Massively Parallel Algorithms
Classification & Prediction
Using Random Forests

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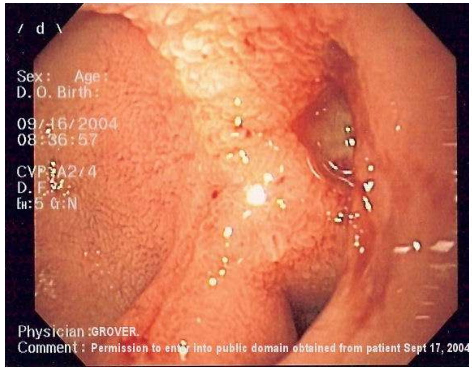
Classification Problem Statement

- Given a set of points $\mathcal{L} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \in \mathbb{R}^d$ and for each such point a label $y_i \in \{l_1, l_2, \ldots, l_n\}$
  - Each label represents a class, all points with the same label are in the same class
- Wanted: a method to decide for a *not-yet-seen* point **x** which label it most probably has, i.e., a method to *predict class labels*
  - We say that we learn a classifier C from the training set $\mathcal{L}$:

$$C : \mathbb{R}^d \rightarrow \{l_1, l_2, \ldots, l_n\}$$

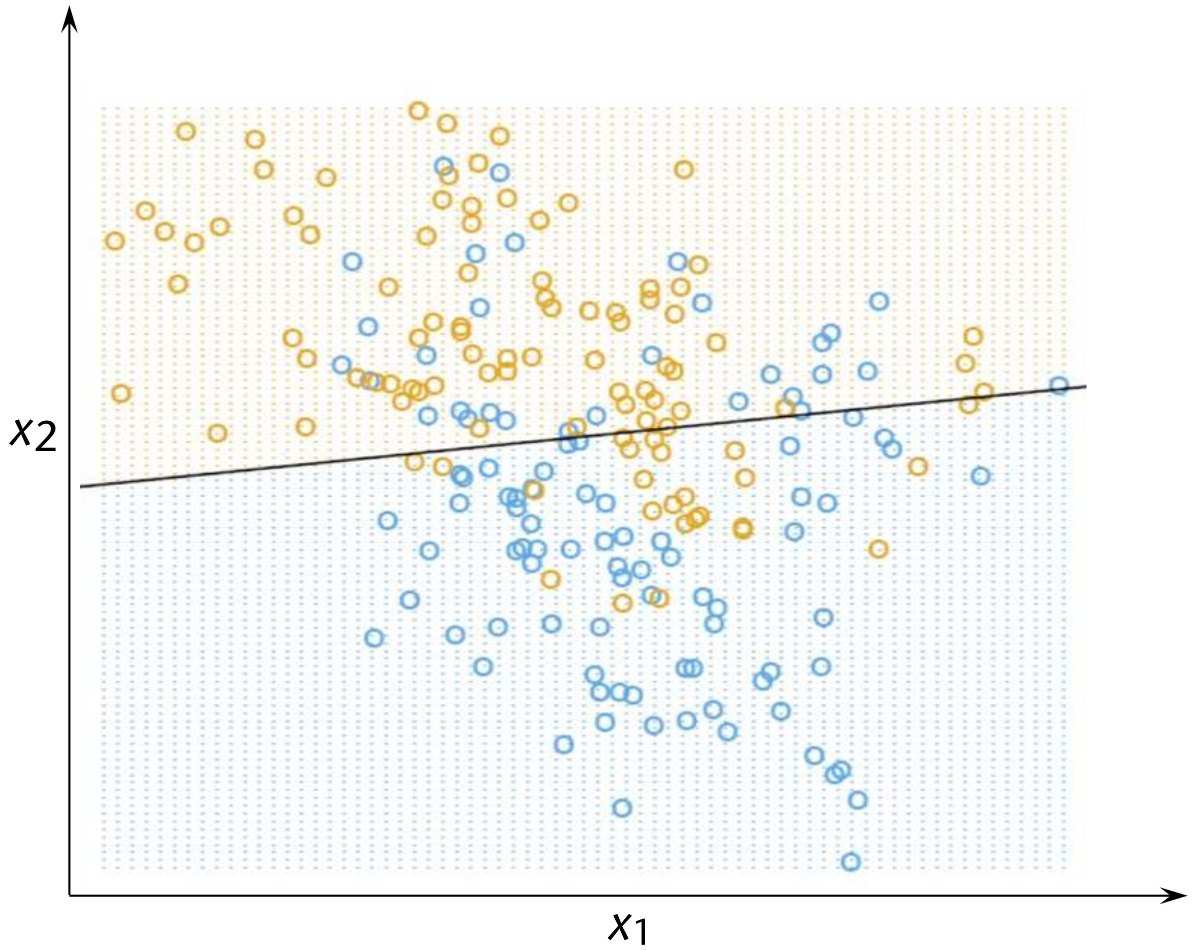
- Typical applications:
  - Computer vision (object recognition, …)
  - Medical diagnosis
  - Credit approval (?)
  - Jurisdiction ?



Ulcer/tumor or not?

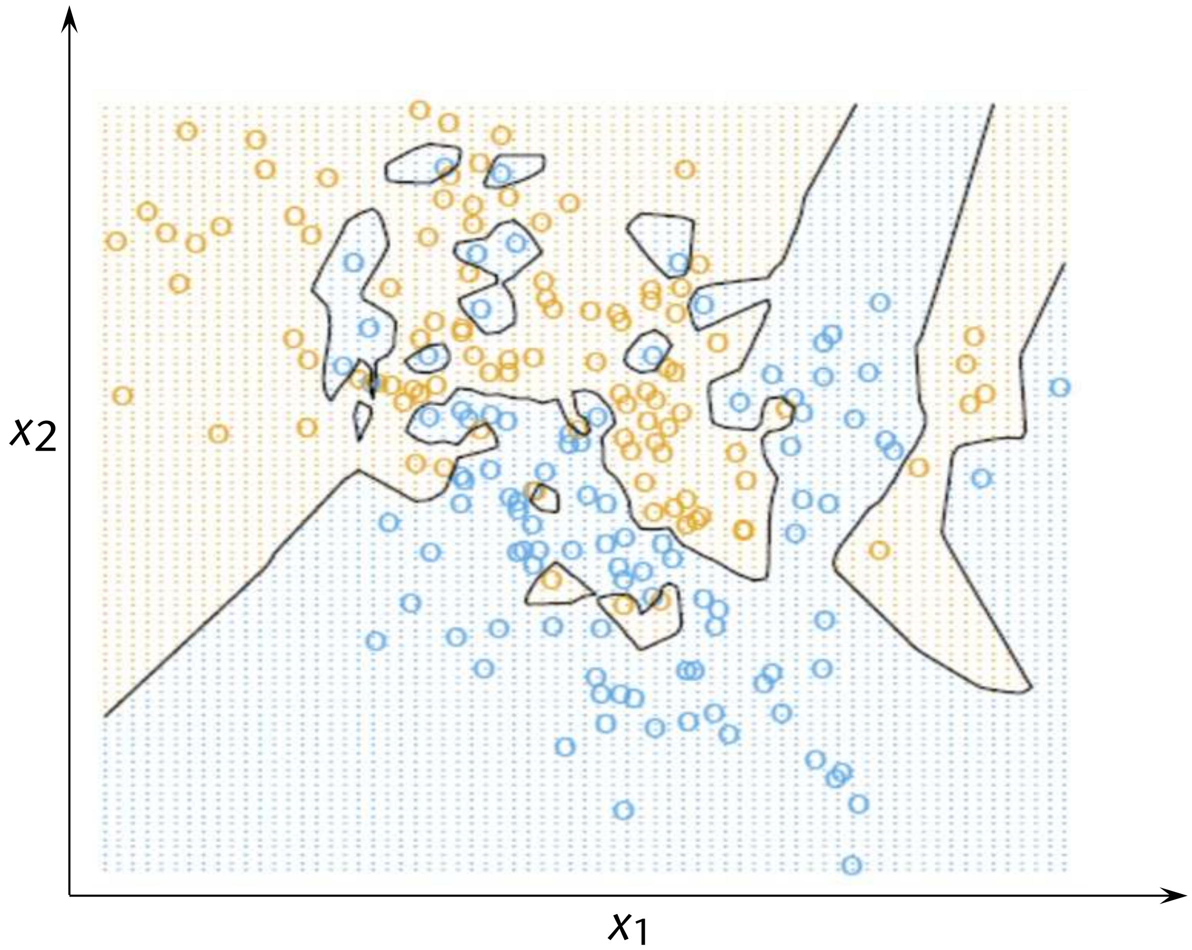
One Possible Solution: Linear Regression

- Assume we have only two classes (e.g., "blue" and "yellow")
- Fit a plane through the data



Another Solution: Nearest Neighbor (NN) Classification

- For the query point **x**, find the nearest neighbor $\mathbf{x}^* \in \{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \in \mathbb{R}^d$
- Assign the class l^* to **x**

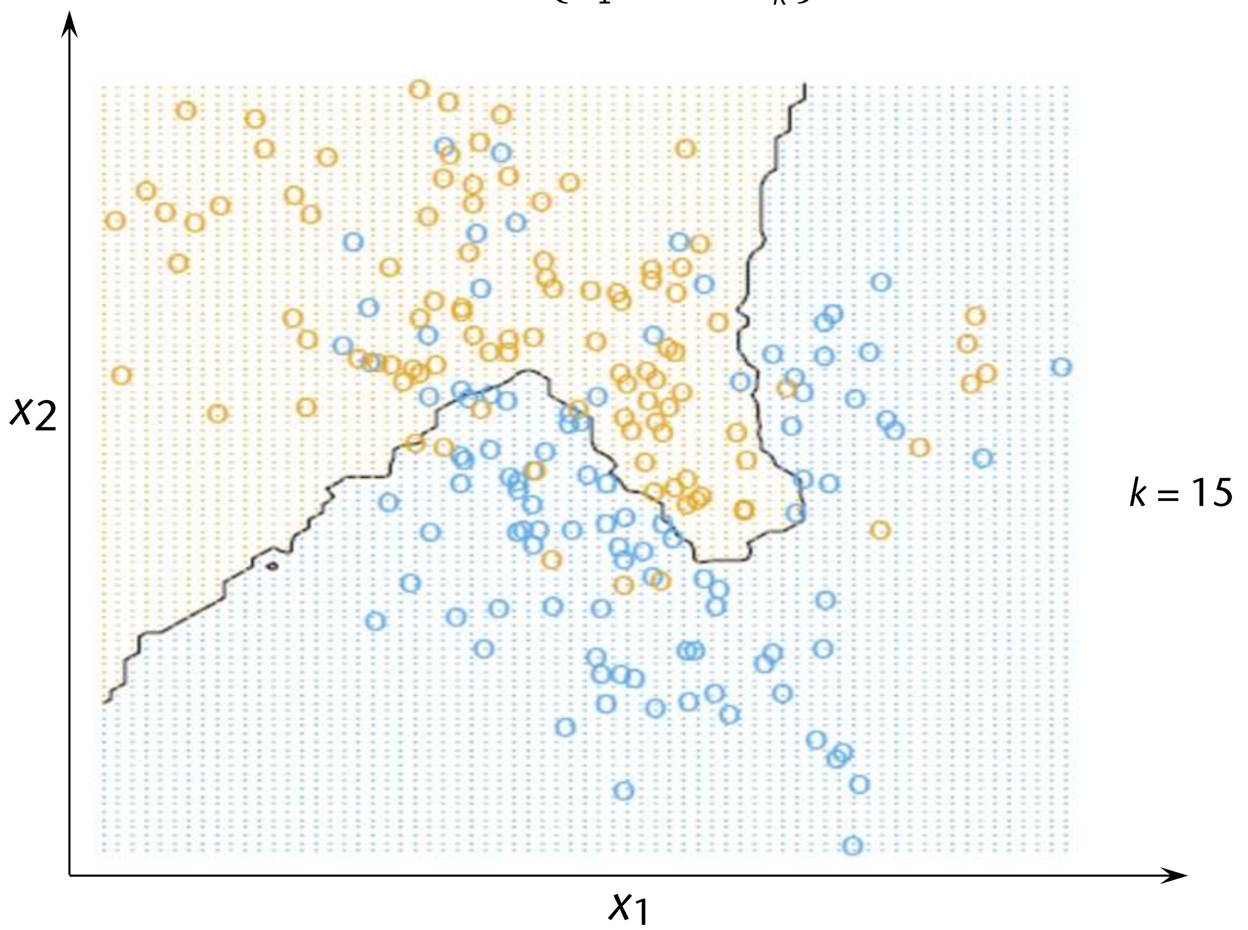


Parallelization

- Trivially:
  - Each thread computes distance $\| \mathbf{x}_i - \mathbf{x} \|$ and stores it in an array
  - All threads perform min reduction
- Can you think of a more clever way?
- What if we have a million queries?

Improvement: *k*-NN Classification

- Instead of the 1 nearest neighbor, find the k nearest neighbors of $\mathbf{x}$, $\{\mathbf{x}_{i_1}, \ldots, \mathbf{x}_{i_k}\} \subset \mathcal{L}$
- Assign the majority of the labels $\{l_{i_1}, \ldots, l_{i_k}\}$ to $\mathbf{x}$



More Terminology

- The coordinates/components $x_{i,j}$ of the points $\mathbf{x}_i$ have special names: independent variables, predictor variables, features, attributes, …
  - Specific name of the $x_{i,j}$ depends on the domain / community
- The space where the $\mathbf{x}_i$ live (i.e., $\mathbb{R}^d$) is called feature space
- The labels y_i are also called target, dependent variable, response variable, …
- The set $\mathcal{L}$ is called the training set / learning set (will become clear later)

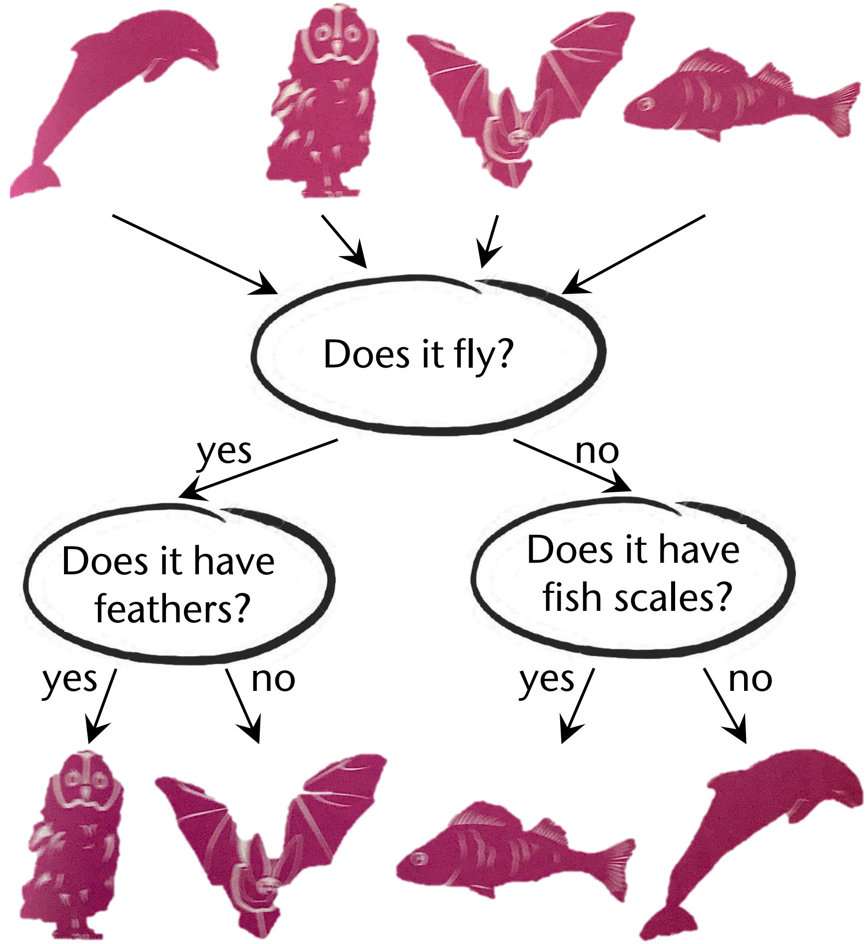
Decision Trees

- Aristotle first described the concept systematically, in order to classify all living things

Branches represent different values of a feature

Each *node* tests one or more feature(s)
This is sometimes called a weak classifier

Leaves represent the classes (decisions)



