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 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; then 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 happens, then the information is large"
- Examples:
  - Observing the outcome of coin flip $\longrightarrow I = -\log \frac{1}{2} = 1$
  - Observing the outcome of dice == 6 $\longrightarrow I = -\log \frac{1}{6} = 2.58$

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 question you need to ask to determine it?
  - In probabilistic terms: what is the *expected amount of information*? ⟶ captured by the notion of entropy
- Definition: Entropy

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

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

- 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

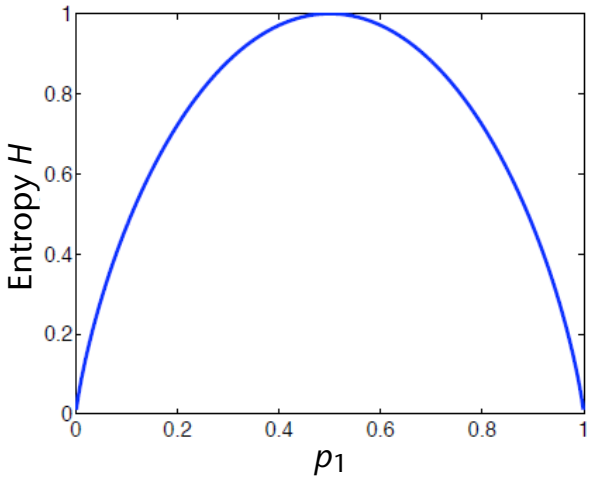
$$H(Y) = -\sum_{i=1}^{8} \frac{1}{8} \log \frac{1}{8} = \log 2^3 = 3 \text{ bits}$$

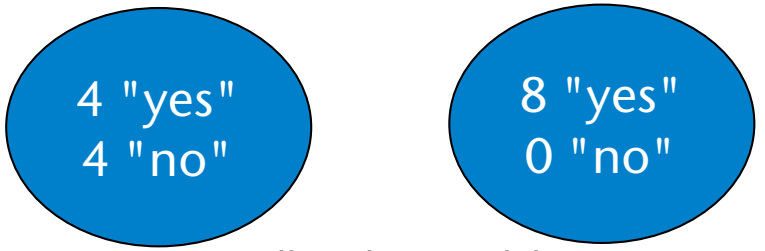
- In general, if there are k different possible outcomes, then

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

  - Equality holds when all outcomes are equally likely

- With $k = 2$ (two outcomes), entropy looks like this:
- The more the probability distribution deviates from uniformity, the lower the entropy
- *Entropy* measures the *impurity*:





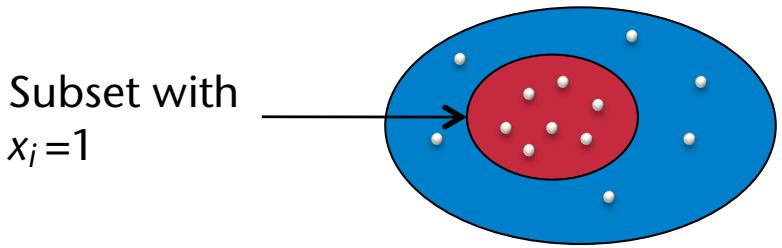
Balls in bin model

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

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., $x_i \in \{1, 2, ..., z\}$
- We now consider only cases 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:

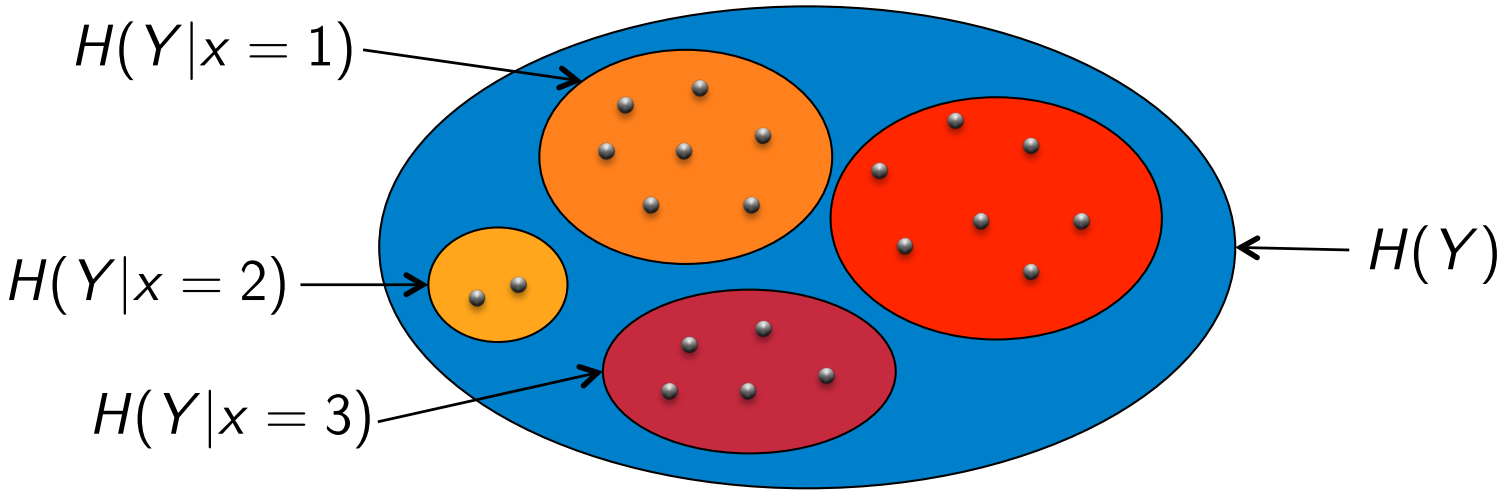
$$H(Y|x_i = 1) = -\sum_i p(y_i|x_i = 1) \log \underbrace{p(y_i|x_i = 1)}_{\text{Probability of } y_i \text{ occurring as a value of } Y, \text{ where we draw } Y \text{ only from the subset that contains only data points that have attribute } x_i=1}$$



- Overall conditional entropy:

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

$$= -\sum_{k=1}^{z} \underbrace{p(x=k)}_{\text{Probability that the attribute } X \text{ has value } k} \sum_{i} p(y_i|x_i=k) \log p(y_i|x_i=k)$$



Information Gain

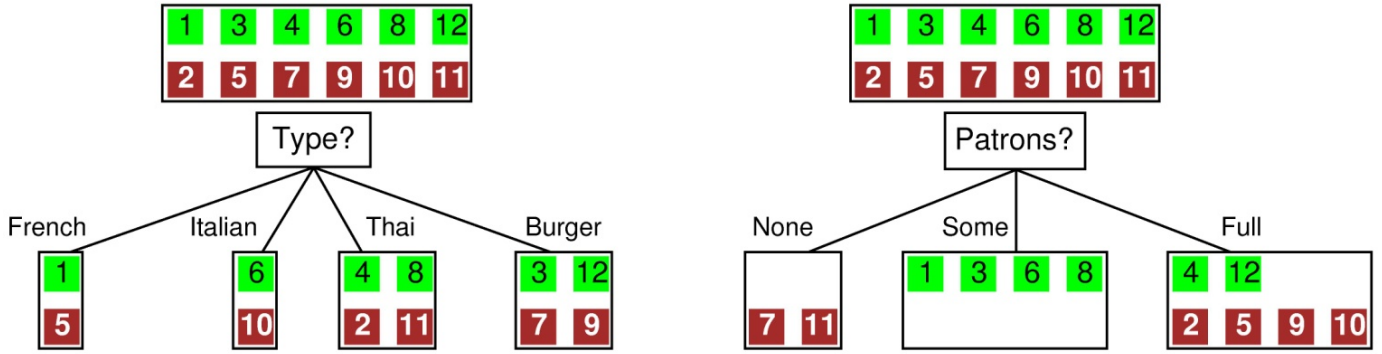
- How much information do we gain *if we disclose the value of one attribute X*?
- Information gain = (information *before* split) – (information *after* split) = *reduction of uncertainty* by knowing attribute *X*
- The information gained by a split in a node of a decision tree:

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

- Goal: choose the attribute with the largest *IG*
  - In case of scalar attributes, also choose the *optimal cutpoint*

