-defined maximum depth.

Which score function should a decision tree used?

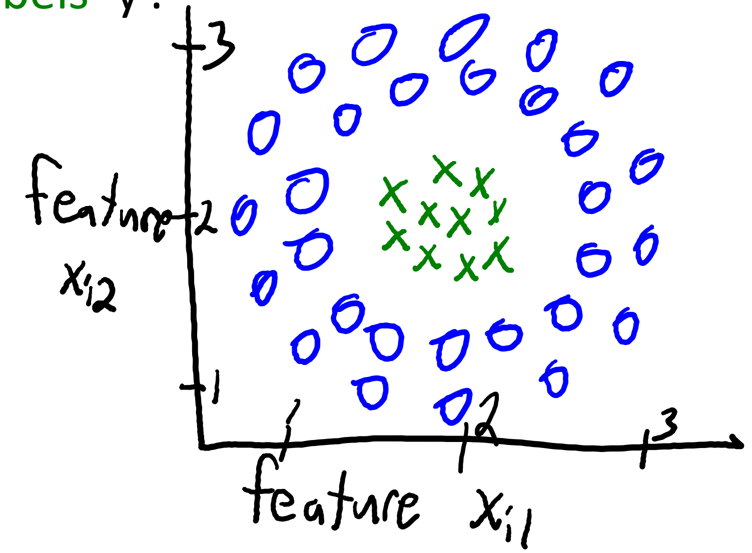
- Shouldn’t we just use accuracy score?
  - For leafs: yes, just maximize accuracy.
  - For internal nodes: maybe not.

- Maybe no simple rule like (egg > 0.5) improves accuracy.
  - But this doesn’t necessarily mean we should stop!

Example Where Accuracy Fails

- Consider a dataset with 2 features and 2 classes (‘x’ and ‘o’).
  - Because there are 2 features, we can draw ‘X’ as a scatterplot.
    - Colours and shapes denote the class labels ‘y’.

$$X = \begin{bmatrix} 1.2 & 2.1 \\ 3.3 & 1.4 \\ 2.0 & 2.1 \\ 2.2 & 2.1 \\ 4.0 & 3.4 \\ \vdots & \vdots \end{bmatrix} \quad y = \begin{bmatrix} \text{'o'} \\ \text{'o'} \\ \text{'x'} \\ \text{'x'} \\ \text{'o'} \\ \vdots \end{bmatrix}$$



- A decision stump would divide space by a horizontal or vertical line.
  - Testing whether $x_{i1} > t$ or whether $x_{i2} > t$.
- On this dataset no horizontal/vertical line improves accuracy.
  - Baseline is ‘o’, but need to get many ‘o’ wrong to get one ‘x’ right.