Another Example

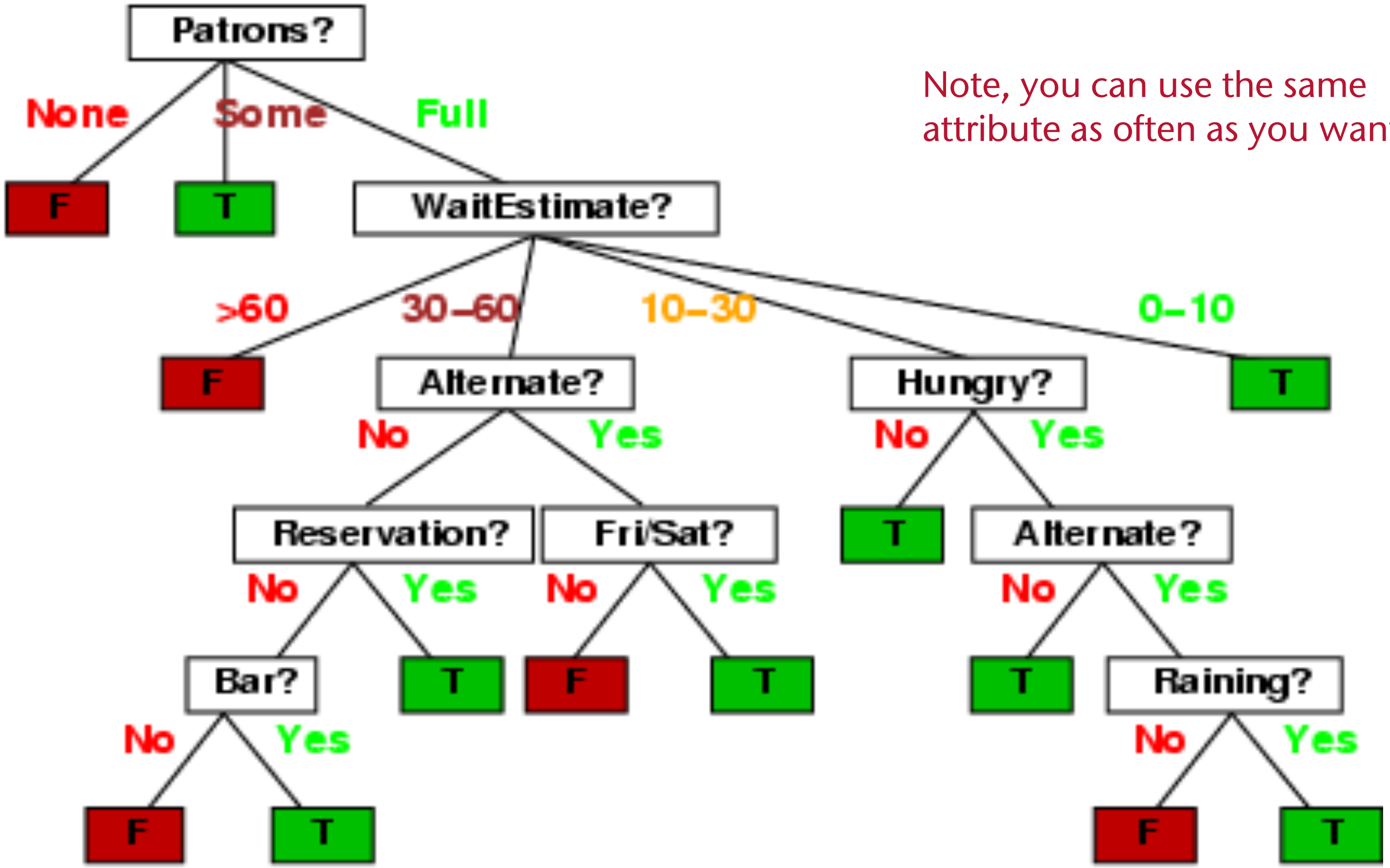
- "Please wait to be seated" ...
- Decide: *wait* or *go* some place else?
- Variables that *could* influence your decision:
  - Alternate: is there an alternative restaurant nearby?
  - Bar: is there a comfortable bar area to wait in?
  - Fri/Sat: is today Friday or Saturday?
  - Hungry: are we hungry?
  - Patrons: number of people in the restaurant (None, Some, Full)
  - Price: price range ($, $$, $$$)
  - Raining: is it raining outside?
  - Reservation: have we made a reservation?
  - Type: kind of restaurant (French, Italian, Thai, Burger)
  - EstimatedWait: estimated waiting time (0-10, 10-30, 30-60, >60)

- You collect data to base your decisions on:

Example	Attributes										Decision
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

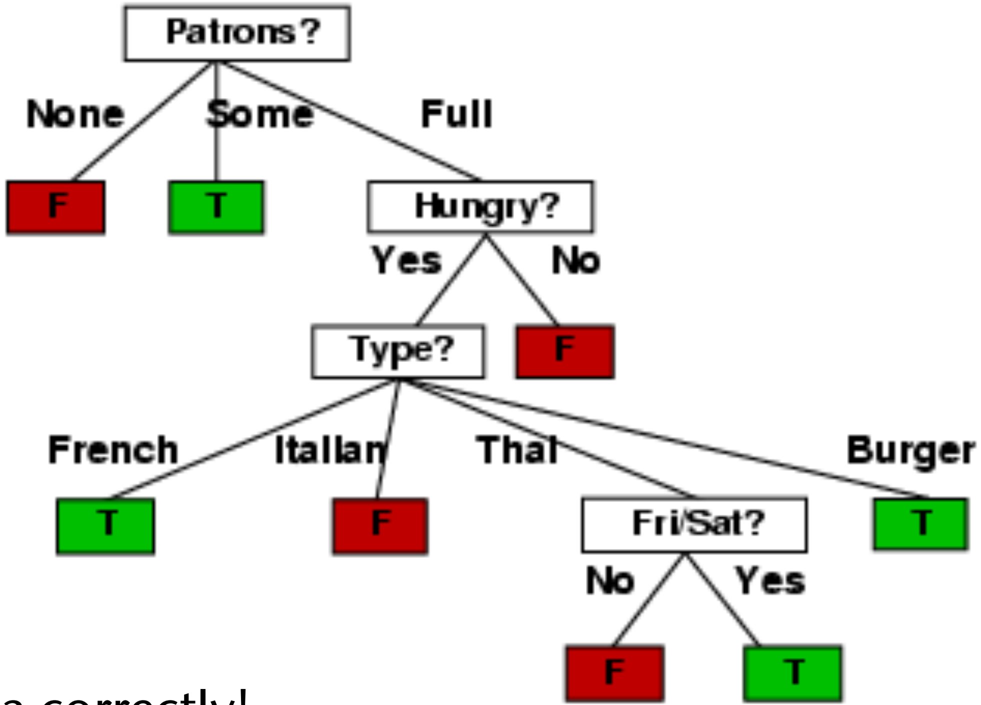
- Feature space: space of all possible feature vectors with all possible combinations of features
  - Here: 10-dimensional, 6 Boolean attributes, 3 discrete attributes, one continuous attribute

- A decision tree that classifies all "training data" correctly:



Note, you can use the same attribute as often as you want

- A better decision tree:



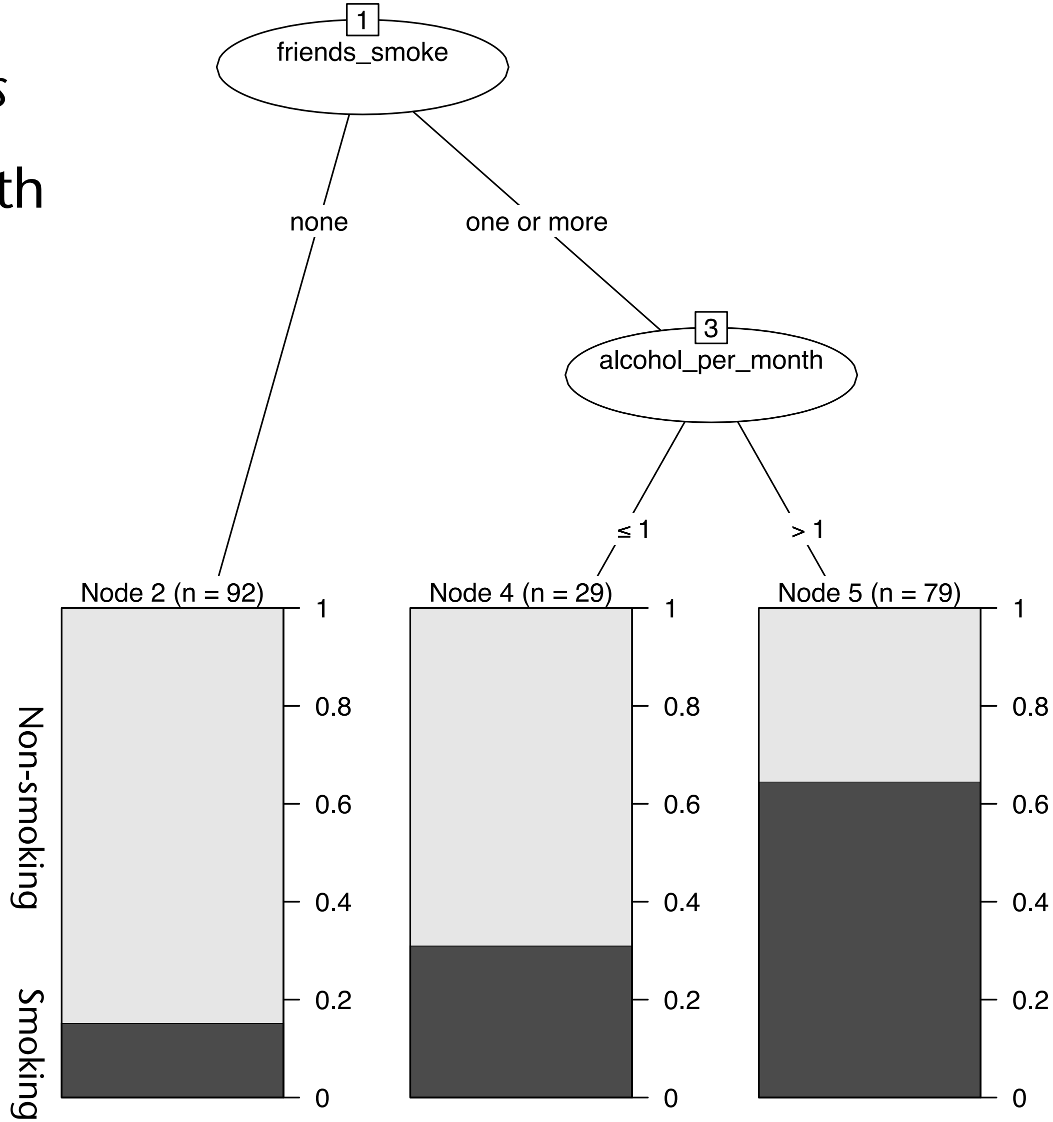
  - Also classifies all training data correctly!
  - Decisions can be made faster
- Questions:
  - How to construct (optimal) decision trees methodically?
  - How well does it generalize/predict? (what is its generalization error?)

Construction (= Learning) of Decision Trees

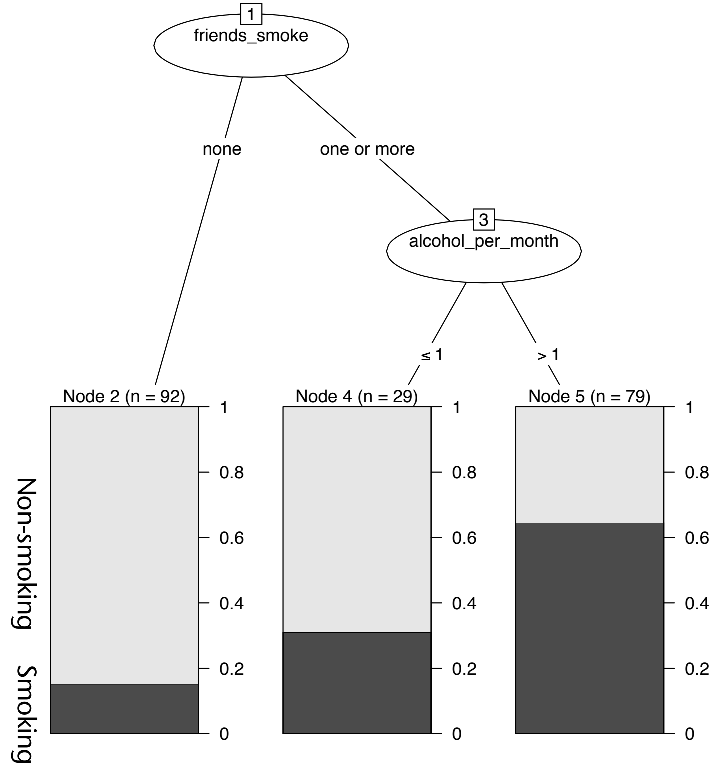
- By way of the following example
- Goal: predict adolescents' intention to smoke within next year
  - Binary response variable *IntentionToSmoke*
- Four predictor variables (= attributes):
  - *LiedToParents* (bool) = subject has ever lied to parents about doing something they would not approve of
  - *FriendsSmoke* (bool) = one or more of the 4 best friends smoke
  - *Age* (int) = subject's current age
  - *AlcoholPerMonth* (int) = # times subject drank alcohol during past month
- Training data:
  - Kitsantas et al.: *Using classification trees to profile adolescent smoking behaviors*. 2007
  - 200 adolescents surveyed

A decision tree

- Root node splits all data points into *two subsets*
- Node 2 = all data points with *FriendsSmoke* = false
- Node 2 contains 92 points, 18% have label "yes", 82% have label "no"
- Ditto for the other nodes

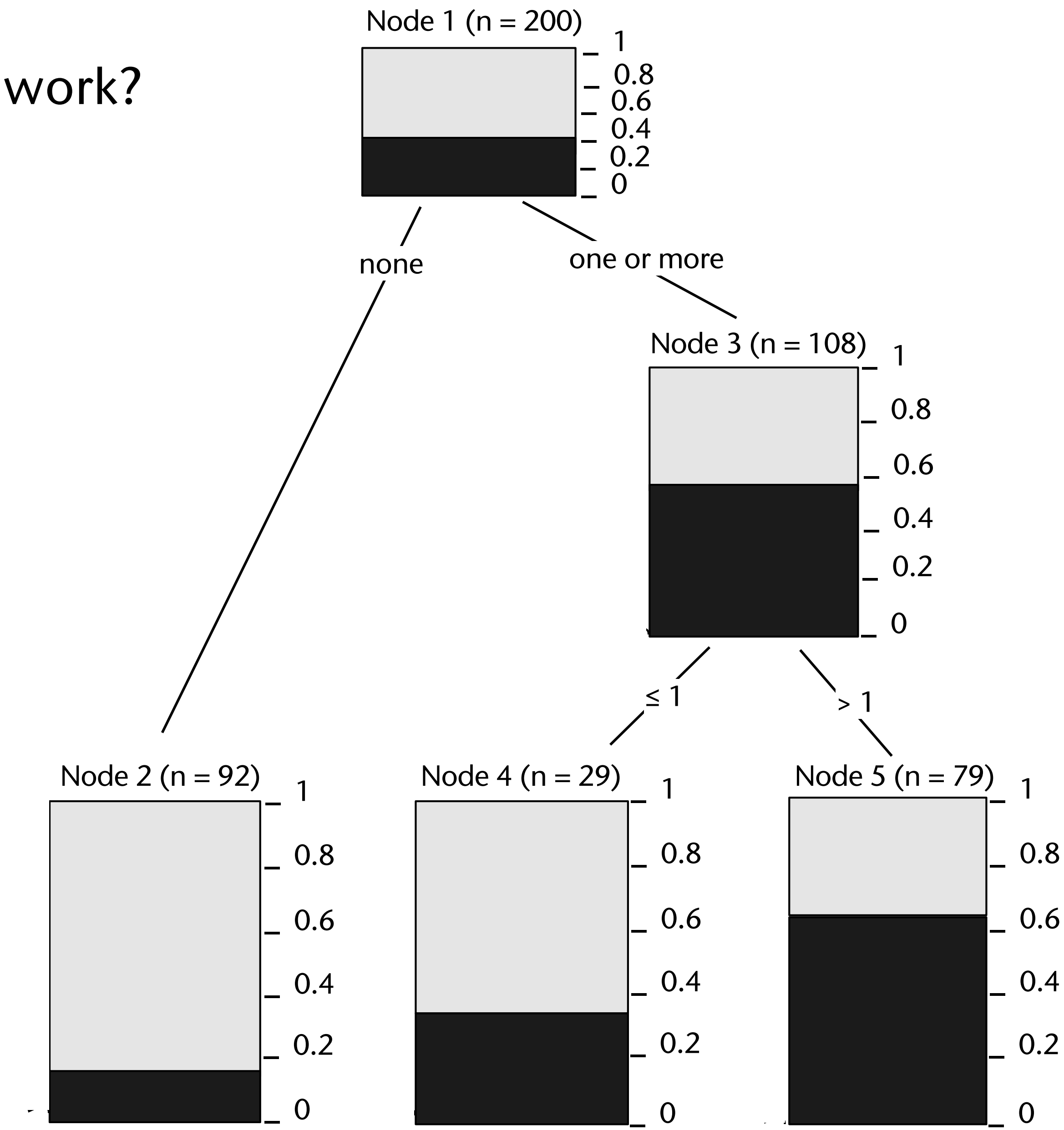


- Observation: a decision tree partitions feature space into rectangular regions (like kd-tree):

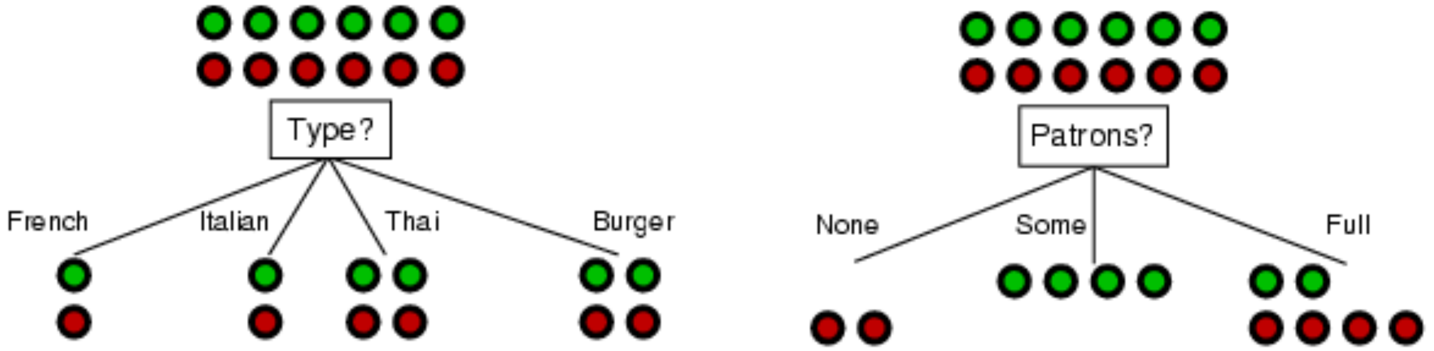


Selection of Splitting Variable and Cutpoint

- Why does our example work?
  - In the root node, *IntentionToSmoke*=yes is 40%
  - In node 2, *IntentionToSmoke*=yes is 18%, while in node 3 *IntentionToSmoke*=yes is 60%
  - So, after first split we can make better predictions

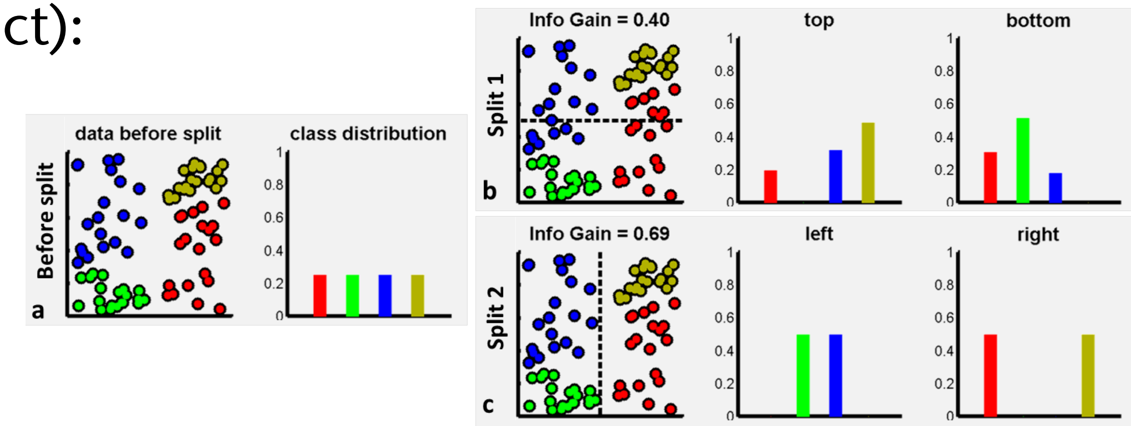


- Ideally, a good attribute (and cutpoint) splits the samples into subsets that are "all positive" or "all negative"
- Example (restaurant):



To wait or not to wait is still at 50%

- Example (abstract):



Goals for Splitting Nodes

- We want:

  (summed "diversity" within children) < ("diversity" in parent)
- Data points should be
  - Homogeneous (by labels) within leaves
  - Different between leaves
- Goal: try to increase purity within subsets
  - *Optimization* goal in each node: find the *attribute* and a *cutpoint* that splits the set of samples into two subsets with *optimal purity*
  - This attribute is the "most discriminative" one for that data (sub-) set
- Question: what is a good measure of purity for two given subsets of our training set?