Example

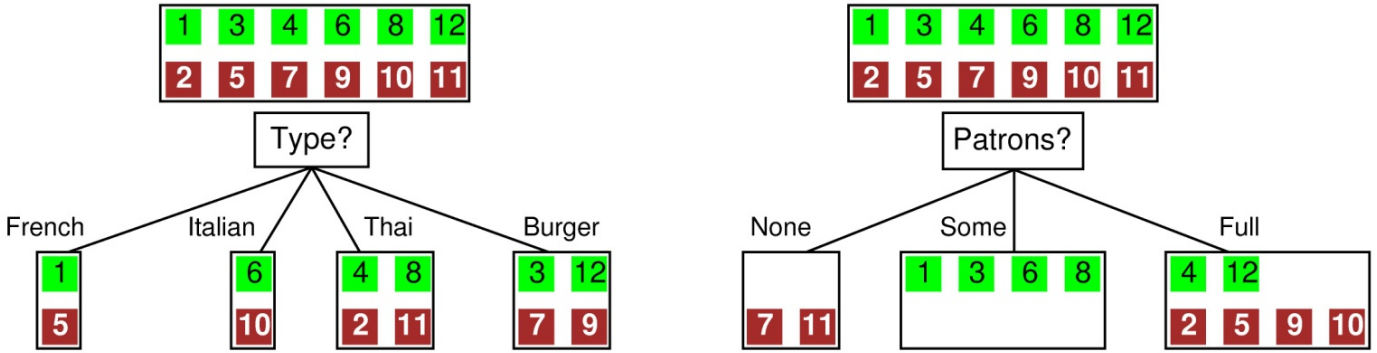
- Consider 2 options to split the root node of the restaurant example



- Random variable $Y \in \{$ "yes", "no" $\}$
- At the root node:

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

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



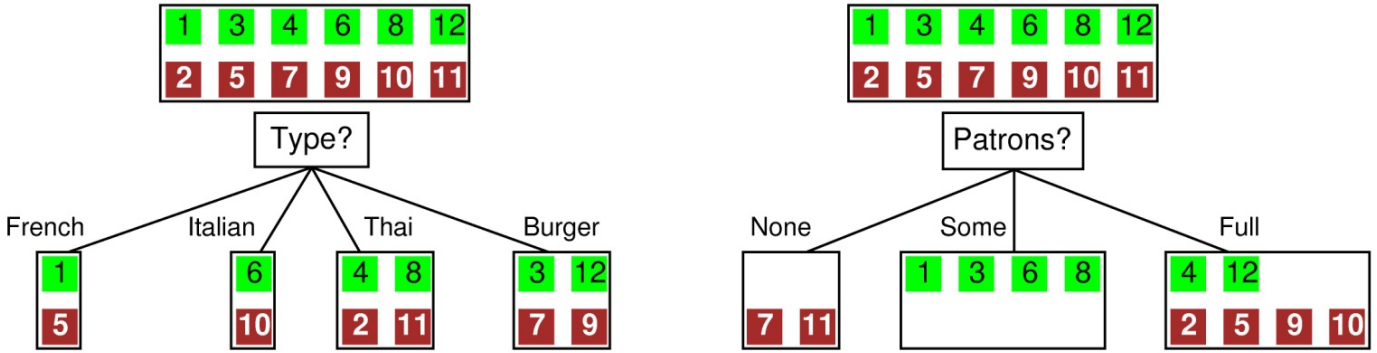
- Conditional entropy for right option:

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

where n = the attribute "#patrons" $\in$ { "none", "some", "full" }

$$H(Y|\#\text{patrons}) = \frac{2}{12}\left(p(y = \text{“no”}) \log p(y = \text{“no”}) + p(y = \text{“yes”}) \log p(y = \text{“yes”})\right) + \frac{4}{12}\left(p(y = \text{“no”}) \log p(y = \text{“no”}) + p(y = \text{“yes”}) \log p(y = \text{“yes”})\right) + \frac{6}{12}\left(p(y = \text{“no”}) \log p(y = \text{“no”}) + p(y = \text{“yes”}) \log p(y = \text{“yes”})\right)$$

$$H(Y|\#\text{patrons}) = \frac{2}{12}(1 \log 1 + 0 \log 0) + \frac{4}{12}(0 \log 0 + 1 \log 1) + \frac{6}{12}\left(\frac{4}{6} \log \frac{6}{4} + \frac{2}{6} \log \frac{6}{2}\right)$$



- Conditional entropy for left option:

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

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

- Compare the information gains:

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

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

  - So, the attribute "#patrons" gives us more information about Y

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

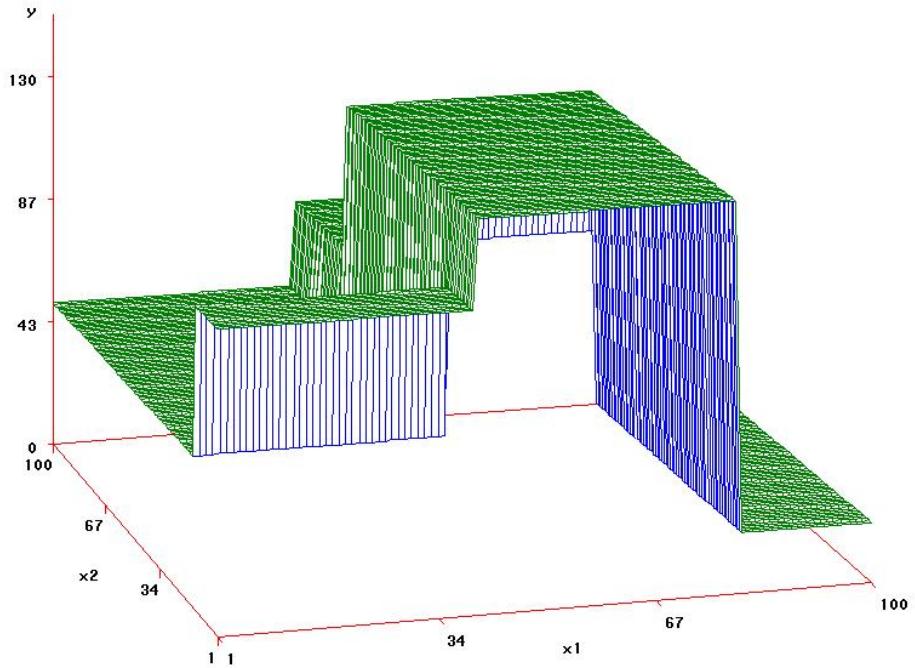
Bits and Pieces

- 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
  - Stop construction here, use majority vote (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