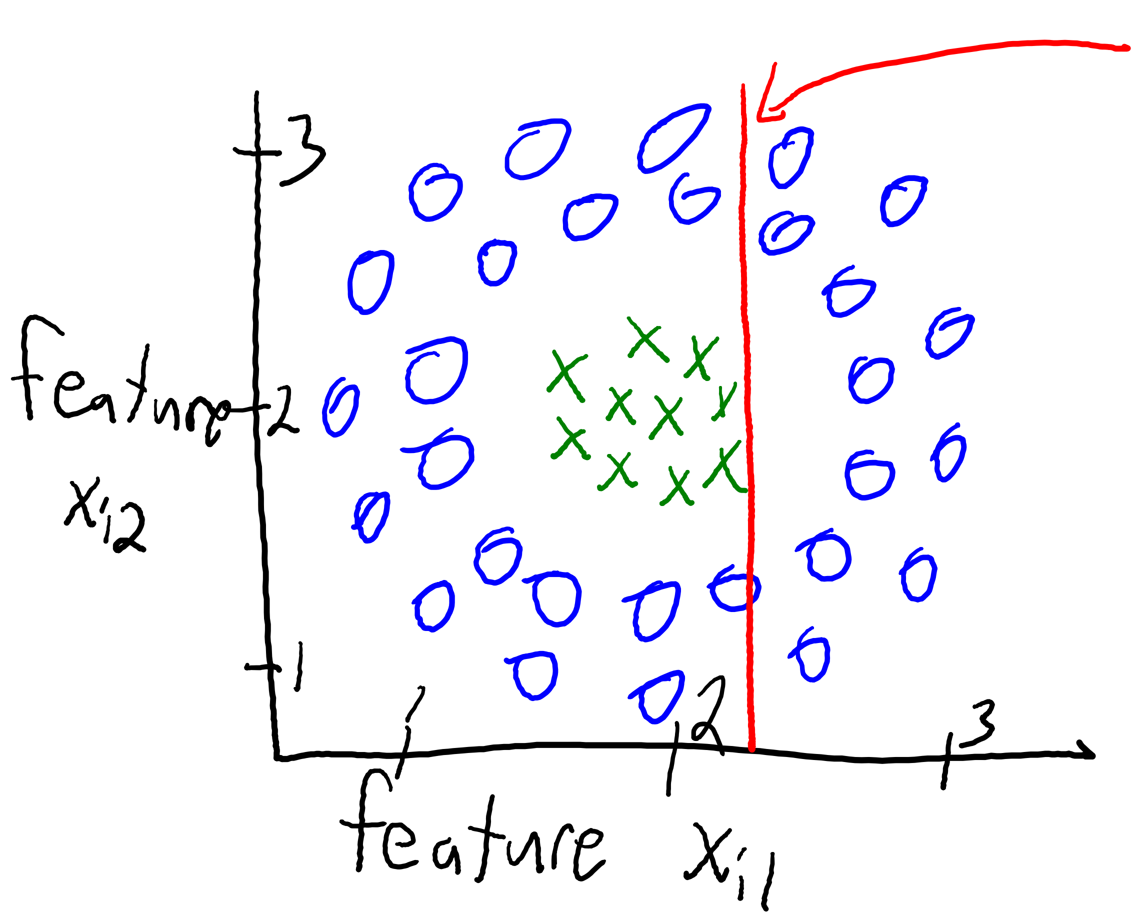
Which score function should a decision tree used?

- Most common score in practice is "information gain".
  - "Choose split that decreases entropy of labels the most".

$$\text{information gain} = \underbrace{\text{entropy}(y)}_{\text{entropy of labels before split}} - \underset{\substack{\uparrow \\ \text{number of examples satisfying rule}}}{\frac{n_{yes}}{n}} \underset{\substack{\uparrow \\ \text{entropy of labels for examples satisfying rule.}}}{\text{entropy}(y_{yes})} - \frac{n_{no}}{n}\text{entropy}(y_{no})$$

- Information gain for baseline rule ("do nothing") is 0.
  - Infogain is large if labels are "more predictable" ("less random") in next layer.
- Even if it does not increase classification accuracy at one depth, we hope that it makes classification easier at the next depth.