Digression: Information Gain in Politics/Journalism

- Politician *X* is accused of doing something wrong
- He is asked (e.g., by journalists): "Did you do it?"
- The opposition (assuming *X* is a member of the ruling party) is asked: "Do you think he did it?"
- The answers are reported in the news …
- What information do you gain?

Information Gain

- Enter the information theoretic concept of information gain
- Imagine different events:
  - The outcome of rolling a dice = 6
  - The outcome of rolling a *biased* dice = 6
  - Each situation has a different amount of uncertainty whether or not the event will occur
- Information = *amount of reduction in uncertainty* (= amount of surprise if a specific outcome occurs)

- Quiz:
  - I am thinking of an integer number in [1,100]
  - How many yes/no questions do you need at most to find it out?
  - Answer: $\lceil \log_2 100 \rceil = 7$
- Definition Information Value:
  - Given a set S, the maximum amount of work required to determine a *specific* element in S by traversing a decision tree is

$$\log_2 |S|$$

  - Call this value the information value of being *told* the element, rather than having to *work* for it (by asking binary questions)

- Let Y be a random variable; we make one observation of the variable Y (e.g., we draw a random ball out of a box) $\longrightarrow$ value y
- The information we obtain if event "$Y = y$" occurs, i.e., the *information value* of that event, is

$$I[Y = y] = \log_2 \left(\frac{\#\text{ balls in box}}{\#\text{ y's in box}} \right) = \log_2 \frac{1}{p(y)} = -\log p(y)$$

  - "If the probability of this event happening is small and it does happen, then the information value is large"
- Examples:
  - Observing the outcome of coin flip $\longrightarrow \; I = -\log \frac{1}{2} = 1$
  - Observing the outcome of dice == $x \longrightarrow \; I = -\log \frac{1}{6} = 2.58$

Entropy

- A random variable Y (= experiment) can assume different values $y_1, \ldots, y_n$ (i.e., the experiment can have different outcomes)
- What is the *average* information we obtain by observing the random variable?
  - In other words: if I pick a value y_i at random, according to their respective probabilities – what is the *average* number of yes/no questions you need to ask to determine it?
  - In probabilistic terms: what is the *expected amount of information*? $\longrightarrow$ captured by the notion of entropy
- Definition: Entropy

  Let Y be a random variable. The entropy of Y is

$$H(Y) = E[I(Y)] = \sum_i p(y_i) I[Y = y_i] = -\sum_i p(y_i) \log p(y_i)$$

  Units = bits

- Interpretation: The number of yes/no questions (= bits) needed *on average* to pin down the value of *y* in a random drawing

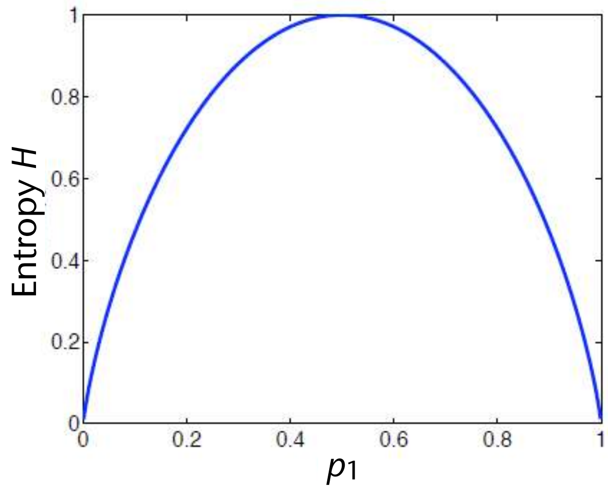
- Example: if *Y* can assume 8 values, and all are equally likely, then

$$H(Y) = -\sum_{i=1}^{8} \frac{1}{8} \log \frac{1}{8} = \log 2^3 = 3 \text{ bits}$$

- In general, if there are k different possible outcomes, then

$$H(Y) \leq \log k$$

  - Equality holds when all outcomes are equally likely
- With $k = 2$ (two outcomes), entropy looks like this ($p_1 + p_2 = 1$) :
- The more the probability distribution deviates from uniformity, the lower the entropy
- *Entropy* measures the *impurity*:



Balls-in-bin model

This distribution is less uniform =
Entropy is lower =
The node is purer

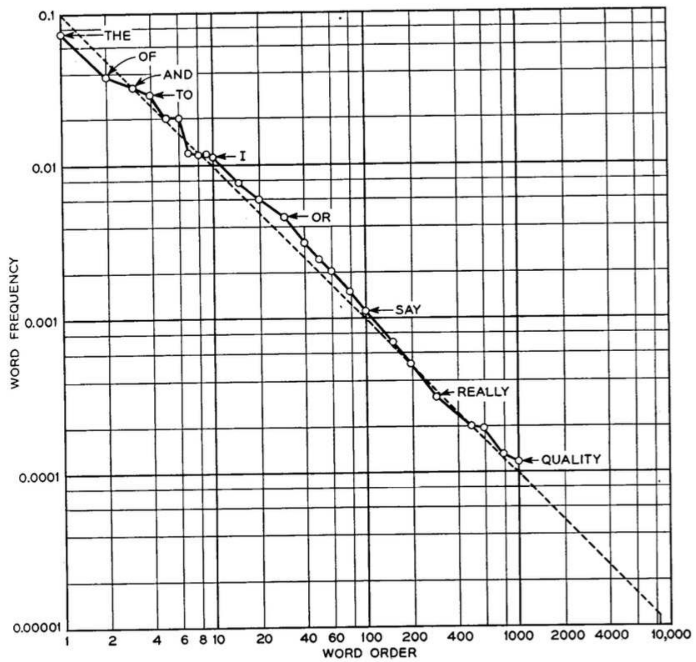
Examples

- Entropy of printed English
  - Let L = random variable, values = letters, picked randomly from a random English text
  - $H(L) = -p(\text{'}E\text{'}) \log p(\text{'}E\text{'}) - p(\text{'}T\text{'}) \log p(\text{'}T\text{'}) - p(\text{'}A\text{'}) \log p(\text{'}A\text{'}) - \ldots$

    $= 4.175$ bits

- Entropy of English words
  - Statistics of large English texts show $p_k \approx 0.1\frac{1}{k}$ where p_k = probability of word of rank k, up to rank 10 000 (Zipf's law)
  - Thus,

$$H \approx \sum_{k=1}^{10\,000} \frac{0.1}{k} \log_2\left(\frac{k}{0.1}\right) = 9.36 \text{ bits}$$

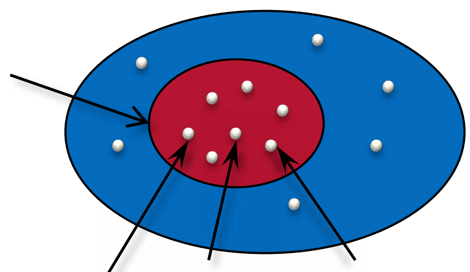


Conditional Entropy

- Now consider a random variable Y (e.g., the different classes/labels) with an attribute X (e.g., the first variable, $x_{i,1}$, of the data points, $\mathbf{x}_i$)
  - With every drawing of Y, we also get a value for the associated attribute X
- Assume that X is discrete, i.e., $x_i \in \{1, 2, ..., z\}$
- Now consider only outcomes of Y that fulfill some *condition*, e.g., $x_i = 1$
- The entropy of Y, provided that it assumes only values with $x_i = 1$:

$$H(Y|x_i = 1) = -\sum_i p(y_i|x_i = 1) \log \underbrace{p(y_i|x_i = 1)}$$

Probability of y_i occurring as a value of Y, where we draw Y only from the subset that contains only data points that have attribute $x_i = 1$

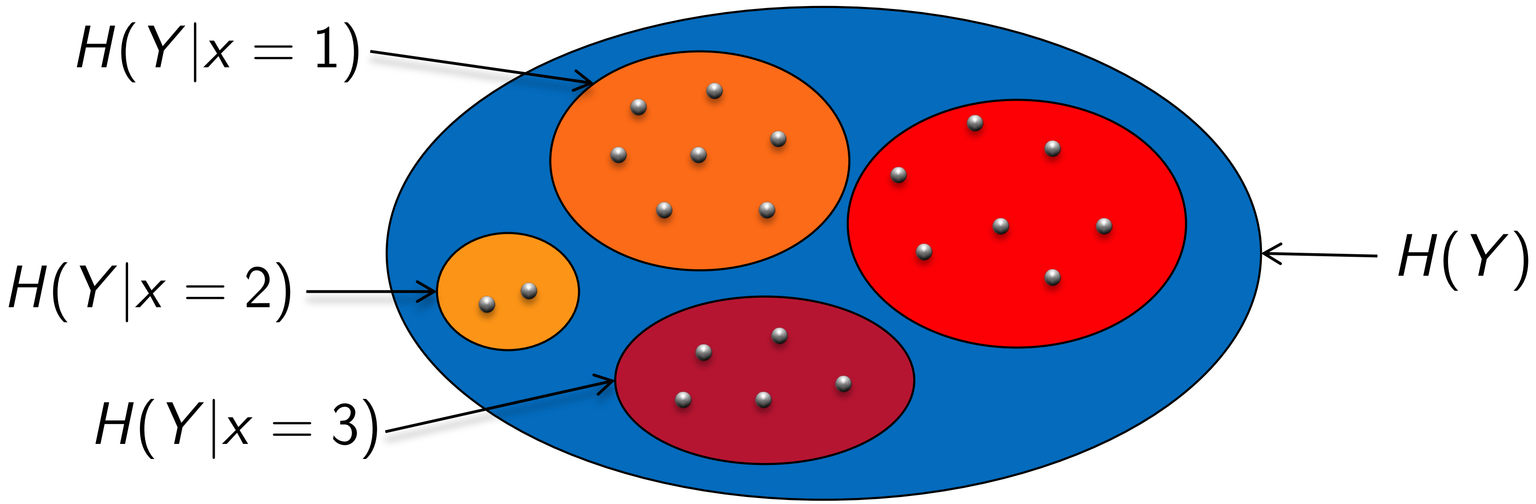


- Overall conditional entropy:

Probability that the attribute X has value k

$$H(Y|X) = \sum_{k=1}^{z} p(x=k) \cdot H(Y|x=k)$$

$$= -\sum_{k=1}^{z} p(x=k) \sum_{i} p(y_i|x_i=k) \log p(y_i|x_i=k)$$



Information Gain

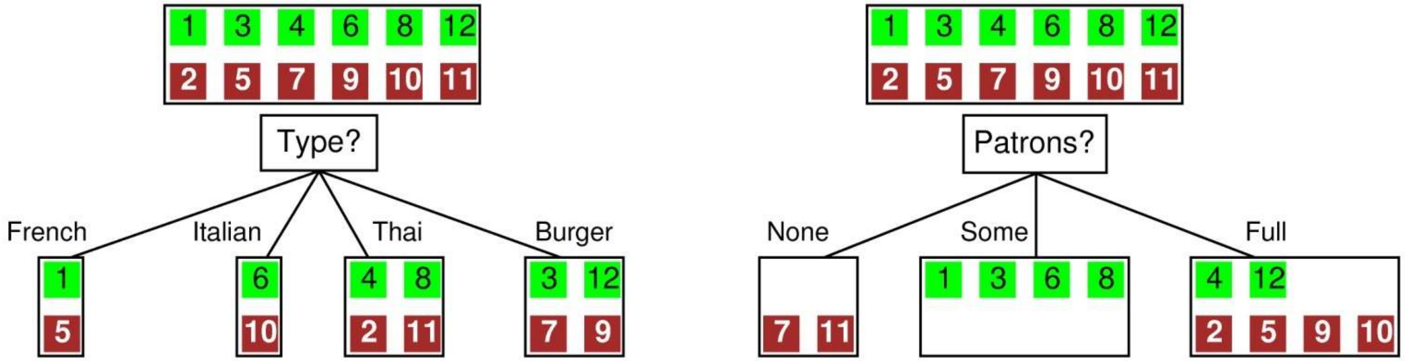
- How much information do we gain *if we disclose (or choose) the value of one attribute X*?
  - Disclosure $\longrightarrow$ splitting of the set of all data points into subsets
- Information gain = (information *before* split) – (information *after* split) = *reduction of uncertainty regarding label y* by learning value of attribute *X*
- The information gained by a split in a node of a decision tree:

$$IG(Y,X) = H(Y) - H(Y|X)$$

  - Hopefully / usually $H(Y|X) < H(Y)$
- Goal: choose the attribute with the largest *IG*
  - In case of scalar attributes, also choose the *optimal cutpoint*
    - In doing so, we basically convert the scalar attribute into a binary one (at that node!)

Example

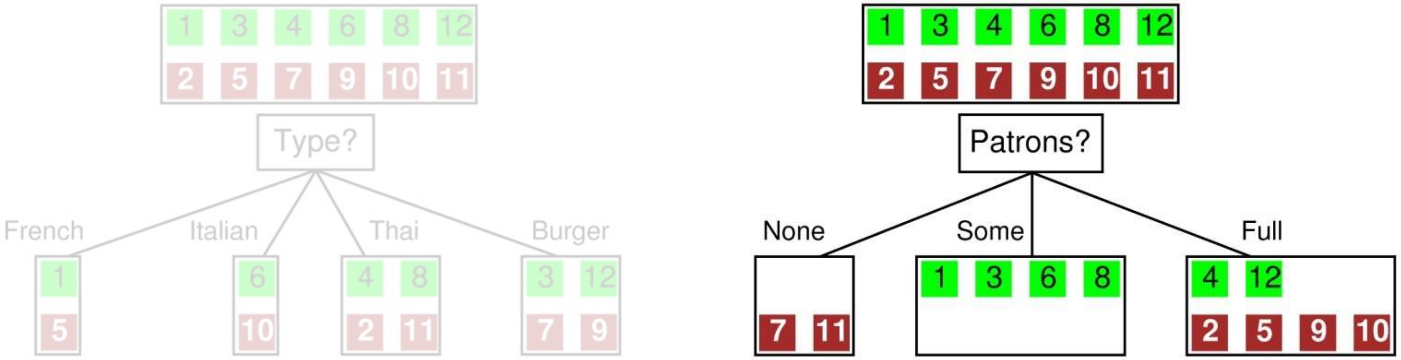
- Consider 2 options to split the root node of the restaurant example