Expressiveness of Decision Trees

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

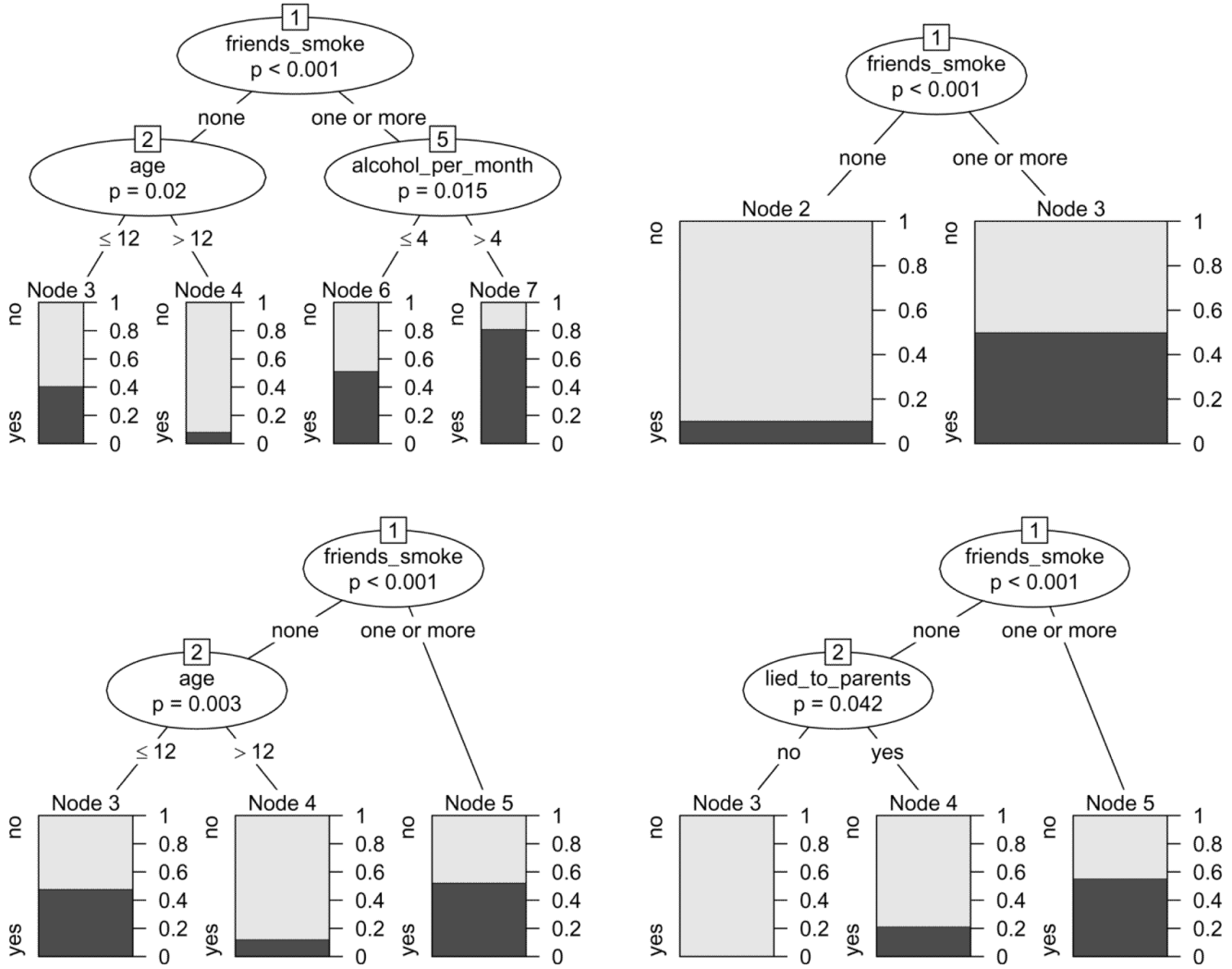


- DTs can approximate *any* function

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 learner performs extremely well on the training data, but very poorly on unseen data ⟶ high generalization error
  - 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 knowledge distributed as:

    7 know 3 of the Monkees

    10 know 2 of the Monkees

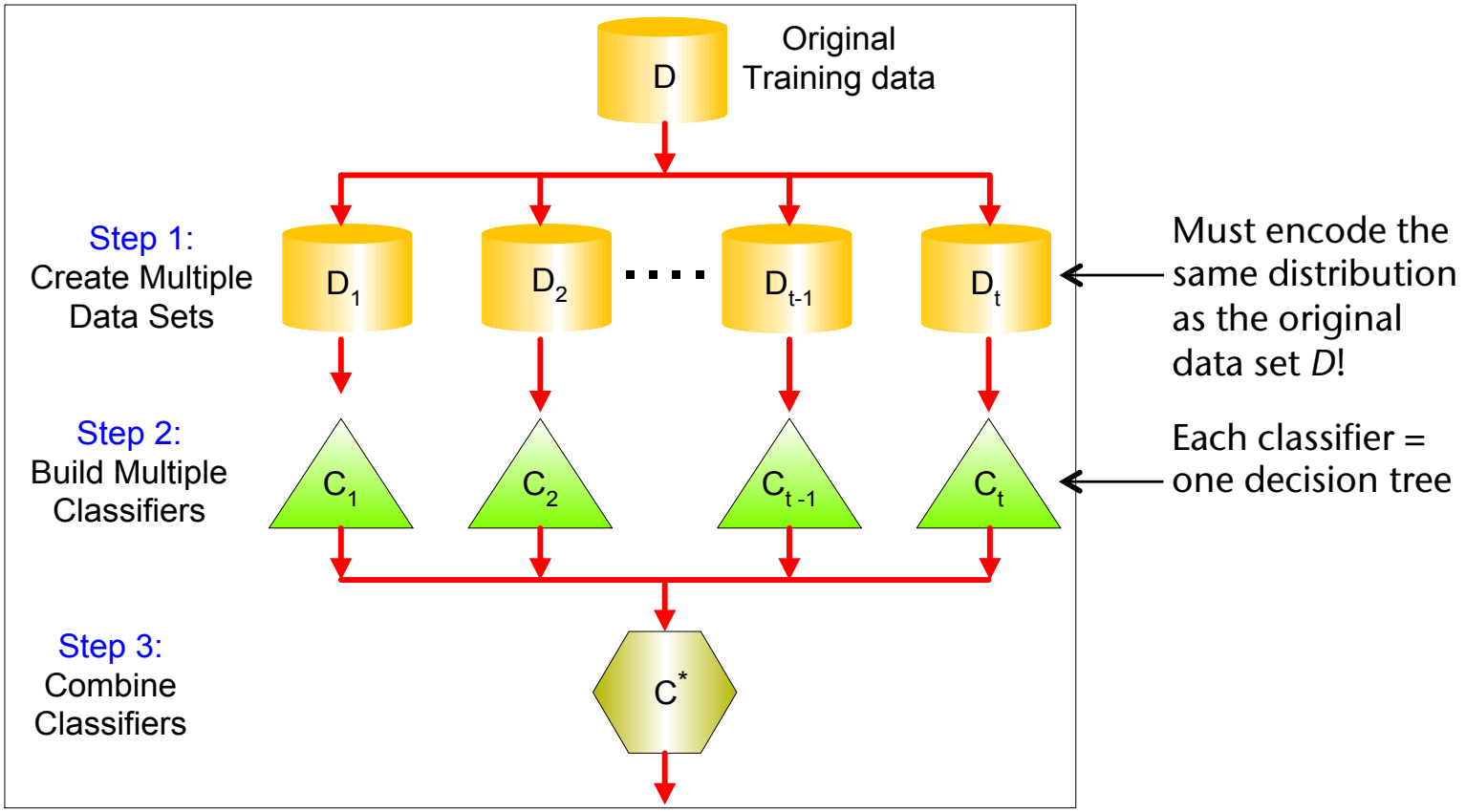
    15 know 1 of the Monkees

    68 have no clue
  - So "Noll" will garner, on average, 34 votes versus 22 votes for each of the other choices

- Implication: one should not expend 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 747
- Prerequisites for crowd wisdom to emerge:
  - Opinions must be independent
  - Some knowledge of the truth must reside with some group members (⟶ *weak classifiers*)

The Random Forest 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)



Details on the Construction of Random Forests

- 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, with replacement, size of new data = size of original data set; or,
2. Subsampling: randomly draw samples, without replacement, size of new data < size of original data set

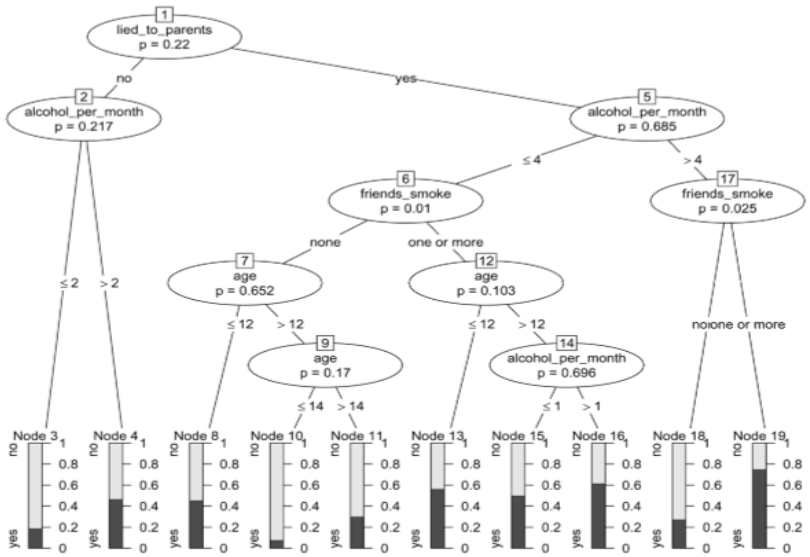
  - New data sets reflect the *same* random process as the orig. data, but they differ slightly from each other and the orig. set due to random variation
  - Resulting trees can differ substantially (see earlier slide)