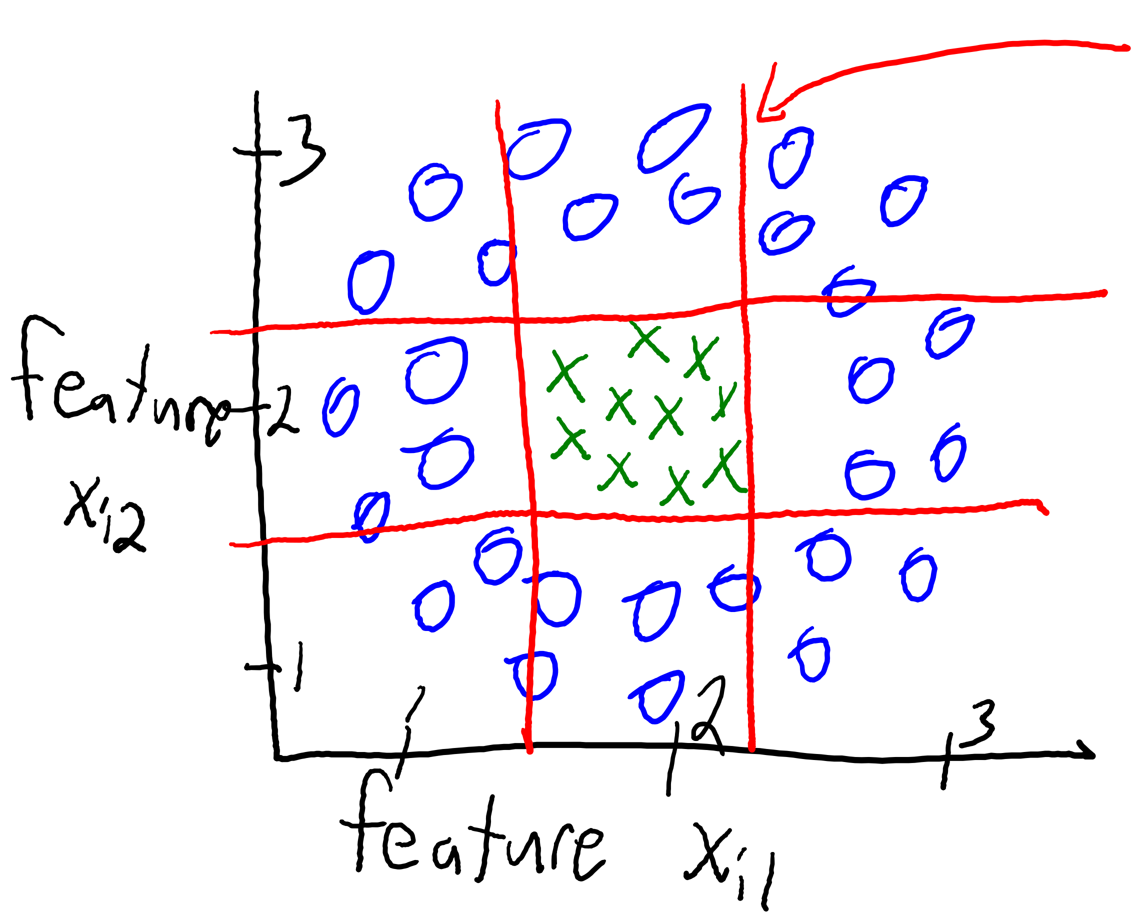
Example Where Accuracy Fails



This split makes labels less random.
(Everything on the right is a 'o')

It did not improve accuracy.
(still classifies everything as 'o')

Example Where Accuracy Fails



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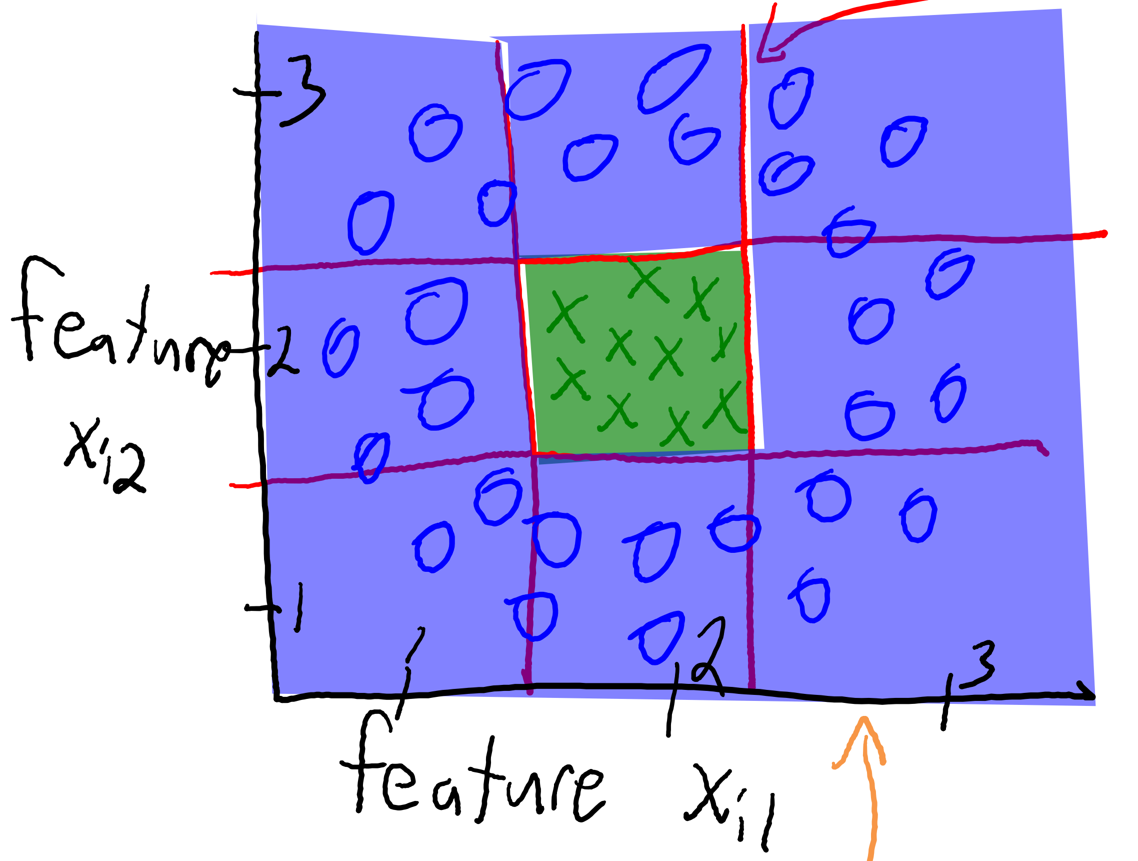
But three more splits maximizing infogain lead to perfect accuracy.