- Labels of random variable $Y \in \{$ "yes", "no" $\}$
- Entropy at the root node:

$$H(Y) = p(y = \text{“yes”}) \log \frac{1}{p(y = \text{“yes”})} + p(y = \text{“no”}) \log \frac{1}{p(y = \text{“no”})}$$

$$= \frac{1}{2} \log 2 + \frac{1}{2} \log 2 = 1$$



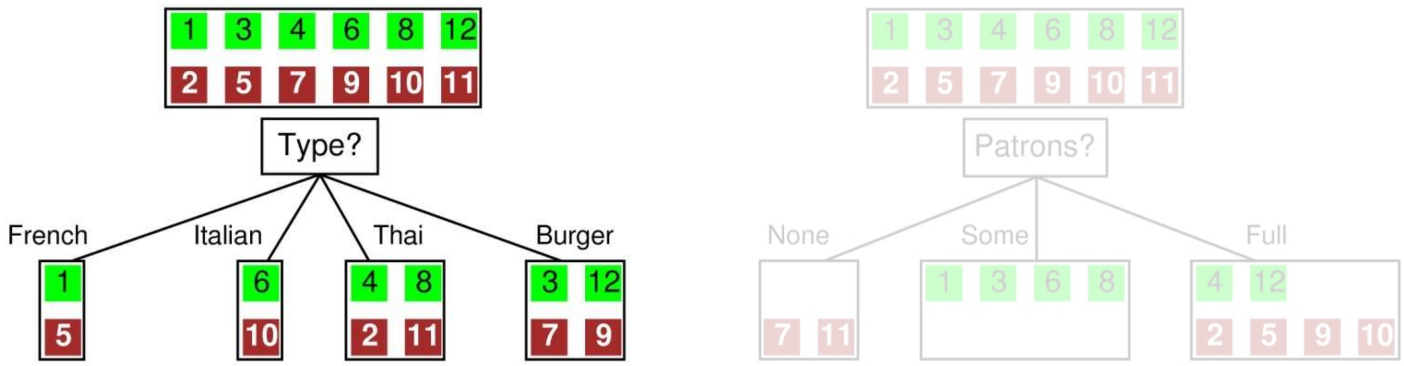
- Conditional entropy for split by #patrons:

$$H(Y \mid n) = p(n=\text{“full”})\cdot H(Y|n=\text{“full”})+ p(n=\text{“some”})\cdot H(Y|n=\text{“some”})+ p(n=\text{“none”})\cdot H(Y|n=\text{“none”})$$

where n = the attribute "#patrons" ∈ { "none", "some", "full" }

$$H(Y|n) = -\frac{6}{12}\big(p(y=\text{“no”})\log p(y=\text{“no”}) + p(y=\text{“yes”})\log p(y=\text{“yes”})\big) -\frac{4}{12}\big(p(y=\text{“no”})\log p(y=\text{“no”}) + p(y=\text{“yes”})\log p(y=\text{“yes”})\big) -\frac{2}{12}\big(p(y=\text{“no”})\log p(y=\text{“no”}) + p(y=\text{“yes”})\log p(y=\text{“yes”})\big)$$

$$H(Y|n) = \frac{6}{12}\Big(\frac{4}{6}\log\frac{6}{4} + \frac{2}{6}\log\frac{6}{2}\Big) + \frac{4}{12}(0\log 0 + 1\log 1) + \frac{2}{12}(1\log 1 + 0\log 0)$$



- Conditional entropy for split by restaurant type:

$$
\begin{aligned}
H(Y|\text{type}) = \; & -\frac{2}{12}\left(p(y=\text{“no”})\log p(y=\text{“no”}) + p(y=\text{“yes”})\log p(y=\text{“yes”})\right) \\
& -\frac{2}{12}\left(p(y=\text{“no”})\log p(y=\text{“no”}) + p(y=\text{“yes”})\log p(y=\text{“yes”})\right) \\
& -\frac{4}{12}\left(p(y=\text{“no”})\log p(y=\text{“no”}) + p(y=\text{“yes”})\log p(y=\text{“yes”})\right) \\
& -\frac{4}{12}\left(p(y=\text{“no”})\log p(y=\text{“no”}) + p(y=\text{“yes”})\log p(y=\text{“yes”})\right)
\end{aligned}
$$

$$
H(Y|\text{type}) = 2\cdot\frac{2}{12}\left(\frac{1}{2}\log\frac{2}{1} + \frac{1}{2}\log\frac{2}{1}\right) \; + \; 2\cdot\frac{4}{12}\left(\frac{2}{4}\log\frac{4}{2} + \frac{2}{4}\log\frac{4}{2}\right)
$$

- Compare the information gains:

$$\begin{aligned} IG(Y, \#\text{patrons}) &= H(Y) - H(Y|\#\text{patrons}) \\ &= 1 - 0.585 \end{aligned}$$

$$\begin{aligned} IG(Y, \text{type}) &= H(Y) - H(Y|\text{type}) \\ &= 1 - 1 \end{aligned}$$

  - Result: learning the value of the attribute "#patrons" gives us more information about the label of Y

- Compute the *IG* obtained by a split induced by *each attribute*
  - In the restaurant case, the optimum is achieved by the attribute "#patrons" for splitting the set of data points at the root

Another Example

- Given the following data points in the parent node:

Attrib.	0	3	7	2	3	2	8	6	1	3
Label	G	G	R	G	G	G	R	R	G	R

  - Entropy: $H = -\frac{4}{10}\log_2\frac{4}{10} - \frac{6}{10}\log_2\frac{6}{10} = 0.97$

- One way to split them:

Attrib.	0	3	7	2	3 |	2	8	6	1	3
Label	G	G	R	G	G |	G	R	R	G	G

  - Entropies: $H_L = -\frac{4}{5}\log_2\frac{4}{5} - \frac{1}{5}\log_2\frac{1}{5} = 0.72$

    $H_R = -\frac{3}{5}\log_2\frac{3}{5} - \frac{2}{5}\log_2\frac{2}{5} = 0.97$

    $$\Big\} \; H_{\text{after}} = \frac{5}{10}H_L + \frac{5}{10}H_R = 0.85$$

  - Information gain: $IG = H_{\text{before}} - H_{\text{after}} = 0.03$

Slight bug in the numbers!

- Another way to split them:

Attrib.	0	1	2	2	3	3	3	6	7	8
Label	G	G	G	G	G	G	R	R	R	R

- Entropies:

$$\left.\begin{aligned} H_L &= -\frac{4}{4}\log_2\frac{4}{4} - \frac{0}{4}\log_2\frac{0}{4} = 0 \\ H_R &= -\frac{2}{6}\log_2\frac{2}{6} - \frac{4}{6}\log_2\frac{4}{6} = 0.92 \end{aligned}\right\} H_{\text{after}} = \frac{4}{10}H_L + \frac{6}{10}H_R = 0.55$$

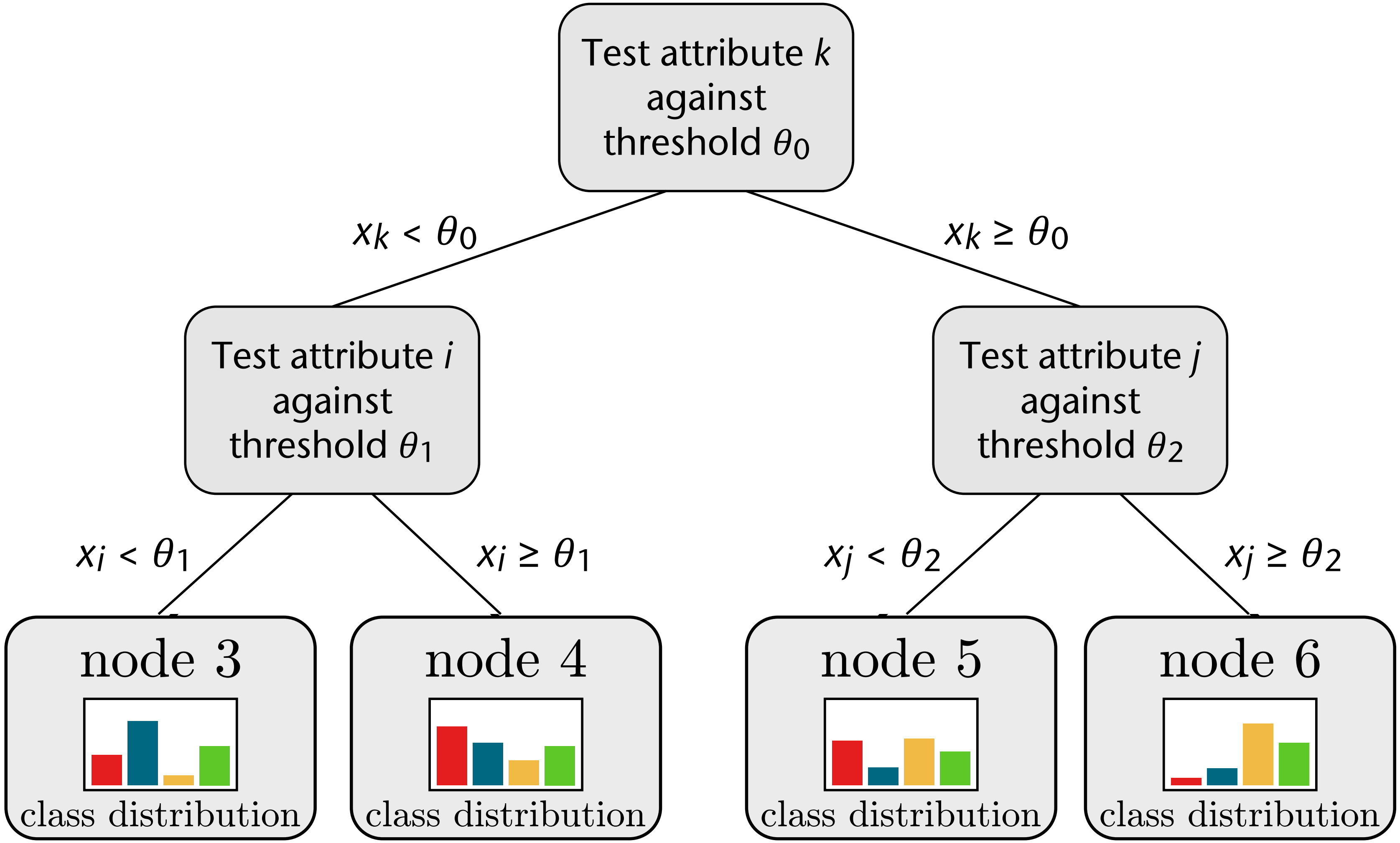
- Information gain: $IG = H_{\text{before}} - H_{\text{after}} = 0.42$

Bits and Pieces

- If there are no attributes left:
  - Can happen during learning of the decision tree, when a node contains data points with same attribute values but different labels
  - This constitutes error / noise in the training data
  - Stop construction here, use majority vote (i.e., discard erroneous point)
- If there are leaves with no data points:
  - While classifying a new data point
  - Just choose the majority vote of the parent node

Classification at Runtime

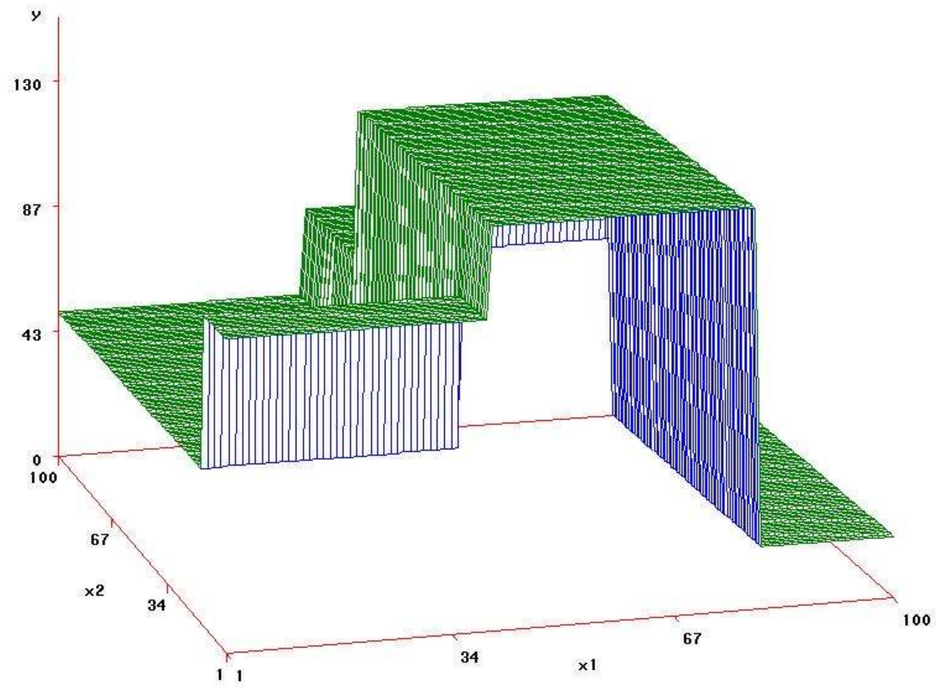
- Given an (unseen) data point **x**, traverse the tree, testing one of its attributes at each node



Expressiveness of Decision Trees

- Assume all variables (attributes and labels) are Boolean
- What is the set of Boolean functions that can be represented by a decision tree?
- Answer: all Boolean functions!
- Proof:
  - Given any Boolean function
  - Convert it to a truth table
  - Consider each row as a data point, output of the fct = label of data point
  - Construct a DT over all data points / rows

- If *Y* is a discrete, numerical variable, then DTs can be regarded as piecewise constant functions over the feature space:

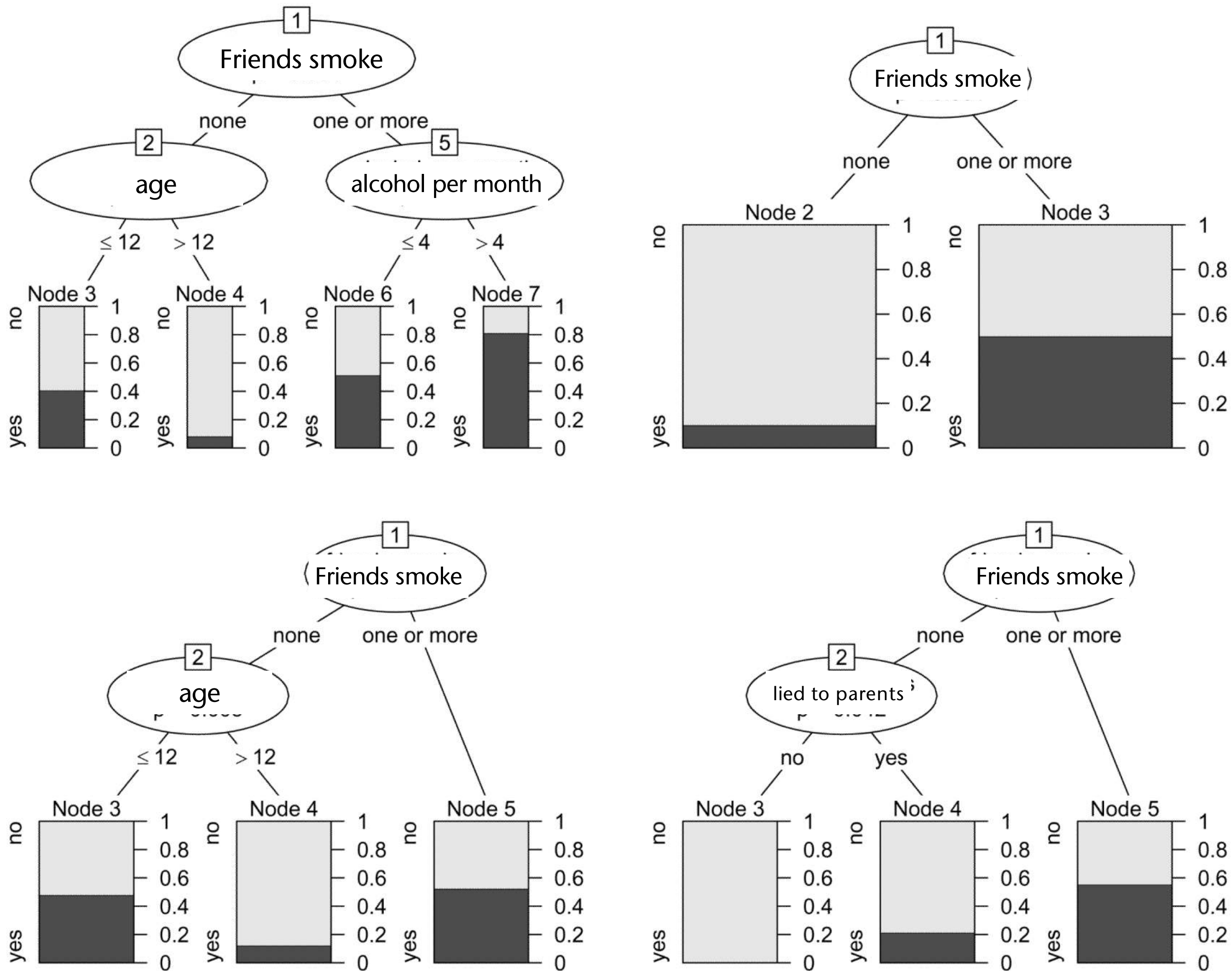


- DTs can approximate *any* function

Problems of Decision Trees

- Error propagation:
  - Learning a DT is based on a series of *local* decisions
  - What happens, if one of the nodes implements the wrong decision? (e.g., because of an outlier)
  - The whole subtree will be wrong!
- Overfitting: in general, it means the classifier performs extremely well on the training data, but very poorly on unseen data ⟶ low generalization capability
  - When overfitting occurs, the DT has "learned the noise in the data"

Example for the instability of single decision trees



"The Wisdom of Crowds"

[James Surowiecki, 2004]

- Francis Galton’s experience at the 1906 West of England Fat Stock and Poultry Exhibition
- Jack Treynor’s jelly-beans-in-the-jar experiment (1987)
  - Only 1 of 56 students' guesses came closer to the truth than the average of the class’ guesses
- Who Wants to Be a Millionaire?
  - Call an expert? ⟶ 65% correct
  - Ask the audience? ⟶ 91% correct

Example (Thought Experiment)

- "Which person from the following list was *not* a member of the Monkees?"