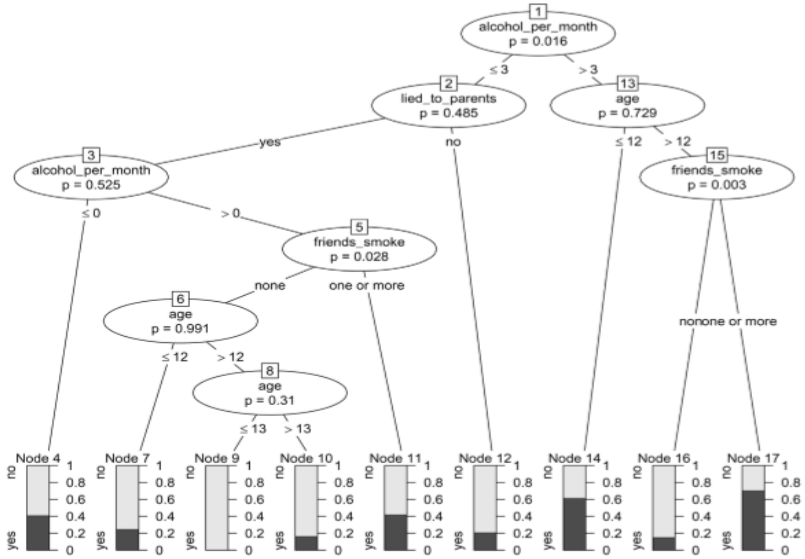
- Growing the trees:
  - Each tree is grown without any stopping criterion, i.e., until each leaf contains data points of only *one single* class
  - At *each node*, a random subset of attributes (= predictor variables/ features) is preselected; *only from those,* the one with the best information gain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

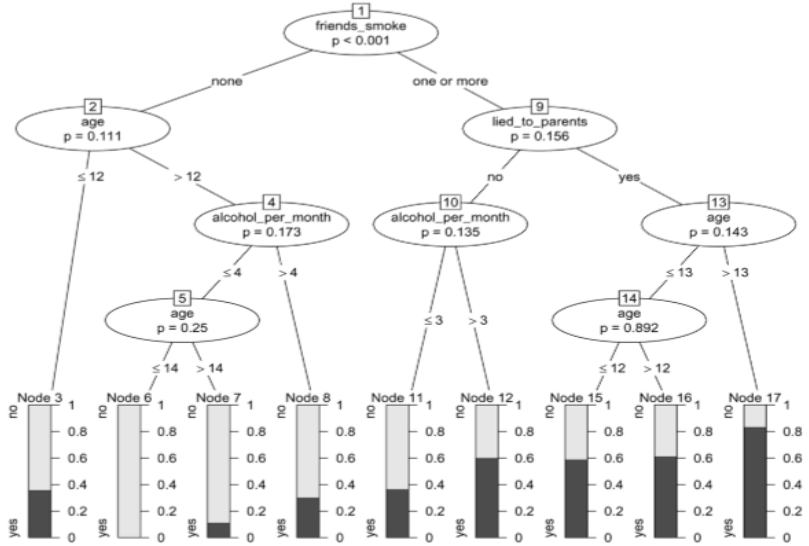
- The learning algorithm:

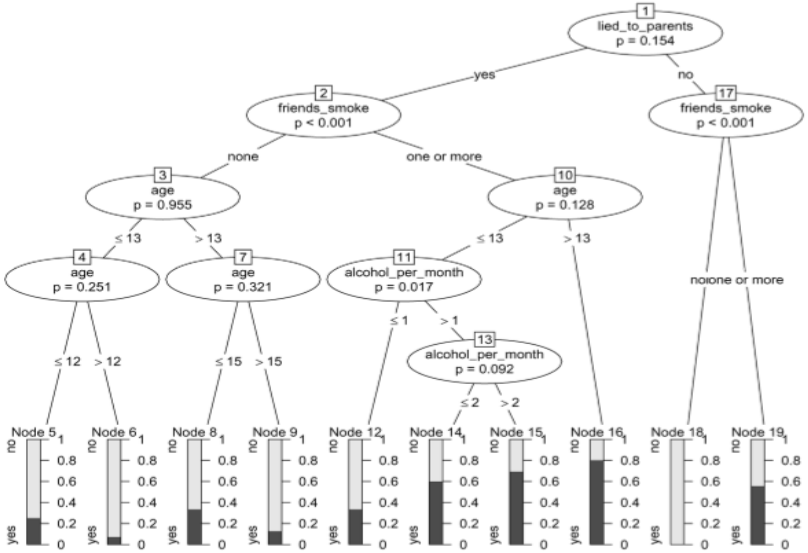
```
input: learning set L
for t = 1...ntree:
   build subset Lt from L by random sampling
   learn tree Tt from Lt:
      at each node:
         randomly choose mtry features
         compute best split from only those features
      grow each tree until leaves are perfectly pure
```

A Random Forest Example for the Smoking Data Set



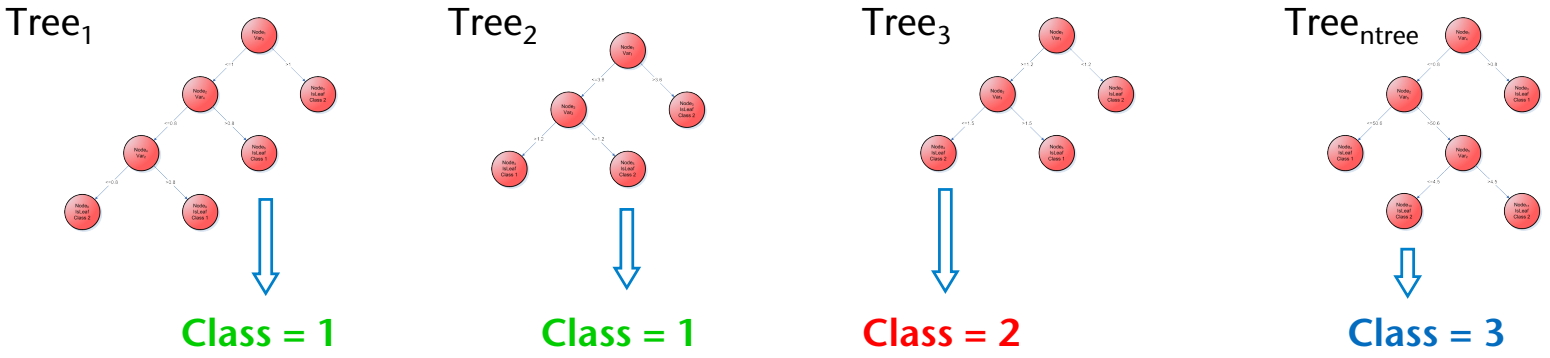






Using a Random Forest for Classification

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



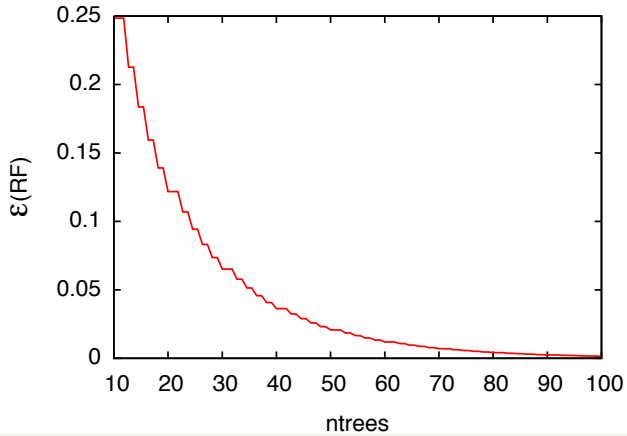
  - Take majority of those class labels
- Sometimes, if labels are numbers, (weighted) averaging makes sense

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:

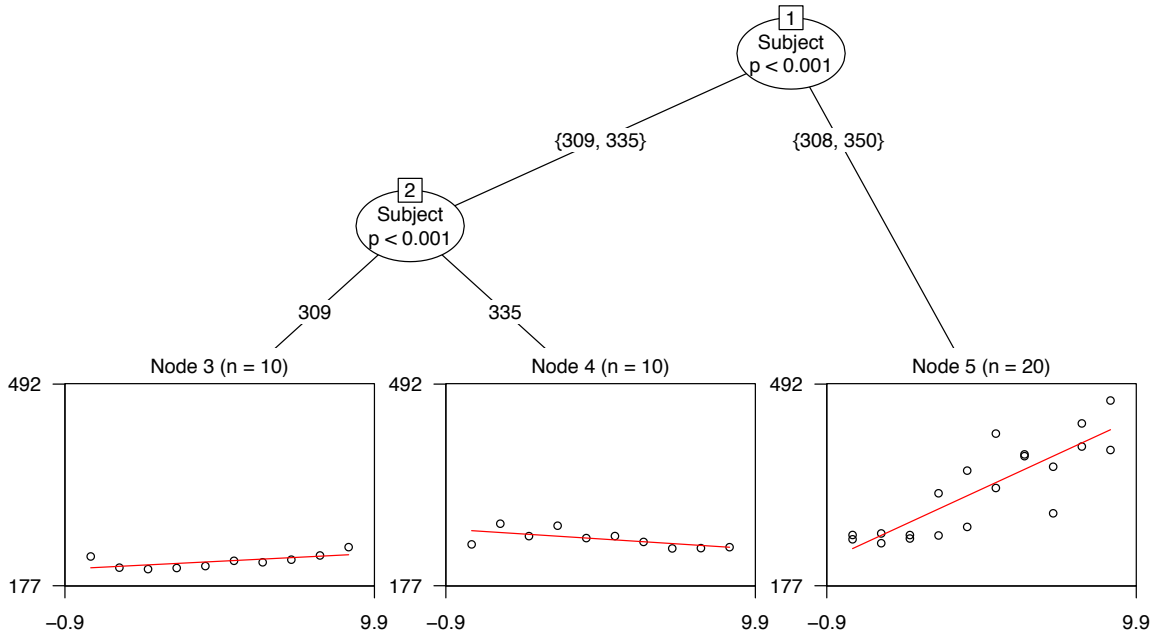
$$\varepsilon_{\text{RF}} = \sum_{i=\lceil \frac{ntree}{2} \rceil}^{ntree} \binom{ntree}{i} \varepsilon^i (1-\varepsilon)^{(ntree-i)}$$

- Example:
  ntree = 60,
  individual error rate $\varepsilon = 0.35 \longrightarrow$
  error rate of RF $\varepsilon_{\text{RF}} \approx 0.01$



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:



Features and Pitfalls of Random Forests

- "Small *n*, large *p*":
  - RFs are well-suited for problems with many more variables (dimensions in the feature space) than observations / training data
- Nonlinear function approximation:
  - RFs can approximate *any* unknown function
- Blackbox:
  - RFs are a black box; it is practically impossible to obtain an analytic function description, or gain insights in predictor variable interactions
- 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 pre-selection of *mtry* variables can help

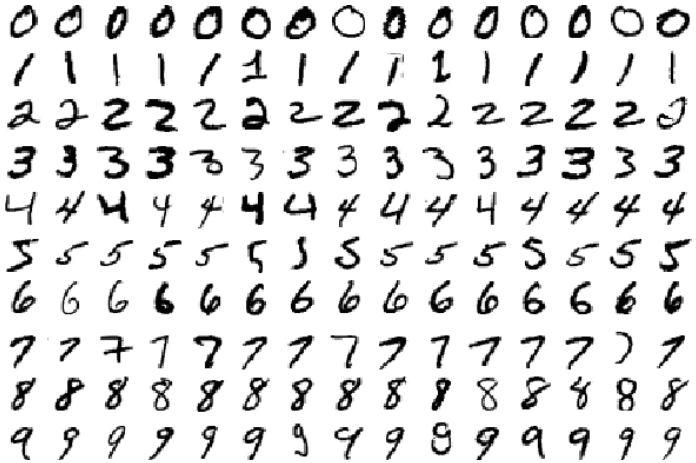
- Out-of-bag error estimation:
  - For each tree T_i, a training data set $\mathcal{L}_i \subset \mathcal{L}$ was used
  - Use $\mathcal{L} \setminus \mathcal{L}_i$ (the out-of-bag data set) to test the prediction accuracy
- Handling missing values:
  - Occasionally, some data points contain a missing value for one or more of its variables (e.g., because the corresponding measuring instrument had a malfunction)
  - When information gain is computed, just omit the missing values
  - During splitting, use a surrogate that best predicts the values of the splitting variable (in case of a missing value)

- 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*

- 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

Application: Handwritten Digit Recognition

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



- 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:

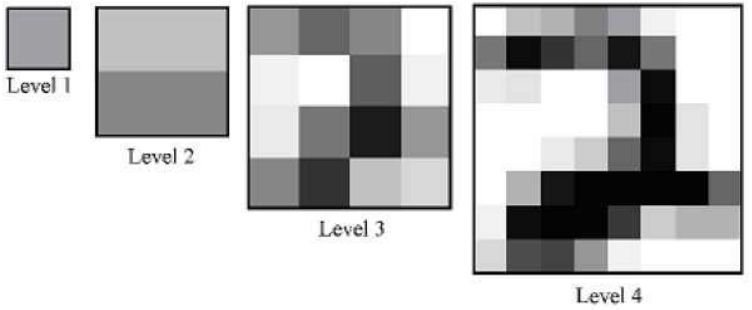
$$H(i,j) = I(i,j) \wedge I(i,j+2)$$
$$V(i,j) = I(i,j) \wedge I(i+2,j)$$
$$N(i,j) = I(i,j) \wedge I(i+2,j+2)$$
$$S(i,j) = I(i,j) \wedge I(i+2,j-2)$$

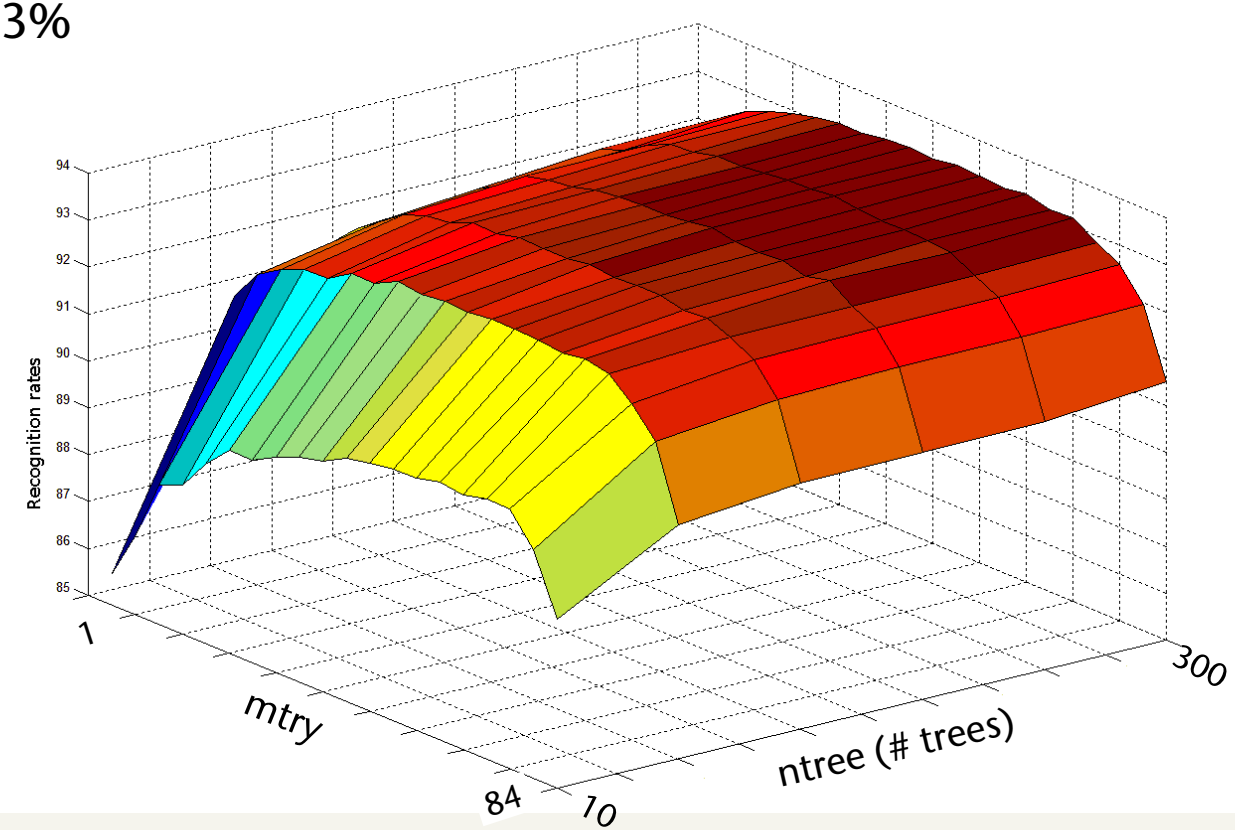
and a few more ...