Example Where Accuracy Fails



This split makes labels less random. (Everything on the right is a 'o')

It did not improve accuracy. (still classifies everything as 'o')

But three more splits maximizing infogain lead to perfect accuracy.

Using colours to show decisions in regions of space

Discussion of Decision Tree Learning

- Advantages:
  - Easy to implement.
  - Interpretable.
  - Learning is fast prediction is very fast.
  - Can elegantly handle a small number missing values during training.
- Disadvantages:
  - Hard to find optimal set of rules.
  - Greedy splitting often not accurate, requires very deep trees.
- Issues:
  - Can you revisit a feature?
    - Yes, knowing other information could make feature relevant again.
  - More complicated rules?
    - Yes, but searching for the best rule gets much more expensive.
  - What is best score?
    - Infogain is the most popular and often works well, but is not always the best.
  - What depth?

Summary

- Supervised learning:
  - Using data to write a program based on input/output examples.
- Decision trees: predicting a label using a sequence of simple rules.
- Decision stumps: simple decision tree that is very fast to fit.
- Greedy recursive splitting: uses a sequence of stumps to fit a tree.
  - Very fast and interpretable, but not always the most accurate.
- Information gain: splitting score based on decreasing entropy.

- Next time: the most important ideas in machine learning.

Entropy Function

```
Input: vector 'y' of length 'n' with numbers {1, 2, ..., k}
    counts = zeros(k)
    for i in 1:n
        counts[y[i]] += 1
    entropy = 0
    for c in 1:k
        prob = counts[c]/n
        entropy -= prob * log(prob)
    return entropy
```

Other Considerations for Food Allergy Example

- What types of preprocessing might we do?
  - Data cleaning: check for and fix missing/unreasonable values.
  - Summary statistics:
    - Can help identify "unclean" data.
    - Correlation might reveal an obvious dependence ("sick" ⇔ "peanuts").
  - Data transformations:
    - Convert everything to same scale? (e.g., grams)
    - Add foods from day before? (maybe "sick" depends on multiple days)
    - Add date? (maybe what makes you "sick" changes over time).
  - Data visualization: look at a scatterplot of each feature and the label.
    - Maybe the visualization will show something weird in the features.
    - Maybe the pattern is really obvious!
- What you do might depend on how much data you have:
  - Very little data:
    - Represent food by common allergic ingredients (lactose, gluten, etc.)?
  - Lots of data:
    - Use more fine-grained features (bread from bakery vs. hamburger bun)?