  (A) Peter Tork (C) Roger Noll

  (B) Davy Jones (D) Michael Nesmith

  - (BTW: Monkeys are a 1960s pop band, comprising 3 band members)
- Correct answer: the non-Monkee is Roger Noll
- Now imagine a crowd of 100 people with this distributed knowledge:

  7 know 3 of the Monkees

  10 know 2 of the Monkees

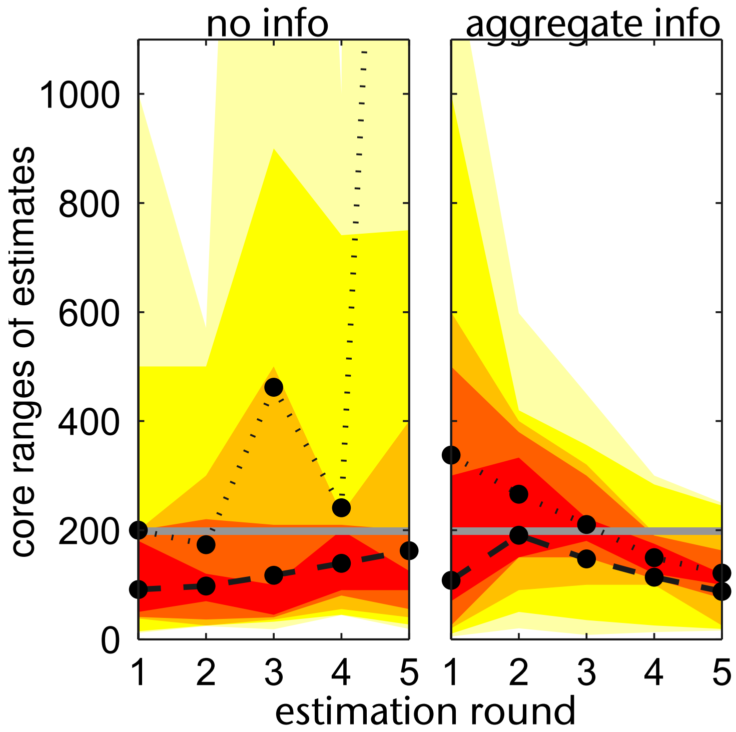
  15 know 1 of the Monkees

  68 have no clue
- So "Noll" will garner, on average, 34 votes versus 22 votes for each of the other choices
  - (68/4 + (15/3)/3*3 + (10/3)/2*3 + 7 = 34)

- Implication: one should not spend energy trying to identify an expert within a group, but instead rely on the group's collective wisdom
- Counter example:
  - Kindergartners guessing the weight of a Boeing 747
- Prerequisites for crowd wisdom to emerge:
  - Some knowledge of the truth must reside with some group members (⟶ *weak classifiers*)
  - Opinions must be independent
  - Knowledge must be objective (no subjective opinions)
  - Works best for quantifiable things (need to calculate the average) ("if you can count it, you can crowd it")

Digression: the Stupidity of Crowds

- Examples:
  - Financial crisis in 2008
  - Bubble formation in social networks
- Social experiment (N = 144) [2011]:
  - Several estimation tasks (country's population, etc.)
  - Conditions:
    - No info: subjects had no information about other participants' guesses
    - Aggregate info: subjects could reconsider their estimate after gaining some information about the estimates of others
  - *Social influence effect*: diversity diminishes, but collective error does not
  - *Confidence effect*: subjects become more certain about their guesses



Bremen

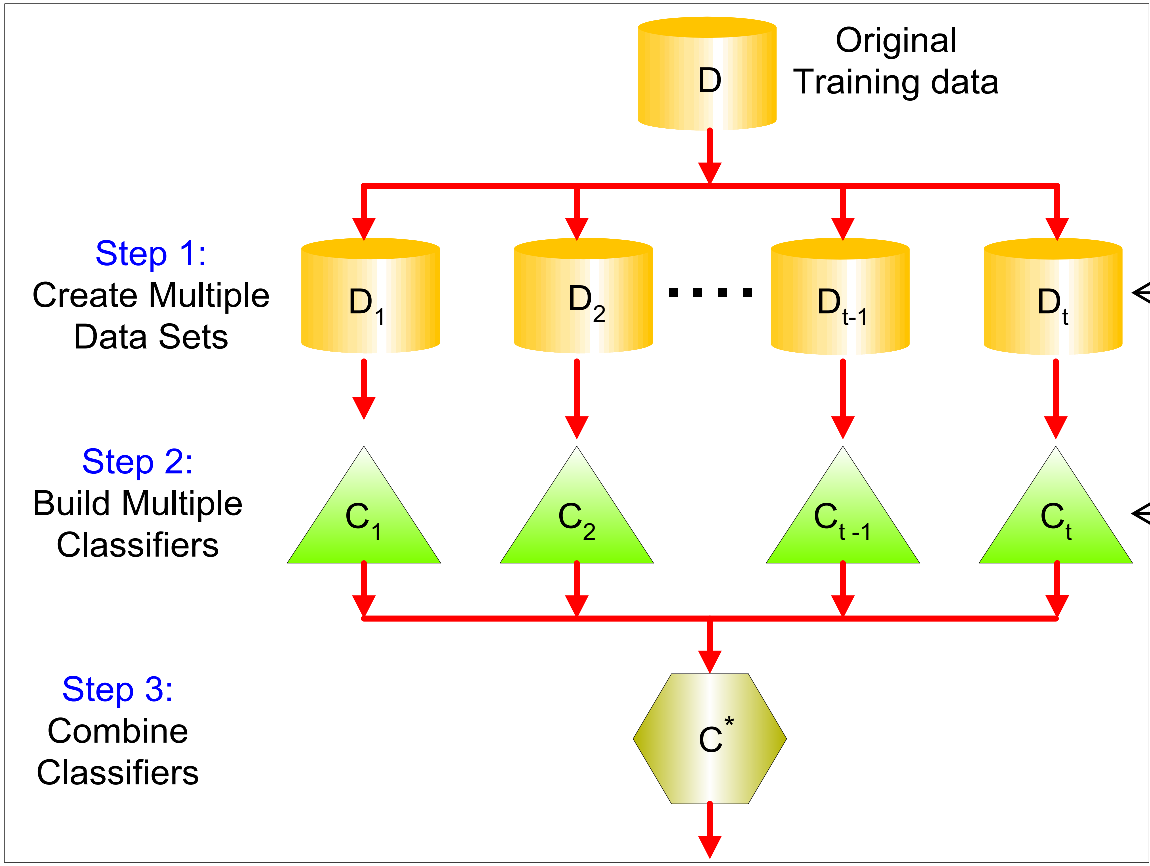
Digression: Francis Galton

- Cousin of Charles Darwin
- "Father" of statistics
- Incidentally, he also invented finger printing
- He also published the "scientific" way to cut cakes in Nature 1906:

Numberphile.com

The Random Forest (RF) Method

- One kind of so-called ensemble (of experts) methods
- Idea: predict class label for unseen data by *aggregating* a set of predictions (= classifiers learned from the training data)



Must encode the same distribution as the original data set *D*!

Each classifier = one decision tree

Randomizations During the Construction of RF's

- Generating the data sets for learning multiple trees:
  - Generate a number of random sub-sets $\mathcal{L}_1, \mathcal{L}_2, \ldots$ from the original training data $\mathcal{L}$, $\mathcal{L}_i \subset \mathcal{L}$. There are basically two methods:

  1. Bootstrapping: randomly draw samples from $\mathcal{L}$, with replacement, size of new data = size of original data set; or,
  2. Subsampling: randomly draw samples from $\mathcal{L}$, without replacement, size of new data < size of original data set

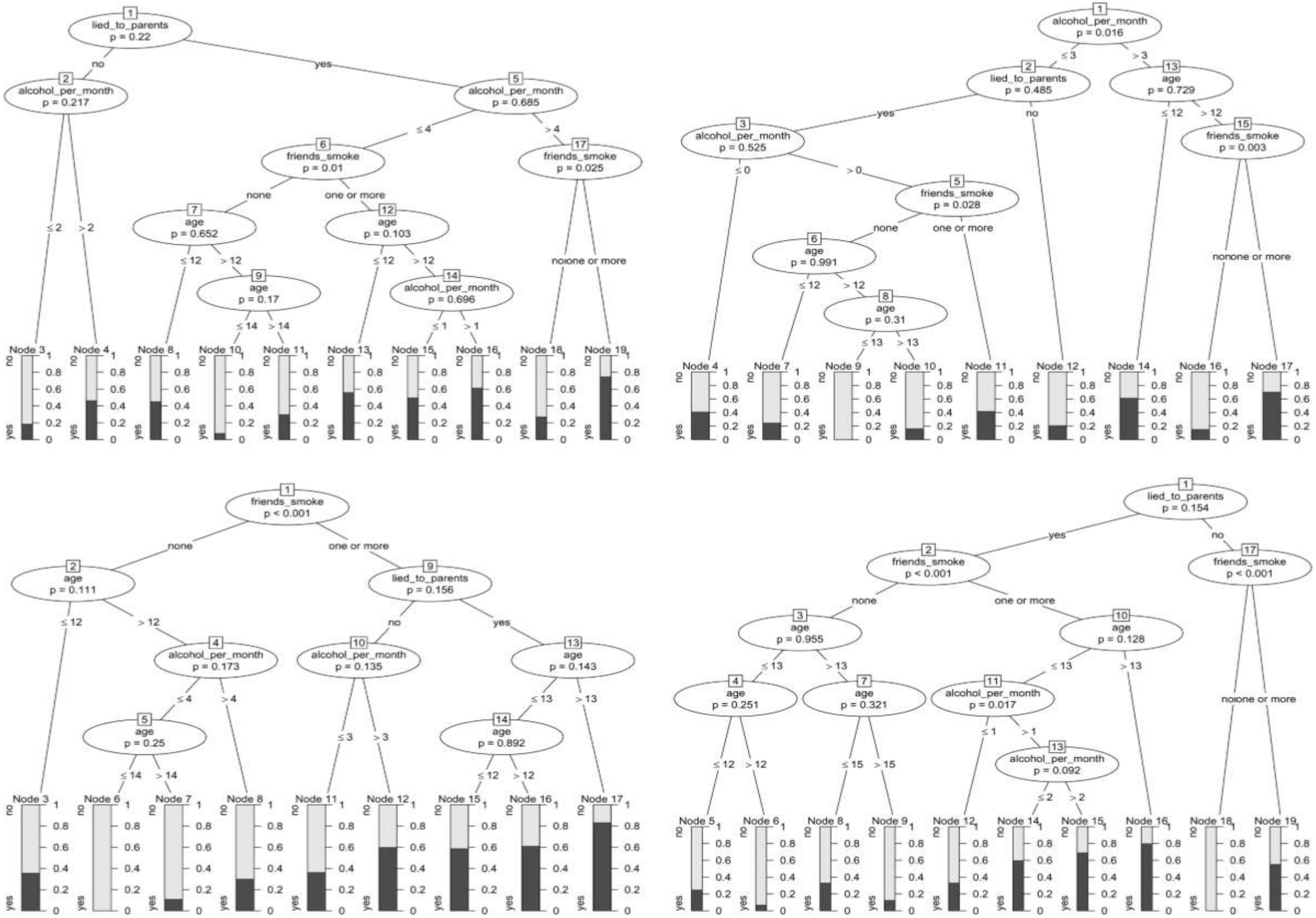
  - New data sets reflect the *same* random process as the orig. data, but they differ slightly from each other and the original set due to random variation
  - Resulting trees can differ substantially (see earlier slide)

- Growing the trees:
  - At *each node*, a random subset of attributes (= predictor variables/ features) is preselected; *only from those,* the one with the best information gain is chosen
    - NB: an individual tree is *not just a DT over a subspace of feature space*!
  - Each tree is grown without any stopping criterion, i.e., until each leaf contains data points of only *one single* class
- Naming convention for 2 essential parameters:
  - Number of trees = *ntree*
  - Size of random subset of variables/attributes at each node = *mtry*
- Rules of thumb:
  - *ntree* = 100 … 300
  - *mtry* = sqrt(d) , with d = dimensions of the feature space

- The learning algorithm:

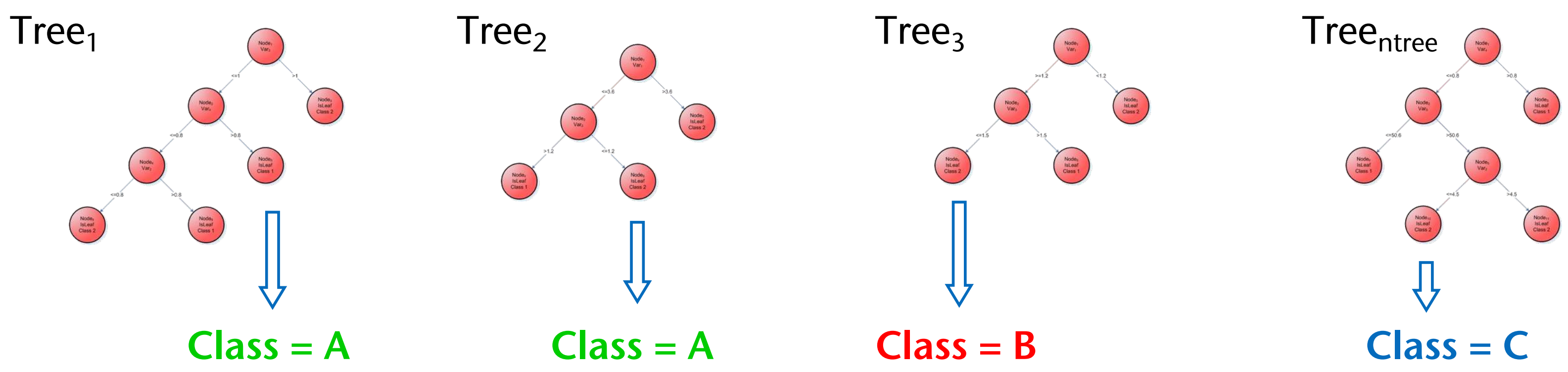
```
input: learning set L
for t = 1...ntree:
   build subset Lt from L by random sampling
   learn tree Tt from Lt:
      at each node:
         randomly choose mtry features
         compute best split from only those features
      grow each tree until leaves are perfectly pure
```

A Random Forest Example for the Smoking Data Set



Using a Random Forest for Classification

- With a new data point:
  - Traverse each tree individually using that point
  - Gives *ntree* many class labels



  - Take majority of those class labels
- Sometimes, if labels are cardinal numbers, (weighted) averaging makes sense

Why Does it Work?

- Make following assumptions:
  - The RF has *ntree* many trees (classifiers)
  - Each tree has an error rate of ε
  - All trees are perfectly independent! (no correlation among trees)
- Probability that the RF makes a wrong prediction:

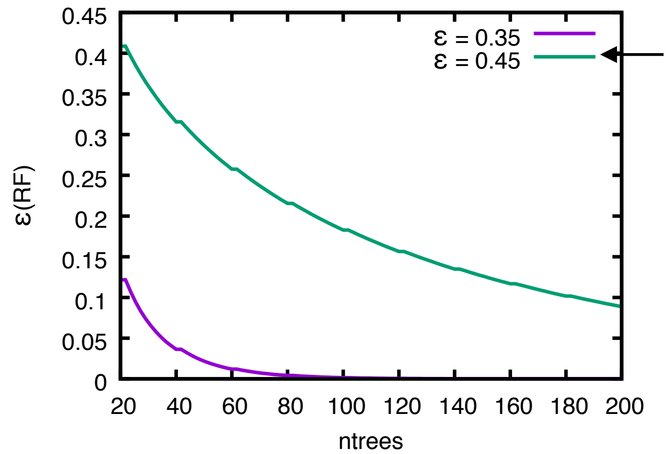
$$\varepsilon_{\text{RF}} = \sum_{i=\left\lceil \frac{ntree}{2} \right\rceil}^{ntree} \binom{ntree}{i} \varepsilon^i (1-\varepsilon)^{(ntree-i)}$$

- Example:

  individual error rate ε= 0.35 ,

  ntree = 60 ⟶

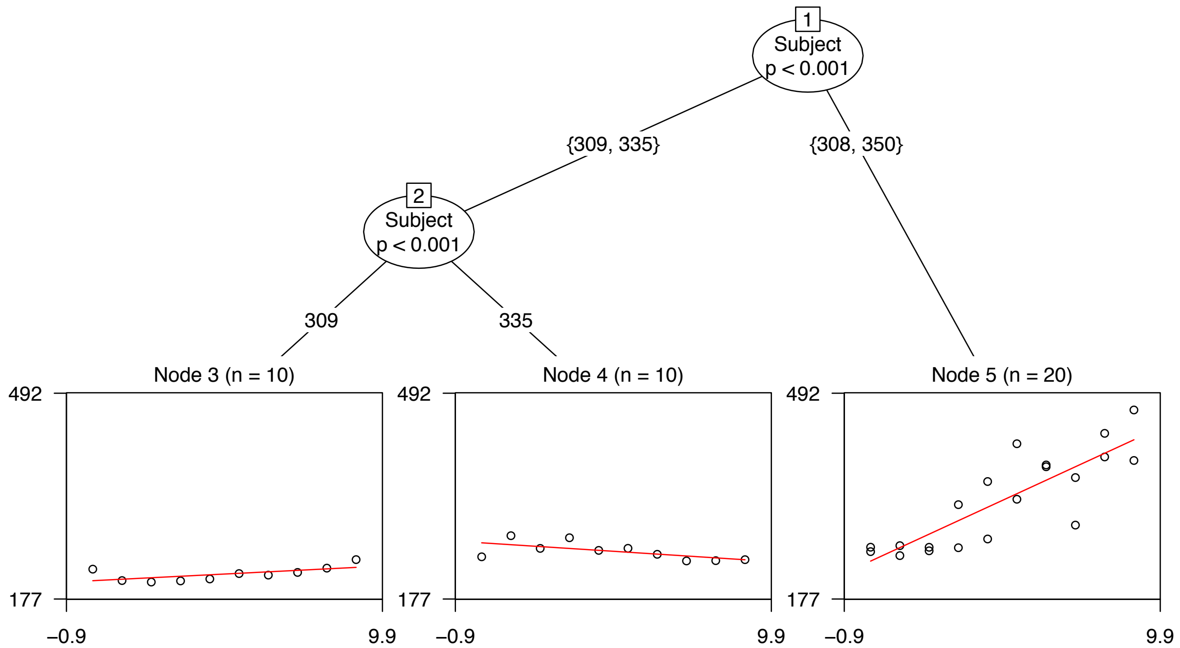
  error rate of RF $\varepsilon_{\text{RF}} \approx 0.01$