- 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%
  - Caveat: it was a precursor of random forests

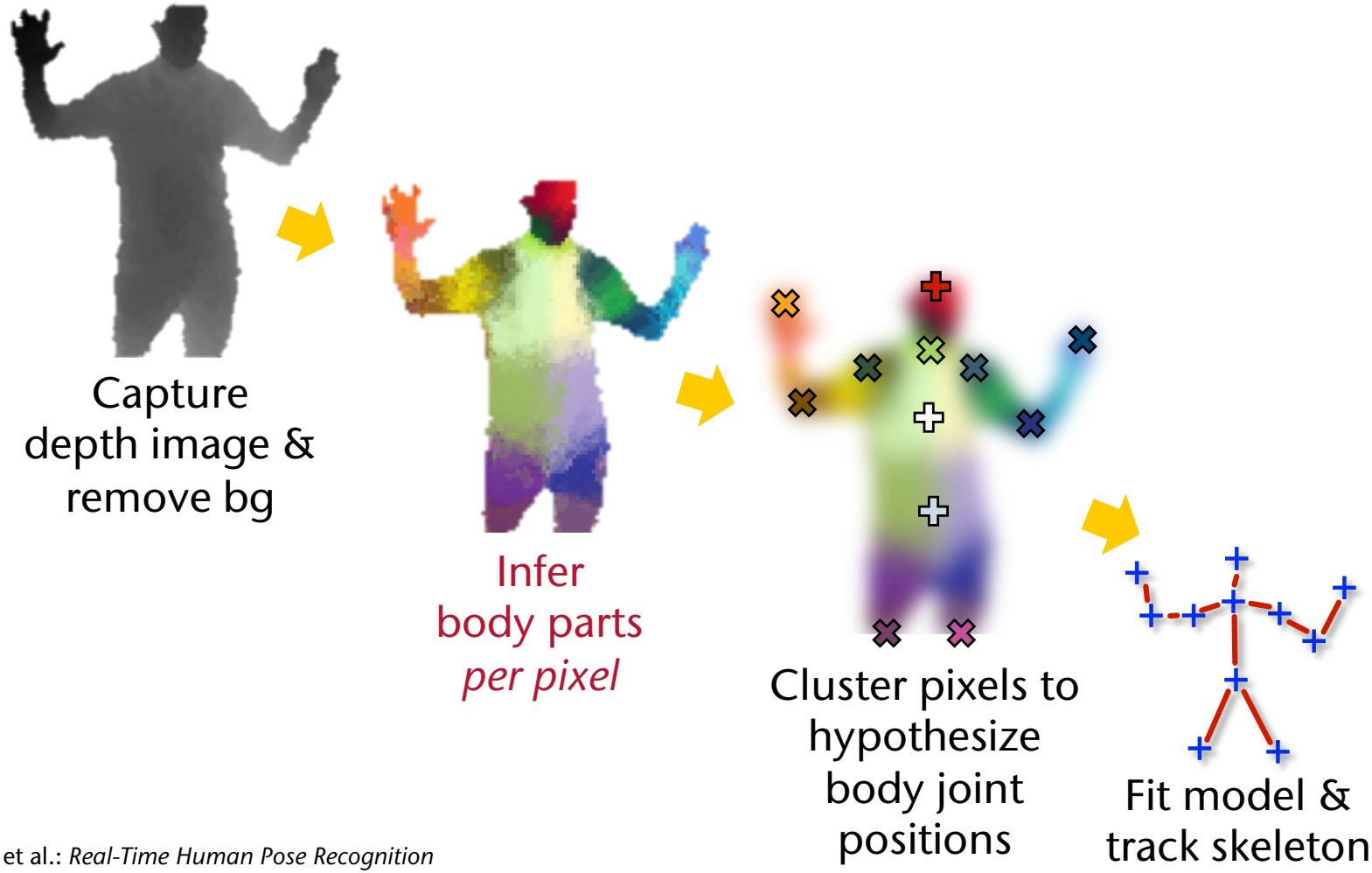
- Other experiments on handwritten digit recognition:
  - Feature vector = all pixels of an image pyramid
  - Recognition rate: ~ 93%
  - Dependence of recognition rate on *ntree* and *mtry*:





Body Tracking Using Depth Images (Kinect)

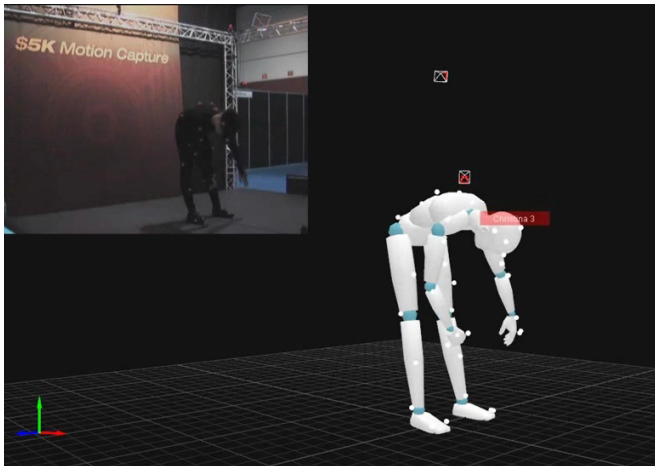
- The tracking / data flow pipeline:



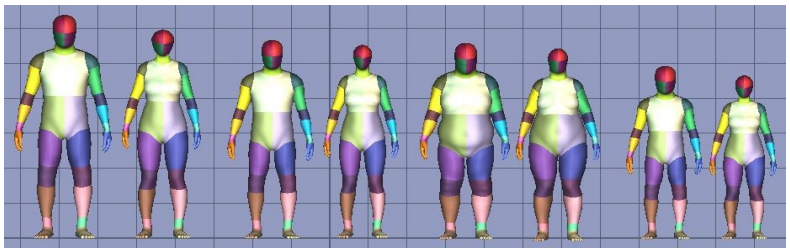
[Shotton et al.: *Real-Time Human Pose Recognition in Parts from Single Depth Images*; CVPR 2011]

The Training Data

Record mocap
500k frames
distilled to 100k poses



Retarget to several models



Render models: store depth & body part ID

Synthetic vs Real Data

synthetic
(train & test)

real
(test)

For each pixel in the depth image, we know its correct class (= label).
Sometimes, such data is also called ground truth data.