Julia Decision Stump Code (not O(n log n) yet)

Input: feature matrix X and label vector y

```
(n, d) = size(X)
minError = sum(y != mode(y))      compute error if you don't split (user-defined function "mode")
minRule = []
for j = 1:d                       for each feature 'j'
    for i = 1:n                       for each example 'i'
        t = X[i,j]                        set threshold to feature 'j' in example 'i'!
        y_above = mode(y[X[:,j].> t])     find mode of label vector when feature 'j' is above threshold
        y_below = mode(y[X[:,j].<= t])    find mode of label vector when feature 'j' is below threshold.
        yhat = fill(y_above, n)           classify all examples based on threshold
        yhat[X[:,j].<= t] = y_below

        error = sum(yhat != y)            count the number of errors.
        if error < minError               store this rule if it has the lowest error so far.
            minError = error
            minRule = [j  t]
```

Going from $O(n^2d)$ to $O(nd \log n)$ for Numerical Features

- Do we have to compute score from scratch?
  - As an example, assume we eat integer number of eggs:
    - So the rules (egg > 1) and (egg > 2) have same decisions, except when (egg == 2).
- We can actually compute the best rule involving 'egg' in O(n log n):
  - Sort the examples based on 'egg', and use these positions to re-arrange 'y'.
  - Go through the sorted values in order, updating the counts of #sick and #not-sick that both satisfy and don't satisfy the rules.
  - With these counts, it's easy to compute the classification accuracy (see bonus slide).
- Sorting costs O(n log n) per feature.
- Total cost of updating counts is O(n) per feature.
- Total cost is reduced from $O(n^2d)$ to O(nd log n).
- This is a good runtime:
  - O(nd) is the size of data, same as runtime up to a log factor.
  - We can apply this algorithm to huge datasets.

How do we fit stumps in O(nd log n)?

- Let’s say we’re trying to find the best rule involving milk:

Egg	Milk	…
0	0.7	
1	0.7	
0	0	
1	0.6	
1	0	
2	0.6	
0	1	
2	0	
0	0.3	
1	0.6	
2	0	

Sick?
1
1
0
1
0
1
1
1
0
0
1

First grab the milk column and sort it (using the sort positions to re-arrange the sick column). This step costs O(n log n) due to sorting.

Now, we’ll go through the milk values in order, keeping track of #sick and #not sick that are above/below the current value. E.g., #sick above 0.3 is 5.

With these counts, accuracy score is (sum of most common label above and below)/n.

Milk
0
0
0
0
0.3
0.6
0.6
0.6
0.7
0.7
1

Sick?
0
0
0
0
0
1
1
0
1
1
1

How do we fit stumps in O(nd log n)?

Milk	Sick?
0	0
0	0
0	0
0	0
0.3	0
0.6	1
0.6	1
0.6	0
0.7	1
0.7	1
1	1

Start with the baseline rule () which is always "satisfied":
If satisfied, #sick=5 and #not-sick=**6**.
If not satisfied, #sick=0 and #not-sick=0.
This gives accuracy of (6+0)/n = 6/11.

Next try the rule (milk > 0), and update the counts based on these 4 rows:
If satisfied, #sick=**5** and #not-sick=2.
If not satisfied, #sick=0 and #not-sick=**4**.
This gives accuracy of (5+4)/n = 9/11, which is better.

Next try the rule (milk > 0.3), and update the counts based on this 1 row:
If satisfied, #sick=**5** and #not-sick=1.
If not satisfied, #sick=0 and #not-sick=**5**.
This gives accuracy of (5+5)/n = 10/11, which is better.
(and keep going until you get to the end…)

How do we fit stumps in O(nd log n)?

Milk
0
0
0
0
0.3
0.6
0.6
0.6
0.7
0.7
1

Sick?
0
0
0
0
0
1
1
0
1
1
1

Notice that for each row, updating the counts only costs O(1).
Since there are O(n) rows, total cost of updating counts is O(n).