Each DT is only 5% better than randomly choosing the class

Variants of Random Forests

- Regression trees:
  - Variable Y (dependent variable) is continuous
    - I.e., no longer a class label
  - Goal is to learn a function $\mathbb{R}^d \rightarrow \mathbb{R}$ that generalizes the training data
  - Example:



- Extremely randomized trees (ERTs):
  - Do not find the optimal threshold for splitting the training set
  - Instead, just pick a random value in the interval of the feature's values
- Oblique random forests:
  - Do not test just one feature
  - Instead, test a linear combination of $k = mtry$ features: $\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_k \end{pmatrix} \begin{pmatrix} x_{i_1} \\ x_{i_2} \\ \vdots \\ x_{i_k} \end{pmatrix} < \theta$
  - Variant "Forest-RC":
    - Randomly choose l different vectors of coefficients $a_i \in [-1,1]$, $i = 1,\ldots,k$
    - Pick that vector of a_i's that maximizes information gain
- Random ferns:
  - All nodes on the same level within a tree test the same attribute against the same threshold
  - Advantage: all decision tests at runtime can be done in parallel
  - Disadvantage: need deeper trees

Features of Random Forests

- "Small *n*, large *d*"
  - RFs are well-suited for problems with many more variables (d = dimensions in the feature space) than observations / training data (n)
- Nonlinear function approximation
  - RFs can approximate *any* unknown function
- RF's can solve the "XOR problem"
  - In an XOR truth table, the two variables show no effect at all
    - With either split variable, the information gain is 0
  - But there is a perfect interaction between the two variables
  - Random selection of $mtry < d$ variables can help in such cases

Tips and Tricks

- Out-of-bag error estimation:
  - For each tree T_i, a training data set $\mathcal{L}_i \subset \mathcal{L}$ was used
  - Use $\mathcal{L} \setminus \mathcal{L}_i$ (the out-of-bag data set) to test the prediction accuracy
- Handling of missing values:
  - Occasionally, some data points contain a missing value for one or more of its variables (e.g., because the corresponding measuring instrument had a malfunction)
  - When information gain is computed, ignore those data points with a missing value at the currently evaluated variable
  - During splitting, use a *surrogate* that best predicts the values of the splitting variable (in case of a missing value)
    - Assume data point has class label l, its m-th variable is missing: compute median of m-th variable of all data points in class l, use this as surrogate for all missing m-th variables of all data points

- Randomness:
  - Random forests are truly random
  - Consequence: when you build two RFs with the same training data, you get slightly different classifiers/predictors
    - Fix the random seed, if you need reproducible RFs
  - Suggestion: if you observe that two RFs over the same training data (with different random seeds) produce noticeably different prediction results, and different variable importance rankings, then you should adjust the parameters *ntree* and *mtry*

Remarks on RFs

- Do random forests overfit?
  - The evidence is inconclusive (with some data sets it seems like they could, with other data sets it doesn't)
  - If you suspect overfitting: try to build the individual trees of the RF to a smaller depth, i.e., not up to completely pure leaves
- Better explainability than CNN’s:
  - RF’s can provide information on which variables/features are important for the decision making (and which are unimportant)

Parallel Construction of Random Forests

- Naïve method: one thread per tree (not massively parallel)
- Better method: one thread per node
- In the following: "data point" actually means "index into data point array", i.e., threads always work with indices only
- General idea:
  - Build all trees breadth-first
  - In each iteration, each thread
    - gets a task = node of one of the DT's, and a list of data points,
    - determines input variable *i* and cutpoint θ for optimal split
  - Produces two new lists and allocates child nodes

The Algorithm in More Detail

```
create ntrees many subsets of training data
assign these subsets to the root nodes
while there are still inner nodes:
  repeat mtry many times:
    pick a random feature i
    sort all data points by value of feature i
    initialize left/right histograms, left h. = empty
    loop with k over data points left to right:
      conceptually move data point k from right to
        left subset ⟶ new θ
      update left/right histograms
      compute new information gain (IG)
      if new IG is better:
        save new θ and IG
    if feature i yields better IG:
      save new feature index i, θ, IG
  create child nodes
  split input data points by feature i and θ
    and create two subsets, one for each child node
```

Executed in parallel

Achieving Higher Parallelism

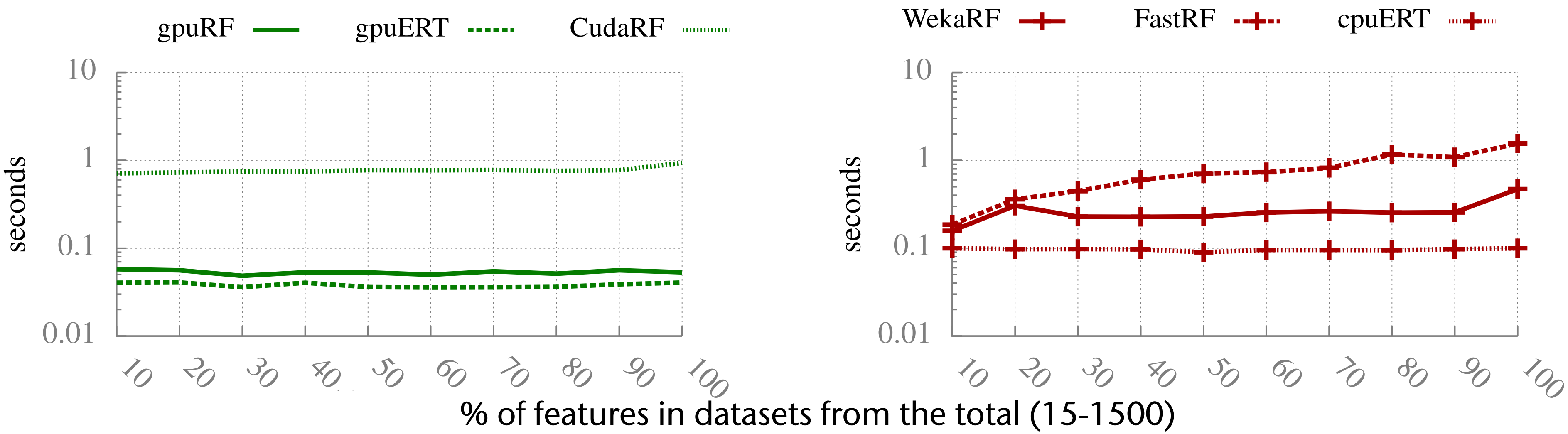
- At each node: calculate IG for *mtry* many features and a fixed number, *s*, of potential cutpoints
- Let n = # inner nodes on the current level
- Launch n blocks of $s \times mtry$ many threads
  - Each thread computes the IG for one specific node, one specific feature i, one specific cutpoint θ
  - Output is a matrix of IG's per node, pick the maximum for the split
    - Segmented max-scan over array of $n \times s \times mtry$ elements, n segments, one segment = $s \times mtry$ many IG values
  - Advantage: all threads in a block work on the same set of data points $\longrightarrow$ load into shared memory

Updating the Histogram

- Given two sets of data points (left and right), and the associated histograms h_l and h_r
- Move one data point from right to left, let $y \in \{y_1, y_2, \ldots, y_l\}$ be its label
- The update method:

```
updateHistograms( hl, hr, y ):
  hr[ y ] -= 1
  hl[ y ] += 1
```

Training Time Depending on Size of Dataset



gpuRF / gpuERT: the presented method for training RF and ERT on the GPU;
cpuERT: same algorithm, but implemented on the CPU running 32 threads;
CudaRF: older method on GPU
WekaRF, FastRF: multi-threaded CPU versions

Dataset	Nr Instances	Nr Features	mtry	Nr Missing values
Adult	32561	14	4	4262
Mushroom	8124	22	5	2480
Spambase	4601	57	6	0
Kr-vs-kp	3196	36	6	0
Eula-Freq	996	1268	11	0
Breast-Cancer-Wis	569	30	5	0
Skin-Disorder	462	1669	11	0
House-Votes	435	16	5	392

Some Code Optimization Tricks (not Only for GPU's)

- Instead of

```
if ( x[i] < threshold )
   child node ptr = left child ptr
else
   child node ptr = right child ptr
```

use

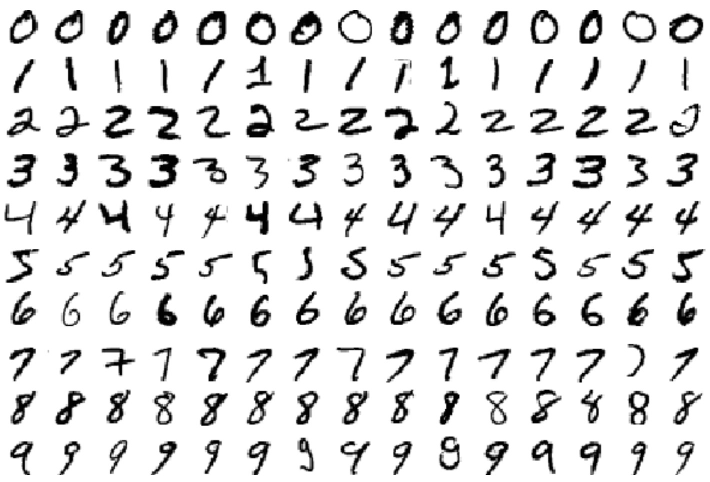
```
child node ptr = left child ptr +
                 static_cast<int>( x[i] >= threshold )
```

- Use half-precision floats for storing the training data set
  - FP16 = 16-bit floating point type **`half`** (since CUDA 7.5)
  - Increases bandwidth, allows 2 × data in shared memory
  - Lower precision is OK, since data set contains noise anyways

- Use `__log2f()` instead of `log2f()`
  - Less precision, but faster
  - Loss in precision does not matter here, because of all the other randomizations
- Use `__fdividef(x,y)` instead of division operator (`x/y`)
  - Twice as fast

Application: Handwritten Digit Recognition

- Data set:
  - Images of handwritten digits
  - 10 classes
  - Normalization: 20x20 pixels, binary images



MNIST data set

- Naïve feature vectors (data points):
  - Each pixel = one variable ⟶ 400-dim. feature space over {0,1}
  - Recognition rate: ~ 70-80 %
- Better feature vectors by *domain knowledge*:
  - For each pixel I(*i*,*j*) compute:

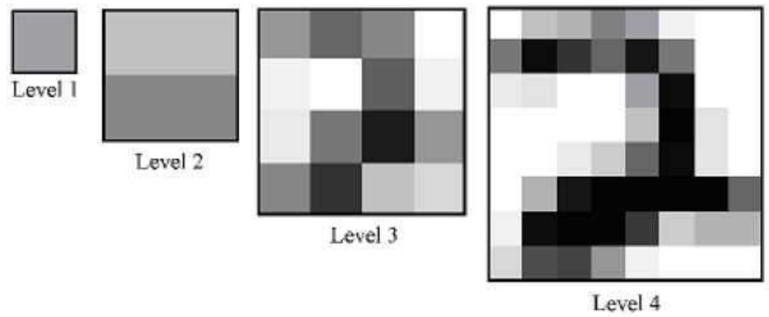
$$H(i,j) = I(i,j) \wedge I(i,j+2)$$
$$V(i,j) = I(i,j) \wedge I(i+2,j)$$
$$N(i,j) = I(i,j) \wedge I(i+2,j+2)$$
$$S(i,j) = I(i,j) \wedge I(i+2,j-2)$$

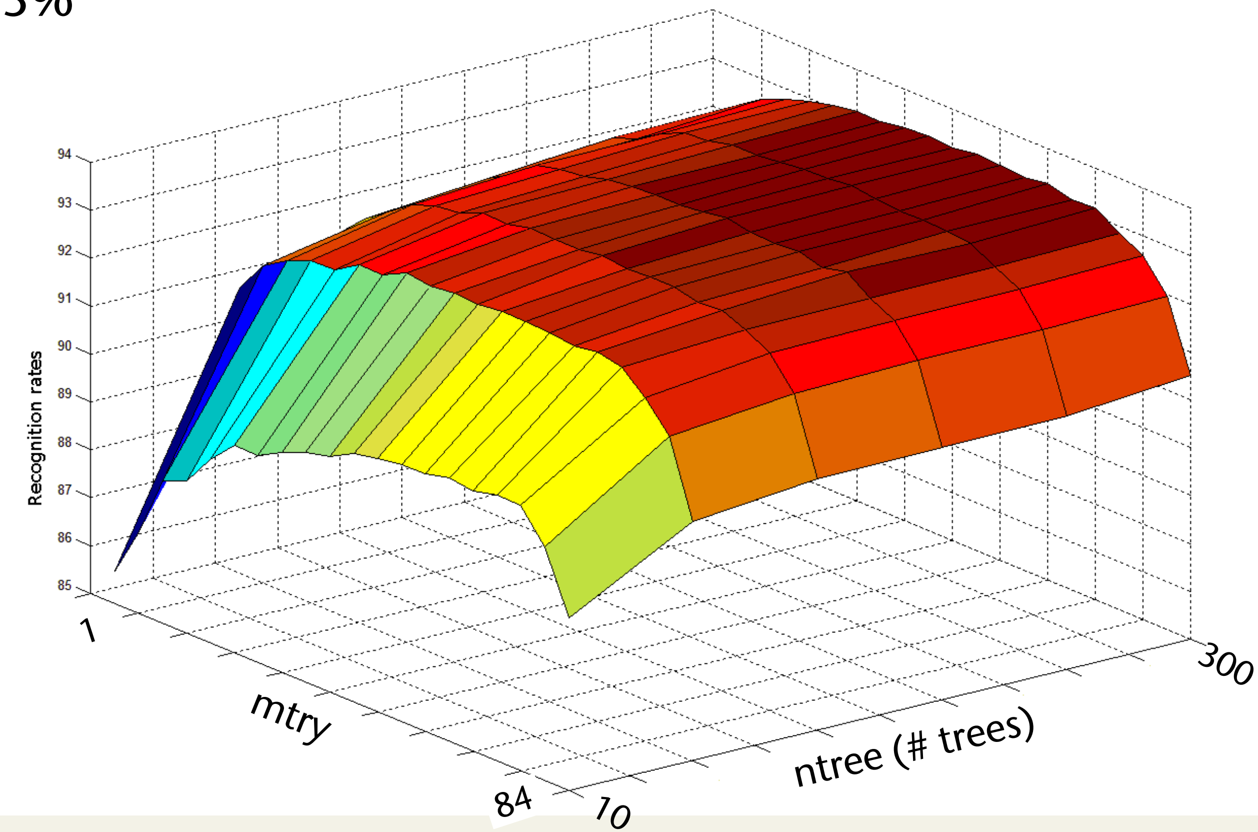
and a few more …

- Feature vector for an image = (all pixels $I(i,j)$, all $H(i,j)$, $V(i,j)$, …)
- Feature space = ca. 1400-dimensional = 1400 variables per data point

- Classification accuracy = ~93%
  - (NB: it was a precursor of random forests)

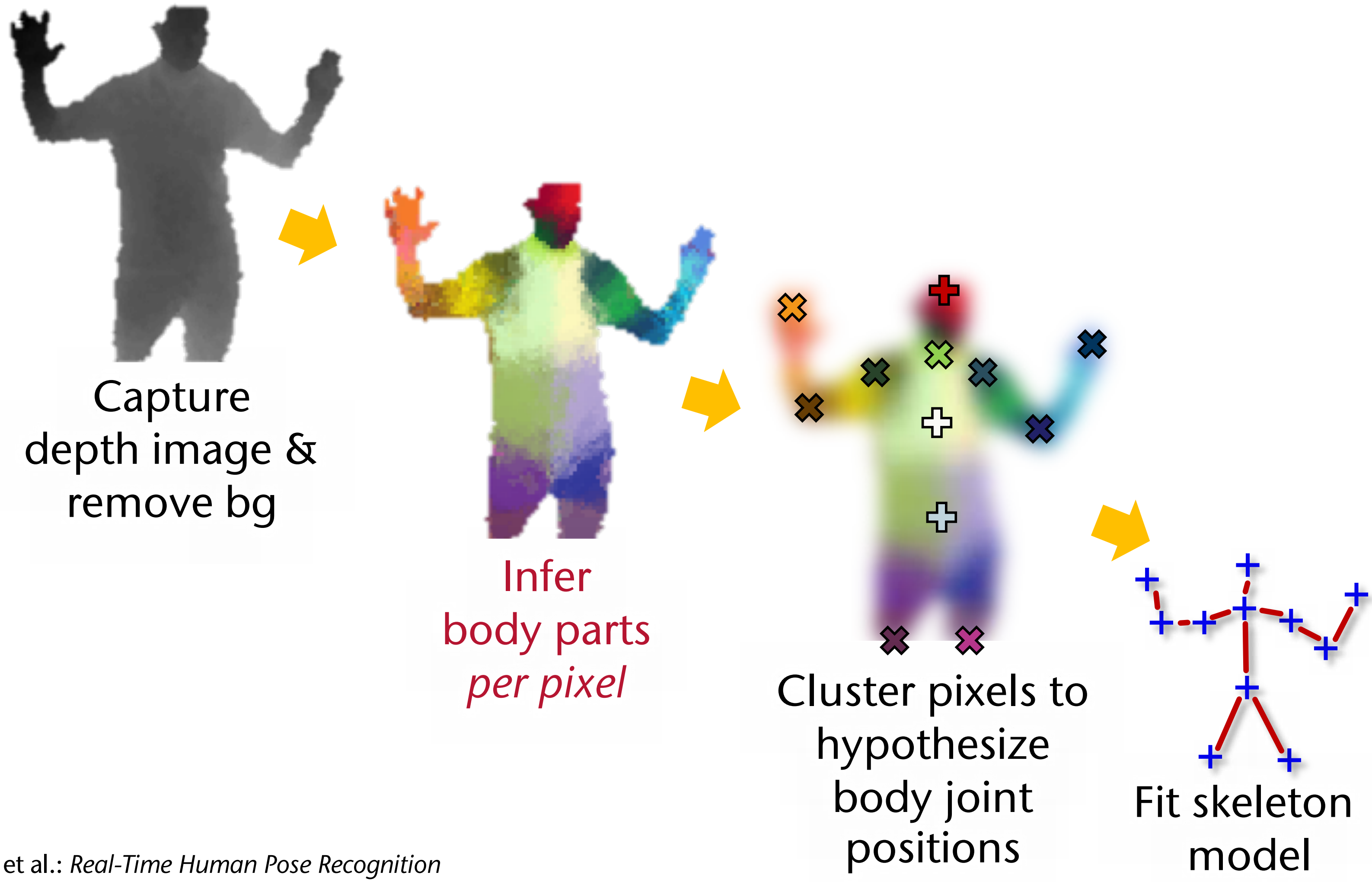
- Other experiments on handwritten digit recognition:
  - Feature vector = all pixels of an image pyramid
  - Recognition rate: ~ 93%
  - Dependence of recognition rate on *ntree* and *mtry*:





Body Tracking Using Depth Images (Kinect)

- The tracking / data flow pipeline:

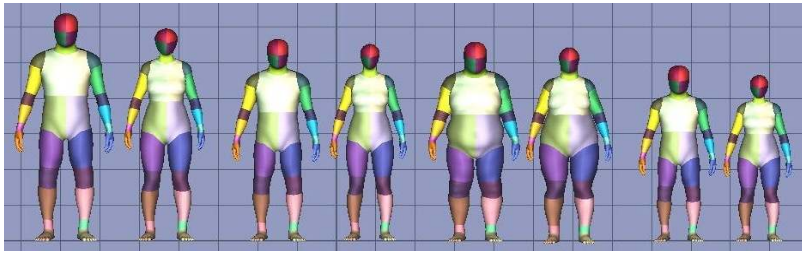


[Shotton et al.: *Real-Time Human Pose Recognition in Parts from Single Depth Images*; CVPR 2011]

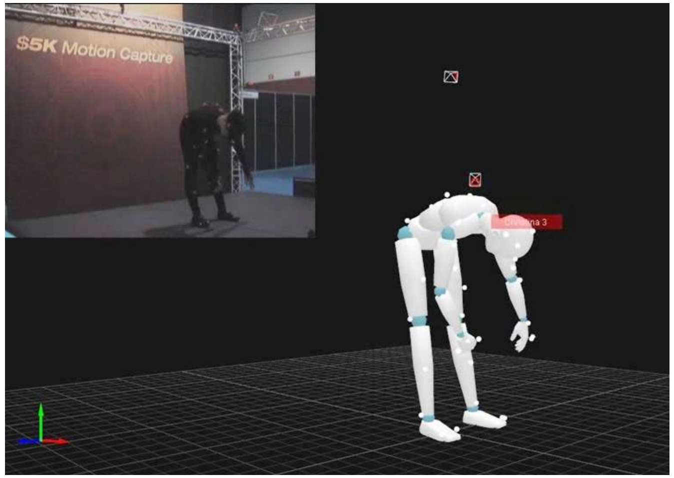
The Training Data

Record mocap
500k frames
distilled to 100k poses

Retarget to several models

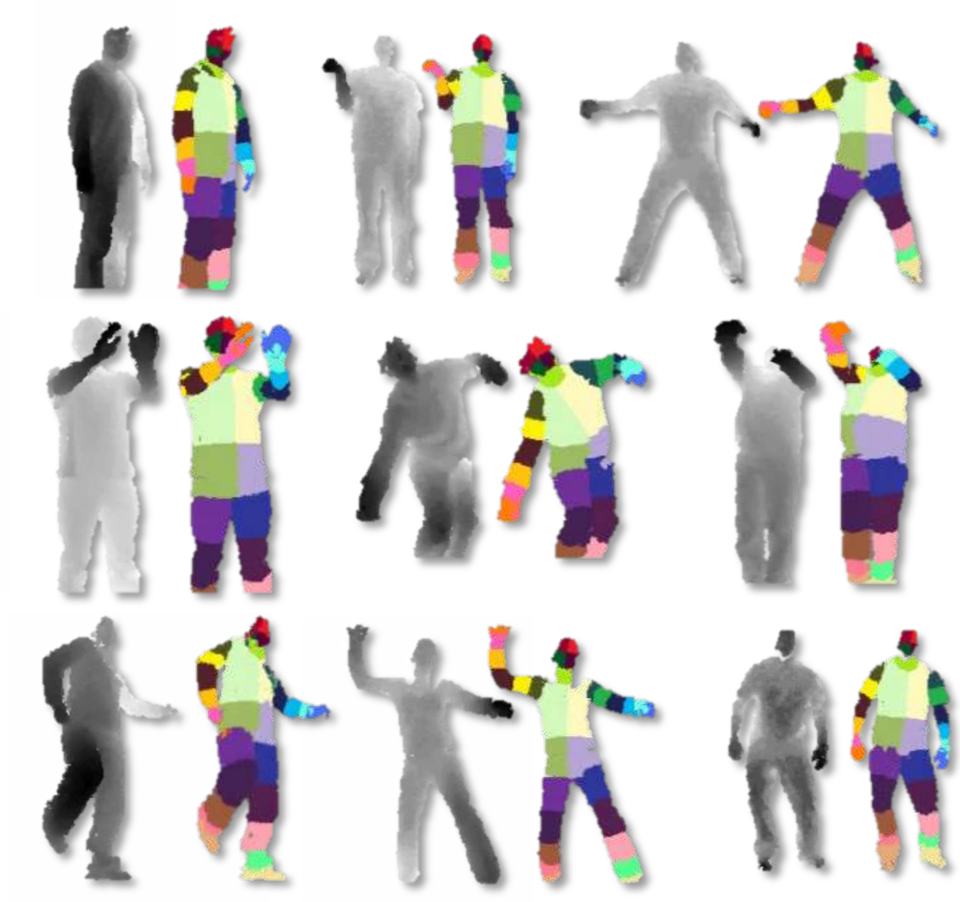


Render models: store depth & body part ID



Synthetic and Real Data

synthetic
(train & test)

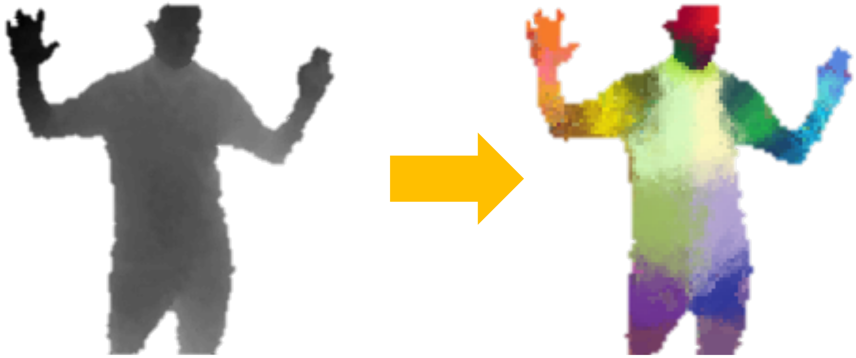


real
(test)

For each pixel in the synthetic depth image, we know its correct class (= label).
Sometimes, such data is also called ground truth data.
For the real test data, the pixels have been *hand labeled*.

Classifying Pixels

- Goal: for each pixel determine the most likely body part (head, shoulder, knee, etc.) it belongs to
- Classifying pixels = compute probability $P(c_\mathbf{x})$ for pixel $\mathbf{x} = (x,y)$, where $c_\mathbf{x}$ = body part
- Task: learn classifier that returns the most likely body part class $c_\mathbf{x}$ for every pixel $\mathbf{x}$
- Idea: consider a neighborhood around **x** (moving window)



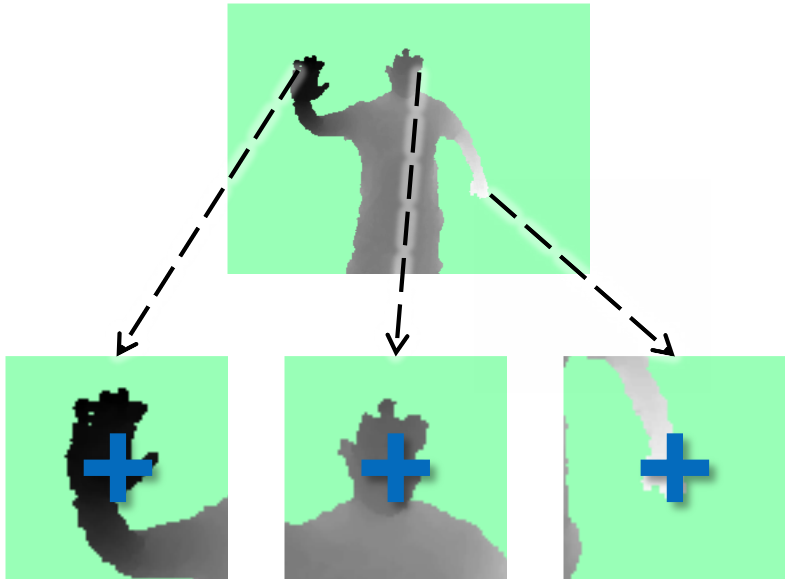


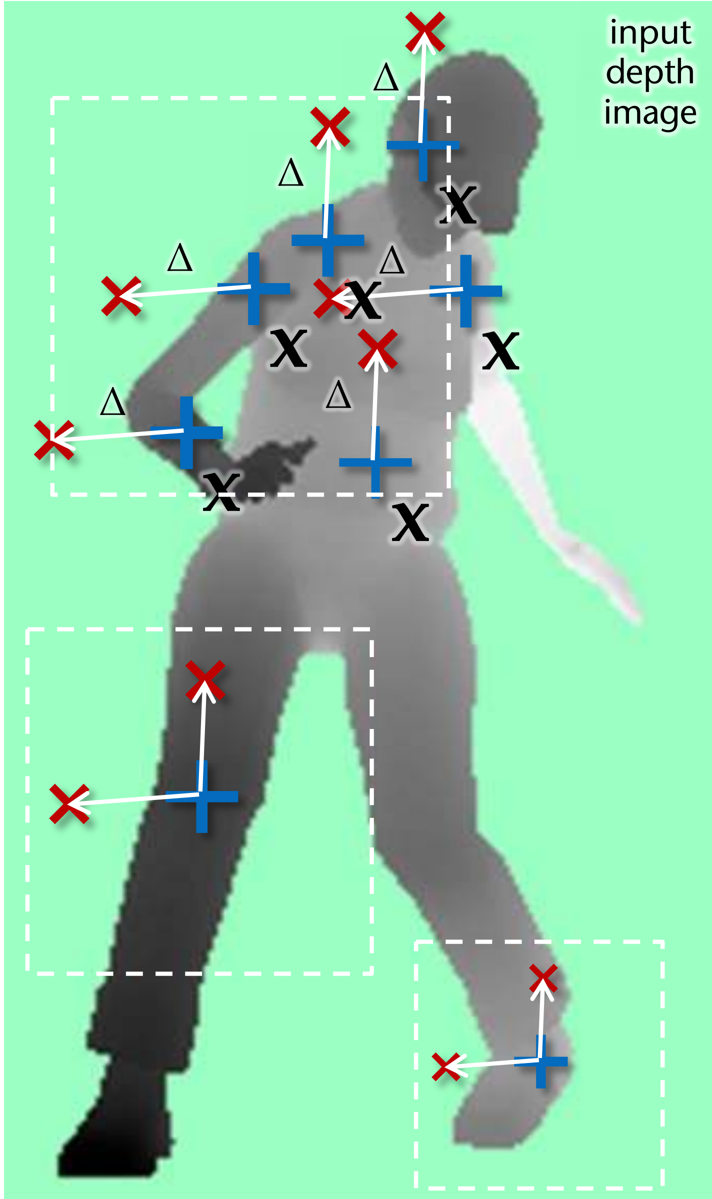
Image windows move with classifier

Fast Depth Image Features

- For a given pixel, consider all depth comparisons inside a window
- The *feature vector* for a pixel **x** are all *feature variables* obtained by all possible depth comparisons inside the window:

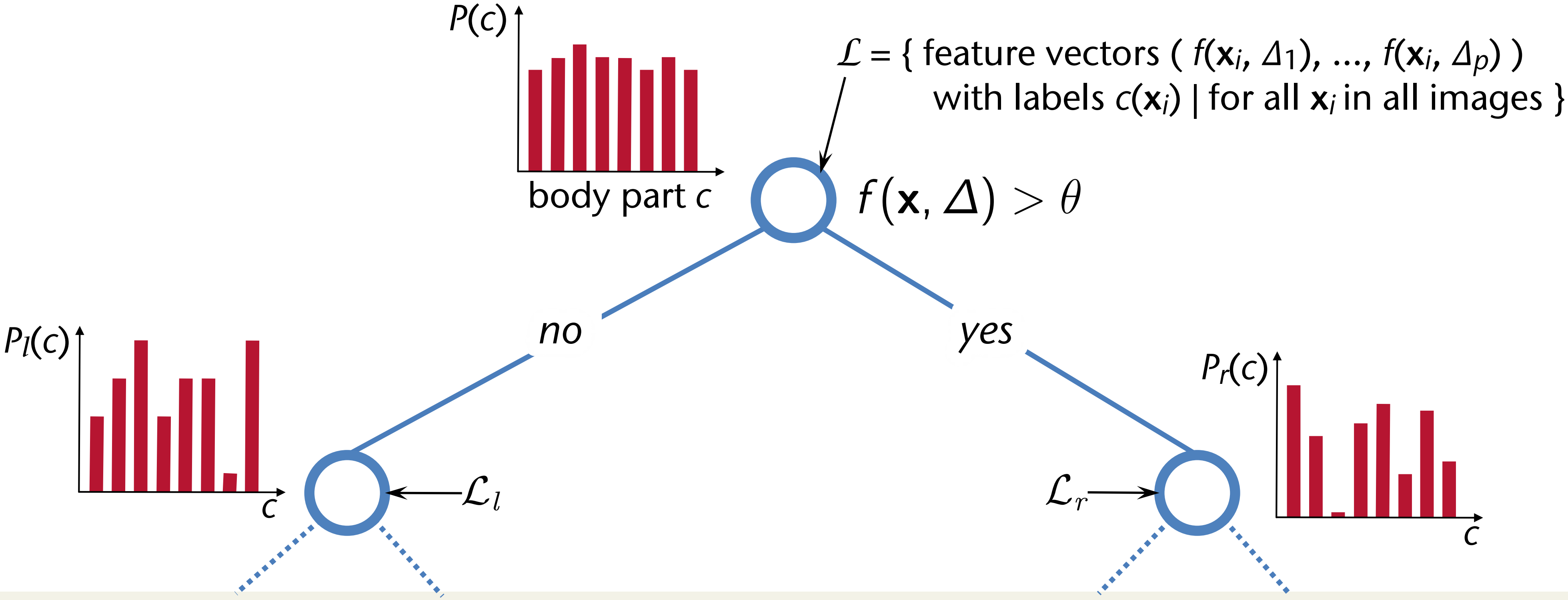
$$f(\mathbf{x}, \Delta) = D(\mathbf{x}) - D\left(\mathbf{x} + \frac{\Delta}{D(\mathbf{x})}\right)$$

  where D = depth image,
  $\Delta = (\Delta_x, \Delta_y)$ = offset vector,
  and D(background) = large constant
  - Note: scale Δ by 1/depth of **x**, so that the window shrinks with distance
- Features are very fast to compute



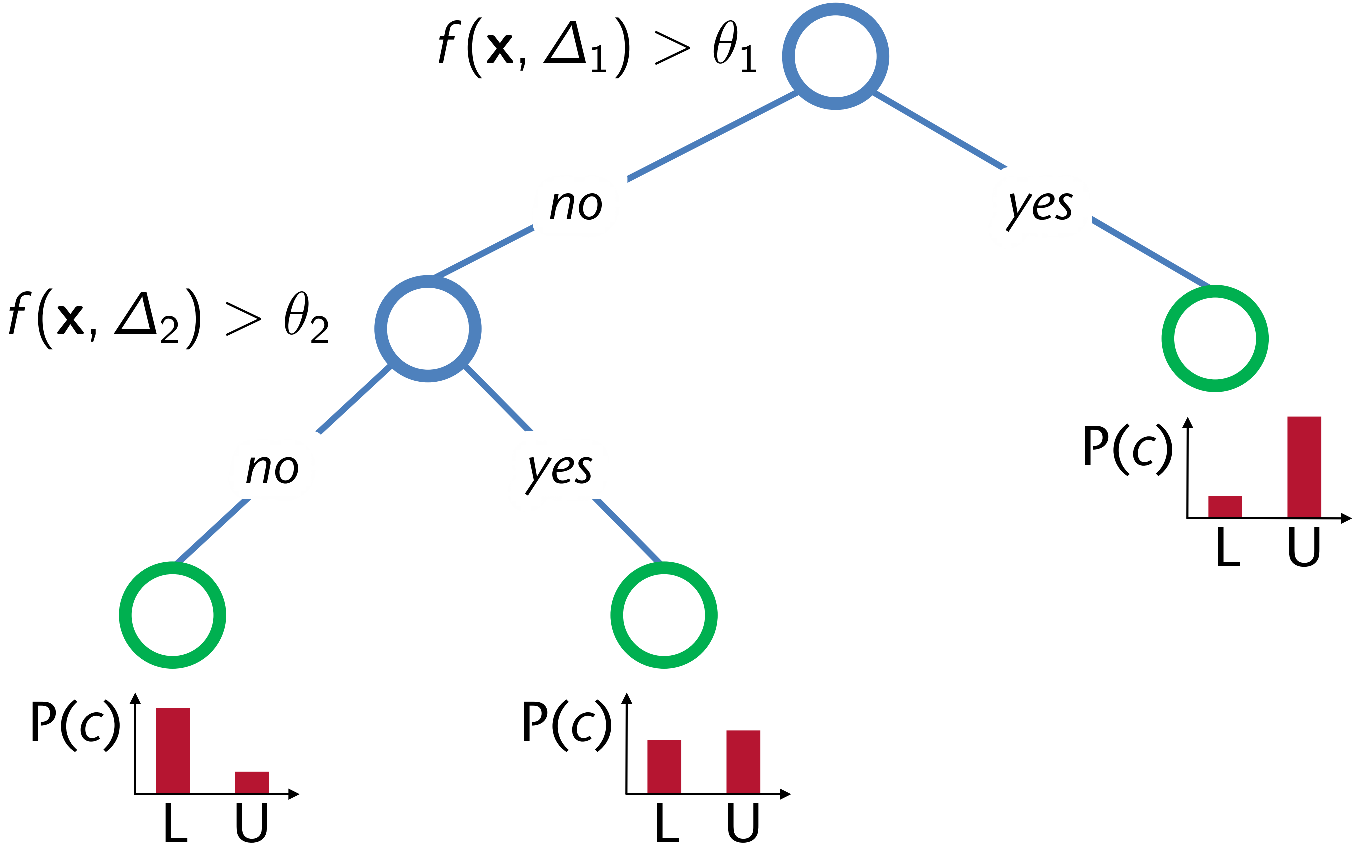
Training of a Single Decision Tree

- Conceptually, the training set $\mathcal{L}$ = { all feature vectors (= all $f(\mathbf{x}, \Delta)$) of all pixels of all training images }, together with the correct labels (= body part)
- Training a decision tree amounts to finding Δ and θ such that the information gain is maximized