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 $\mathbf{x}$ (moving window)

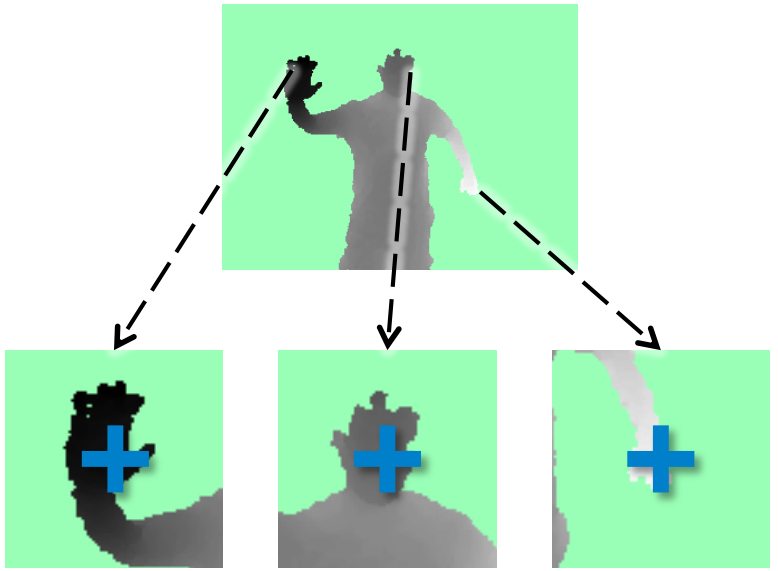
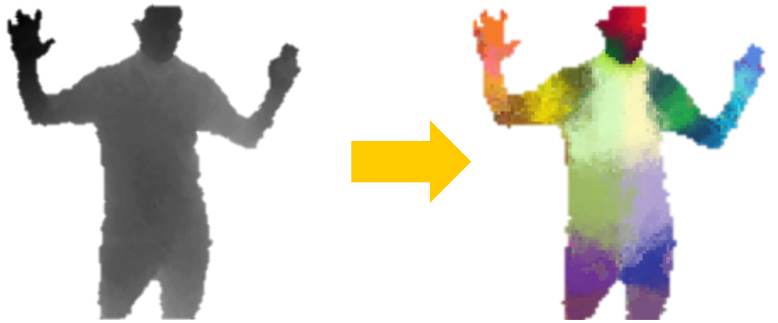


image windows move with classifier



Fast Depth Image Features

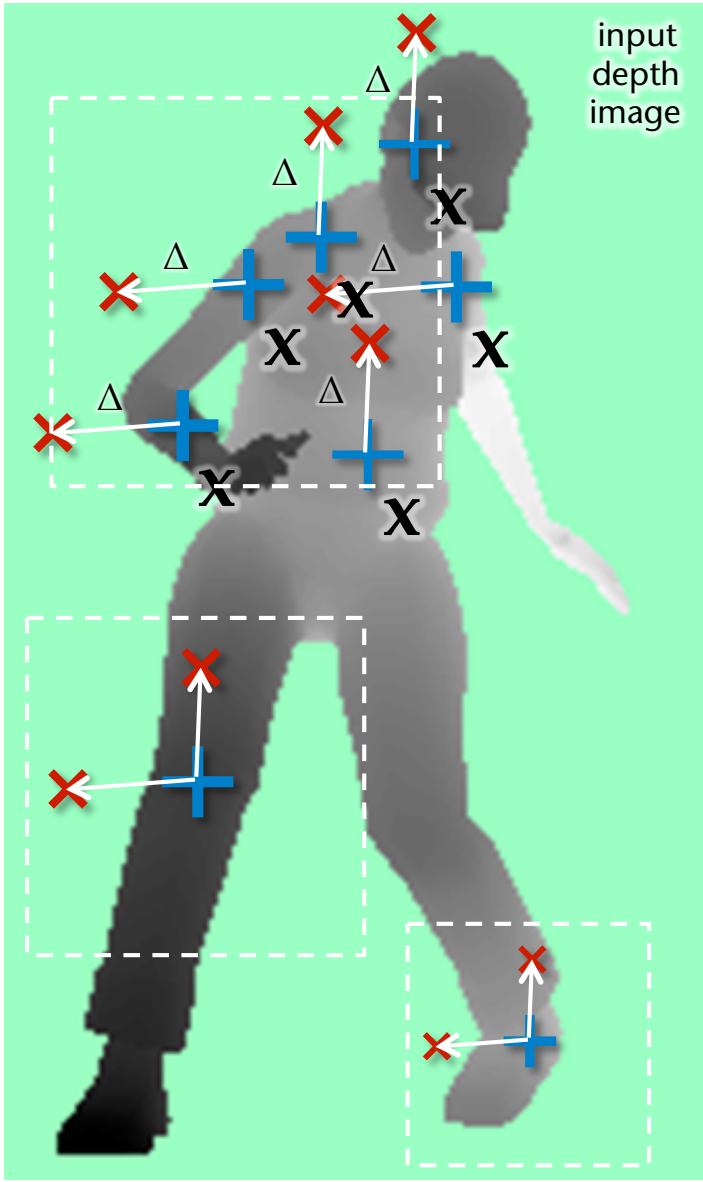
- For a given pixel, consider all depth comparisons inside a window
- The *feature vector* for a pixel **x** are all *feature variables* obtained by all possible depth comparisons inside the window:

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

where D = depth image,
$\Delta = (\Delta_x, \Delta_y)$ = offset vector,
and D(background) = large constant

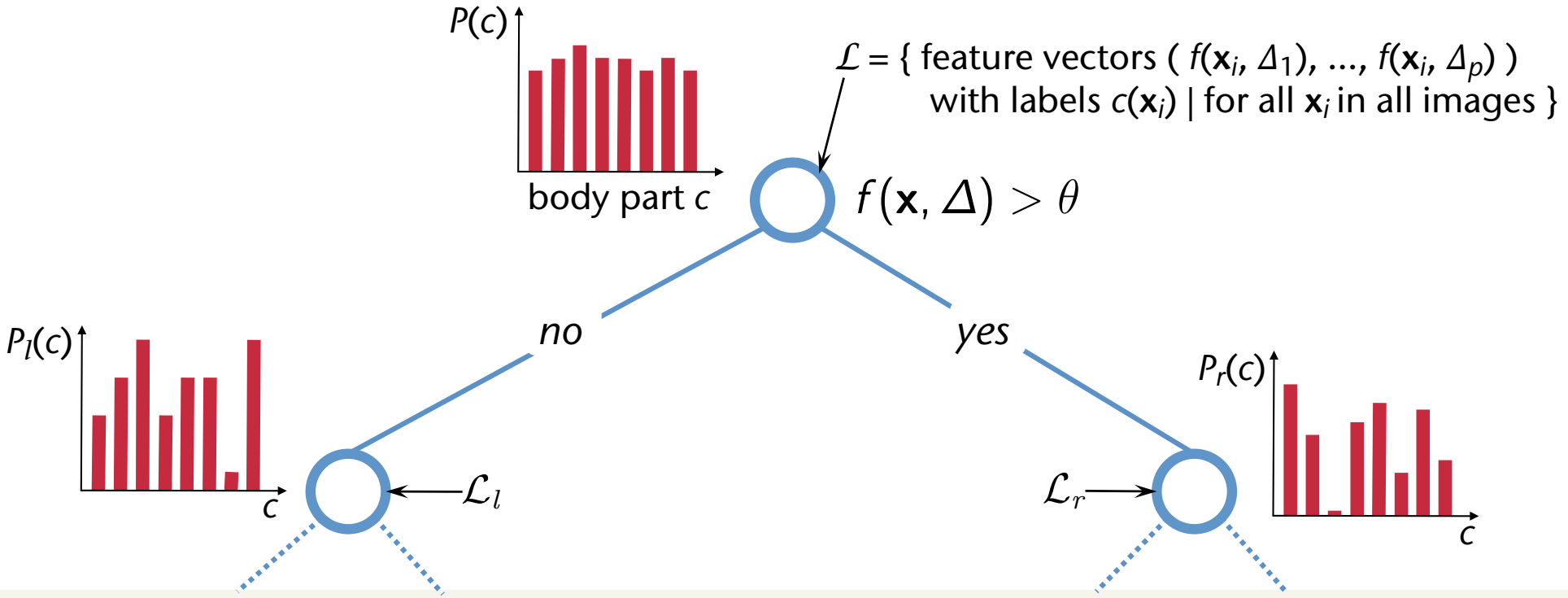
  - Note: scale Δ by 1/depth of **x**, so that the window shrinks with distance