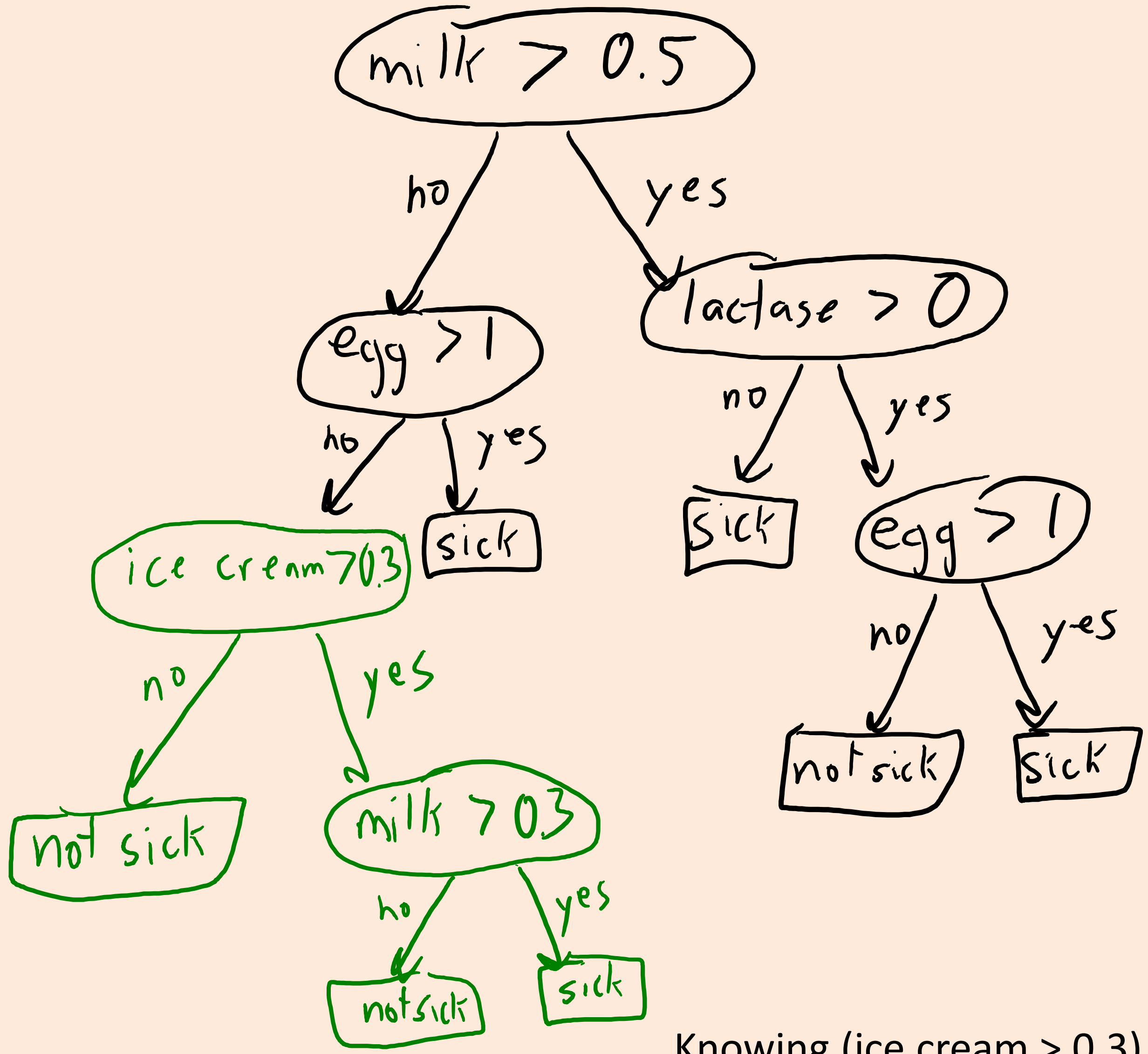
Instead of 2 labels (sick vs. not-sick), consider the case of 'k' labels:
- Updating the counts still costs O(n), since each row has one label.
- But computing the 'max' across the labels costs O(k), so cost is O(kn).