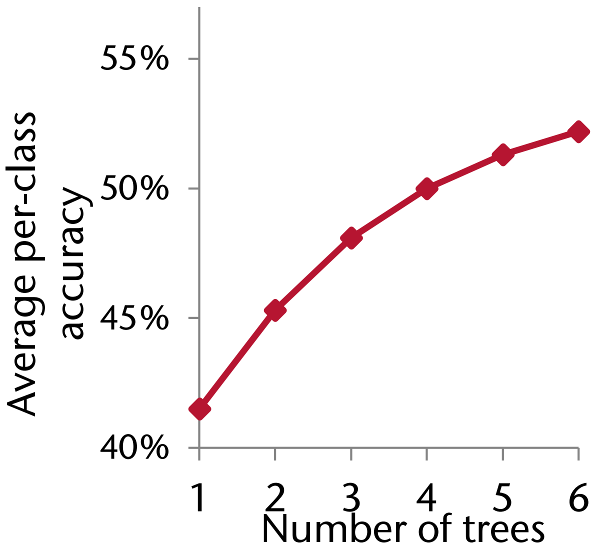
Classification of a Pixel at Runtime

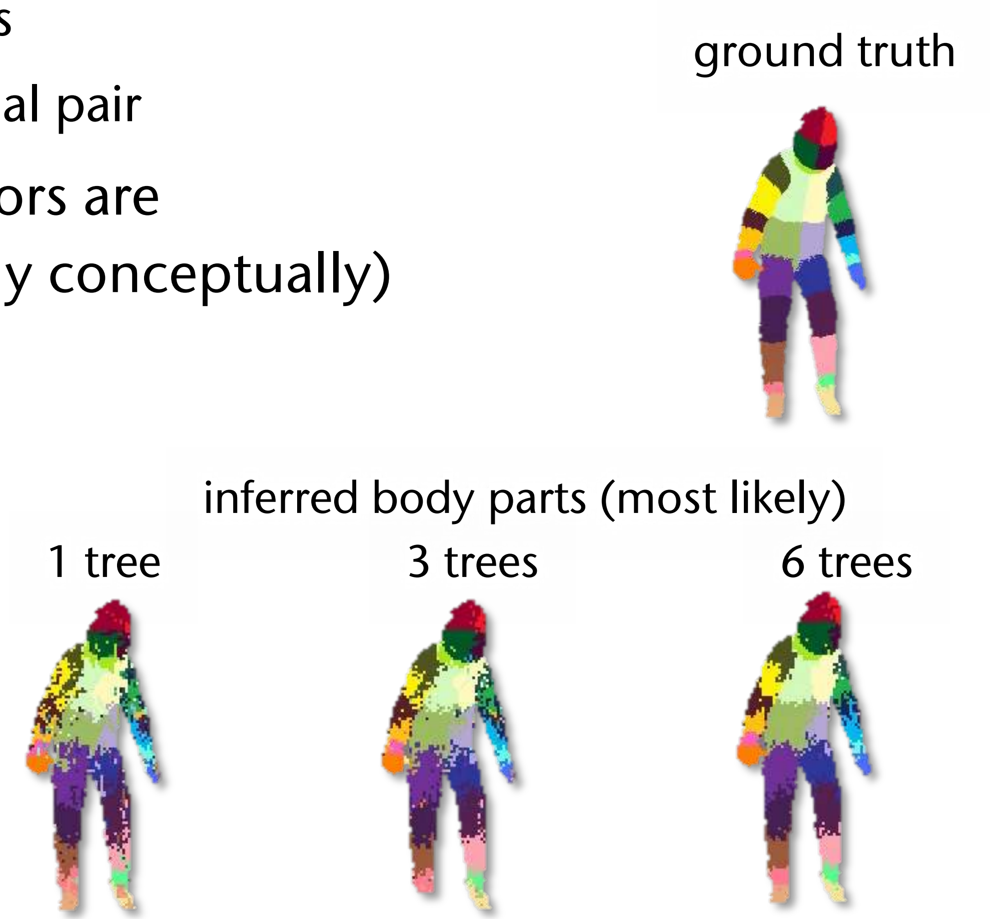
- Toy example: distinguish lower (L) and upper (U) parts of the body
- Note: each node only needs to store Δ and θ !
- For every pixel $\mathbf{x}$ in the depth image,
  we traverse the DT:



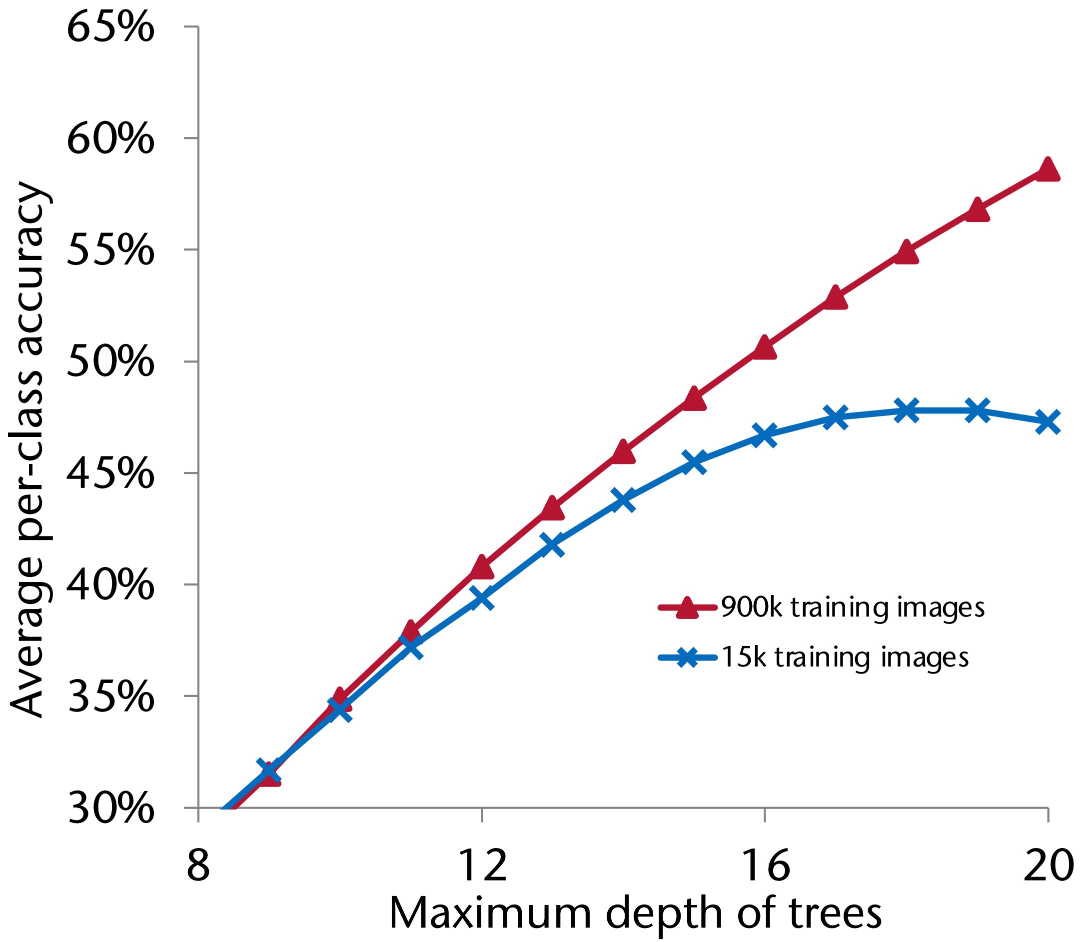
Training a Random Forest

- Train *ntree* many trees, for each one introduce lots of randomization:
  - Random subset of pixels of the training images (~ 2000)
  - At each node to be trained, choose a random set of *mtry* many Δ values
  - Optimize θ for each Δ, pick optimal pair
- Note: the complete feature vectors are never explicitly constructed (only conceptually)

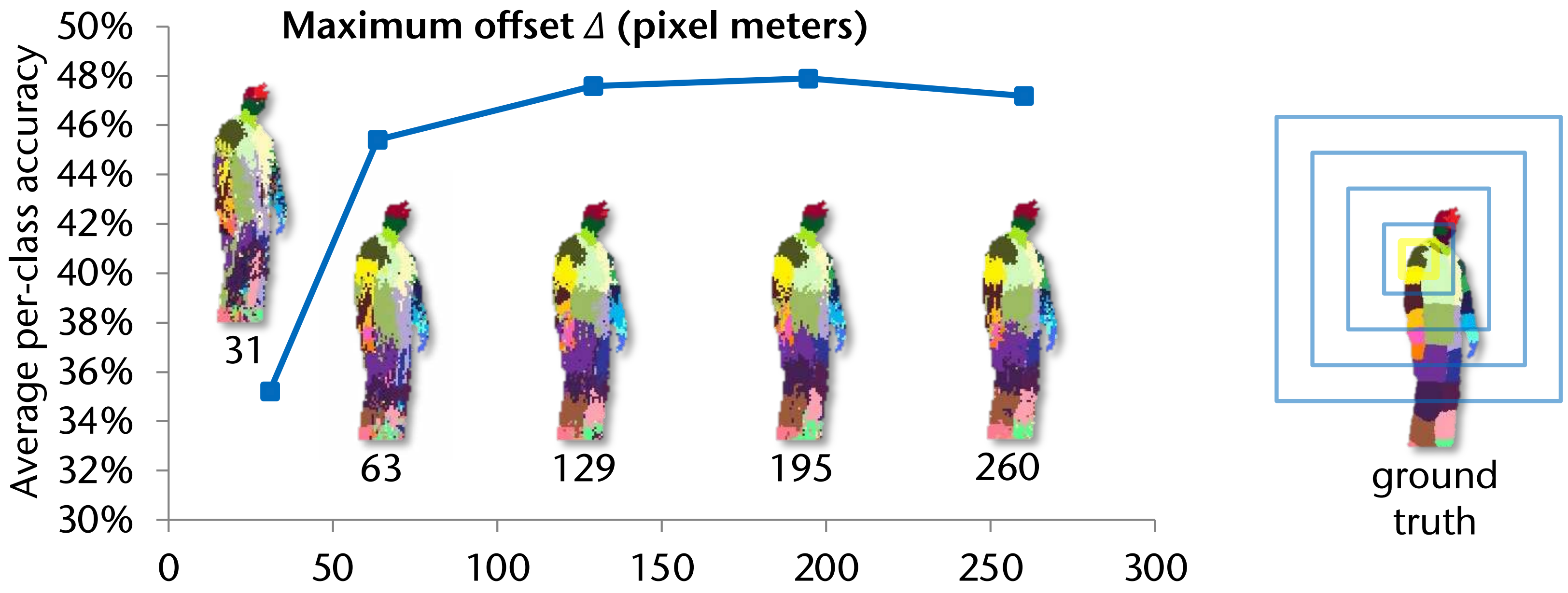


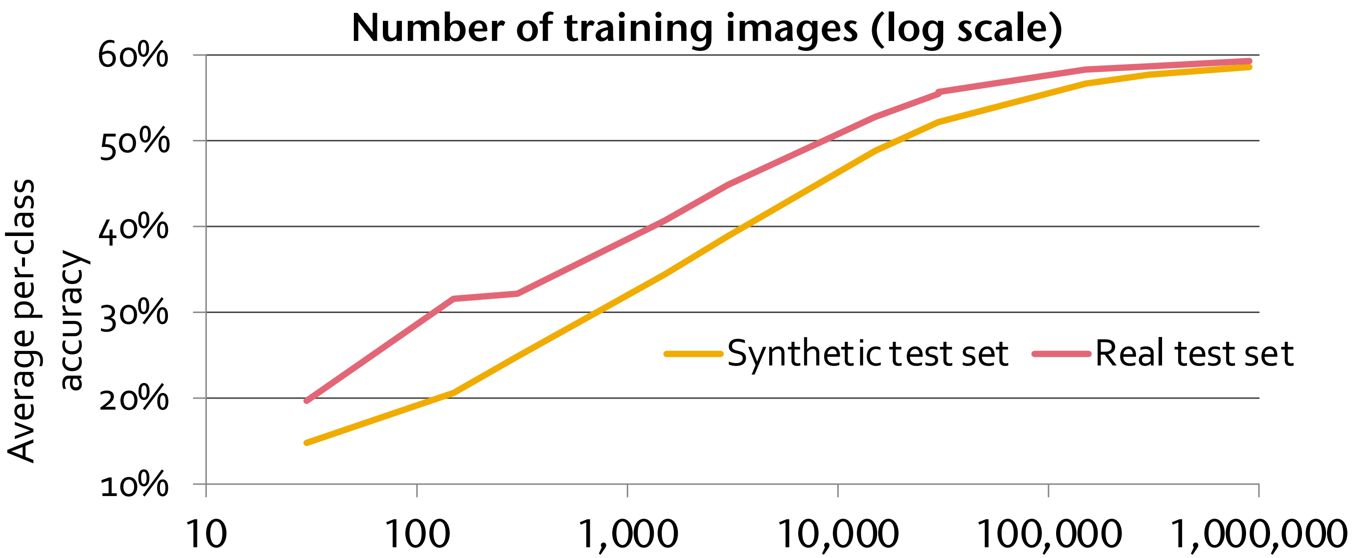


- Depth of trees: check whether it is really best to grow all DTs in the RF to their maximum depth



More Parameters

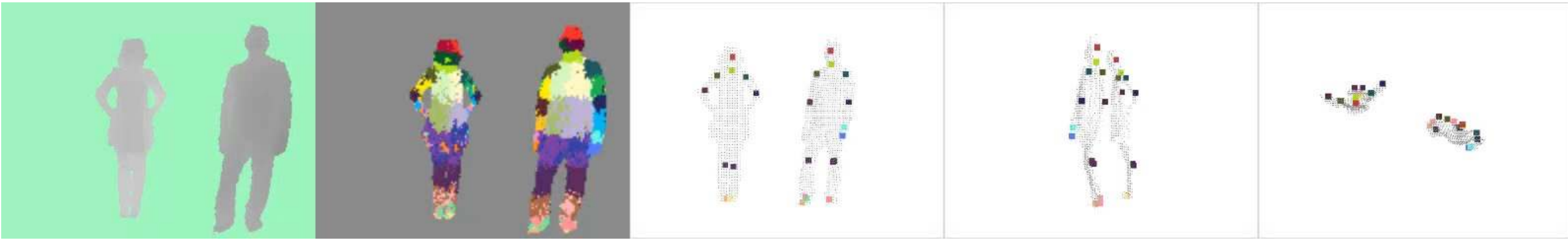


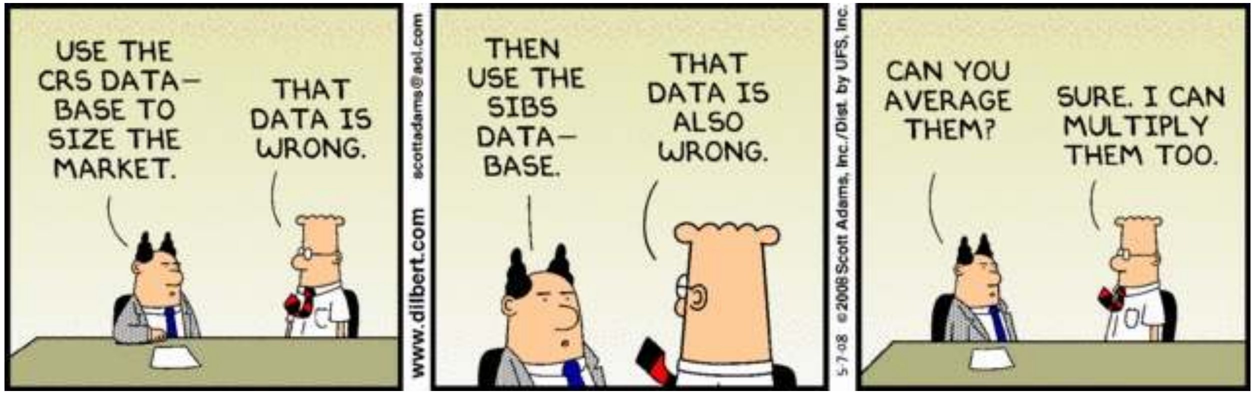


Video

Input depth image (bg removed)

Inferred body parts posterior

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