With 'k' labels, you can decrease cost using a "max-heap" data structure:
- Cost of getting max is O(1), cost of updating heap for a row is O(log k).
- But k <= n (each row has only one label).
- So cost is in O(log n) for one row.

Since the above shows we can find best rule in one column in O(n log n), total cost to find best rule across all 'd' columns is O(nd log n).

Can decision trees re-visit a feature?

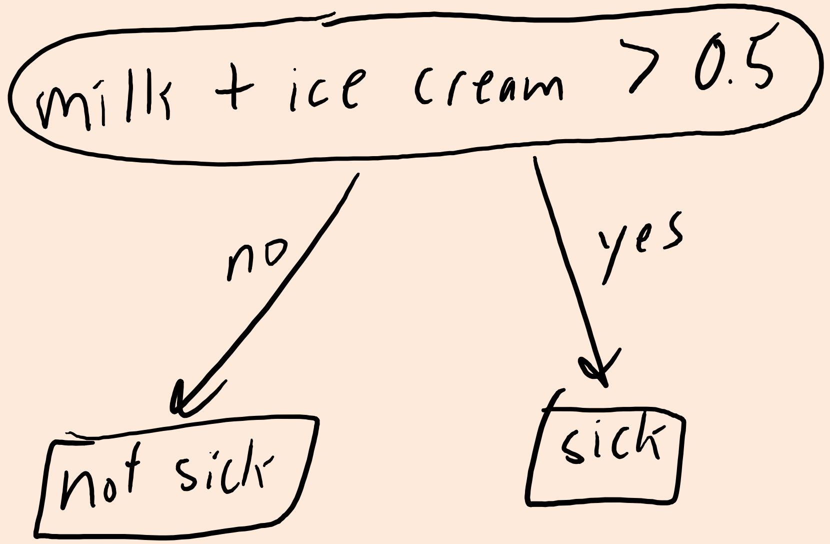
- Yes.



Knowing (ice cream > 0.3) makes small milk quantities relevant.

Can decision trees have more complicated rules?

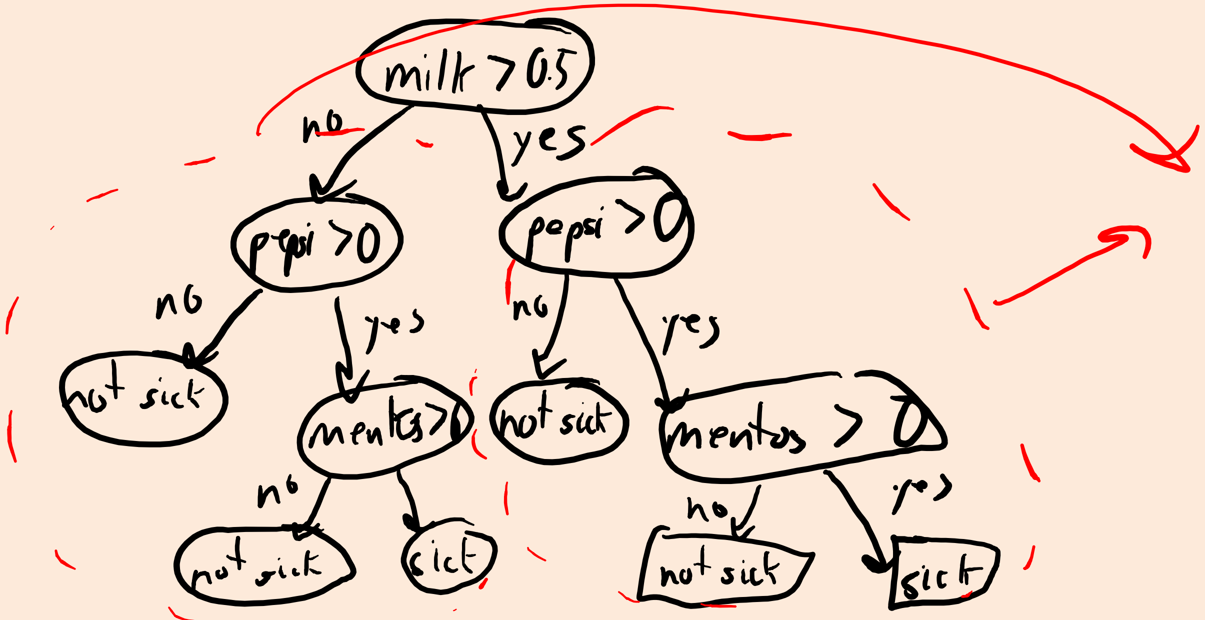
- Yes:



- But searching for best rule can get expensive.

Does being greedy actually hurt?

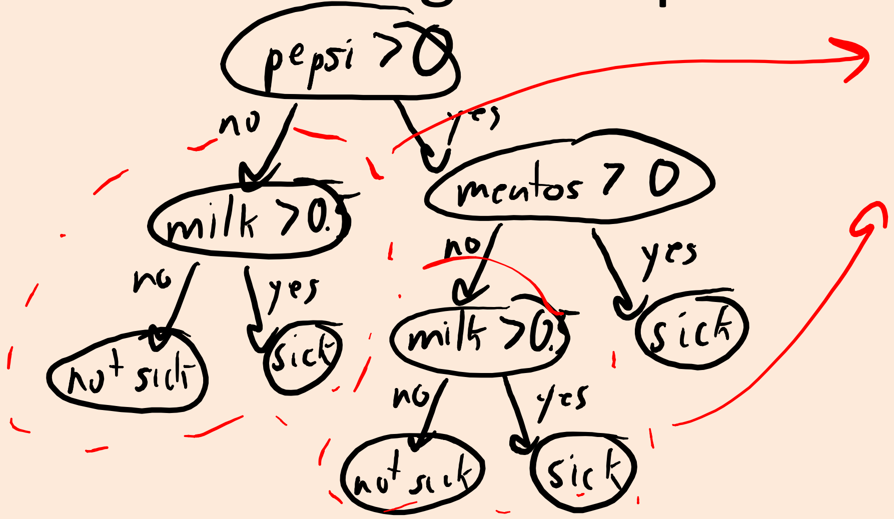
- Can't you just go deeper to correct greedy decisions?
  - Yes, but you need to "re-discover" rules with less data.
- Consider that you are allergic to milk (and drink this often), and also get sick when you (rarely) combine diet coke with mentos.
- Greedy method should first split on milk (helps accuracy the most):



Get same sub-tree, you need learn it twice and with less data.

Does being greedy actually hurt?

- Can't you just go deeper to correct greedy decisions?
  - Yes, but you need to "re-discover" rules with less data.
- Consider that you are allergic to milk (and drink this often), and also get sick when you (rarely) combine diet coke with mentos.
- Greedy method should first split on milk (helps accuracy the most).
- Non-greedy method could get simpler tree (split on milk later):



Still has repeated structure, but you should have more data to estimate these splits.

Decision Trees with Probabilistic Predictions

- Often, we'll have multiple 'y' values at each leaf node.
- In these cases, we might return probabilities instead of a label.

- E.g., if in the leaf node we 5 have "sick" examples and 1 "not sick":
  - Return $p(y = \text{"sick"} \mid x_i) = 5/6$ and $p(y = \text{"not sick"} \mid x_i) = 1/6$.

- In general, a natural estimate of the probabilities at the leaf nodes:
  - Let 'n_k' be the number of examples that arrive to leaf node 'k'.
  - Let 'n_{kc}' be the number of times (y == c) in the examples at leaf node 'k'.
  - Maximum likelihood estimate for this leaf is $p(y = c \mid x_i) = n_{kc}/n_k$.

Alternative Stopping Rules

- There are more complicated rules for deciding when *not* to split.

- Rules based on minimum sample size.
  - Don’t split any nodes where the number of examples is less than some ‘m’.
  - Don’t split any nodes that create children with less than ‘m’ examples.
    - These types of rules try to make sure that you have enough data to justify decisions.

- Alternately, you can use a validation set (see next lecture):
  - Don’t split the node if it decreases an approximation of test accuracy.