- Features are very fast to compute



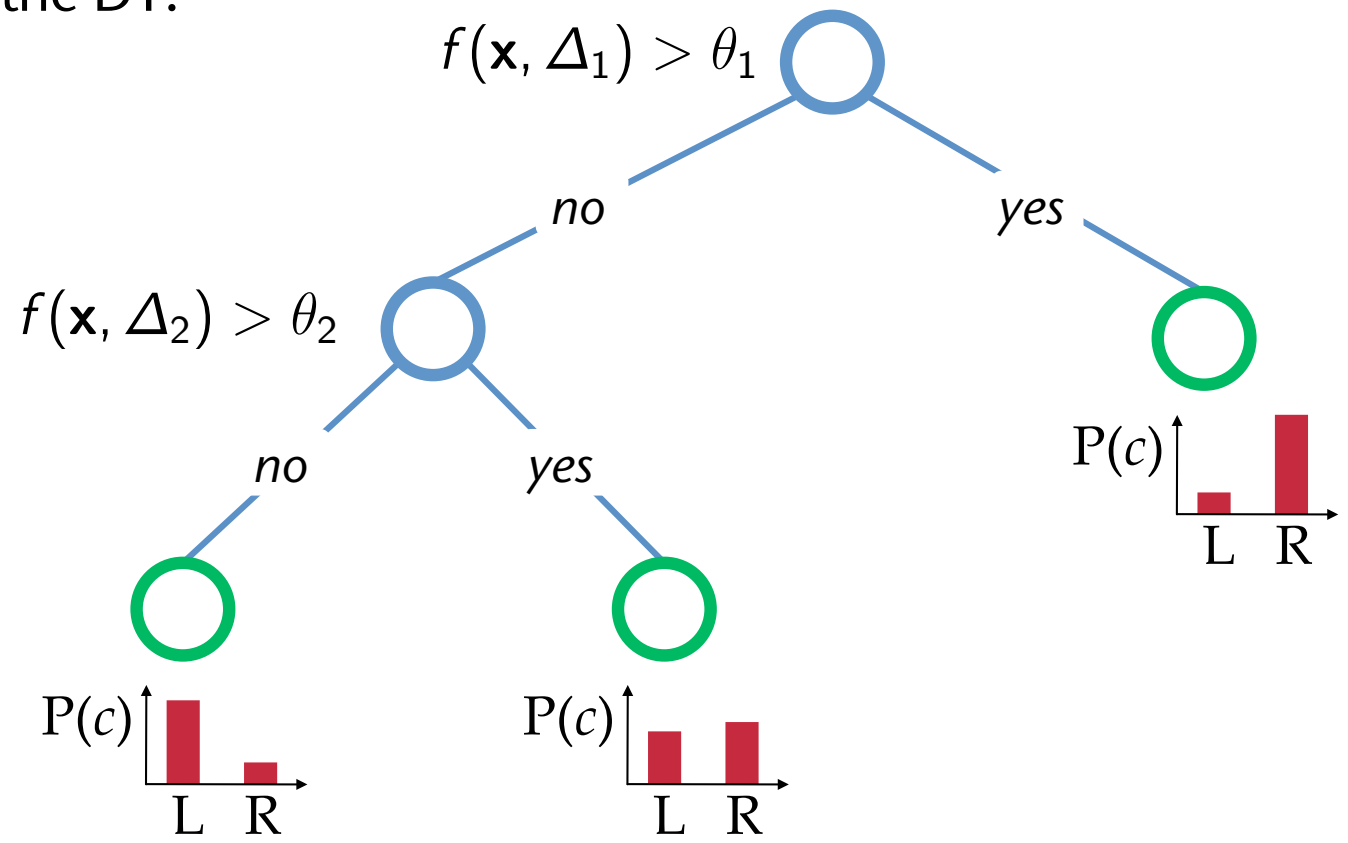
Training of a Single Decision Tree

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



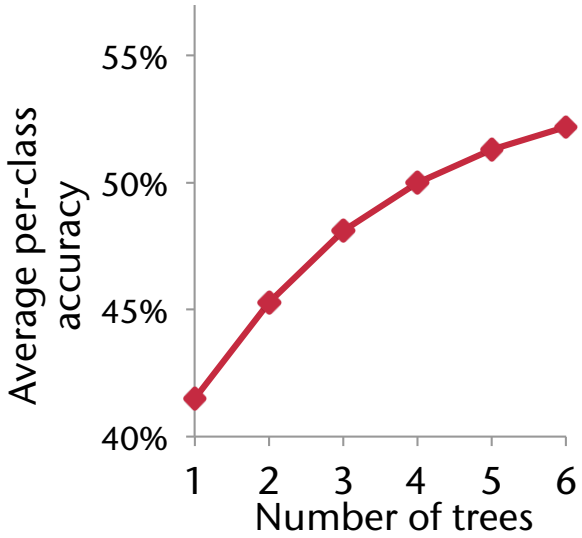
Classification of a Pixel at Runtime

- Toy example: distinguish left (L) and right (R) sides of the body
- Note: each node only needs to store Δ and θ!
- For every pixel **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, θ) values
- Note: the complete feature vectors are never explicitly constructed (only conceptually)



ground truth

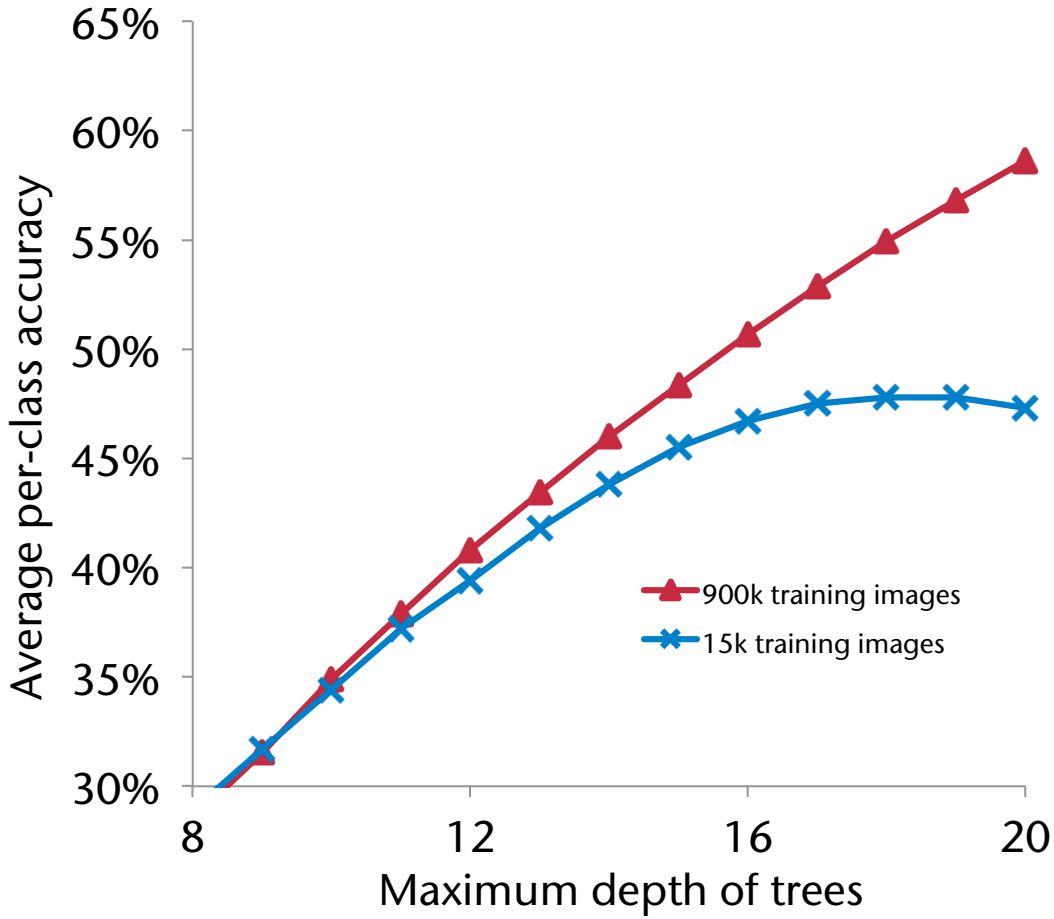
inferred body parts (most likely)

1 tree

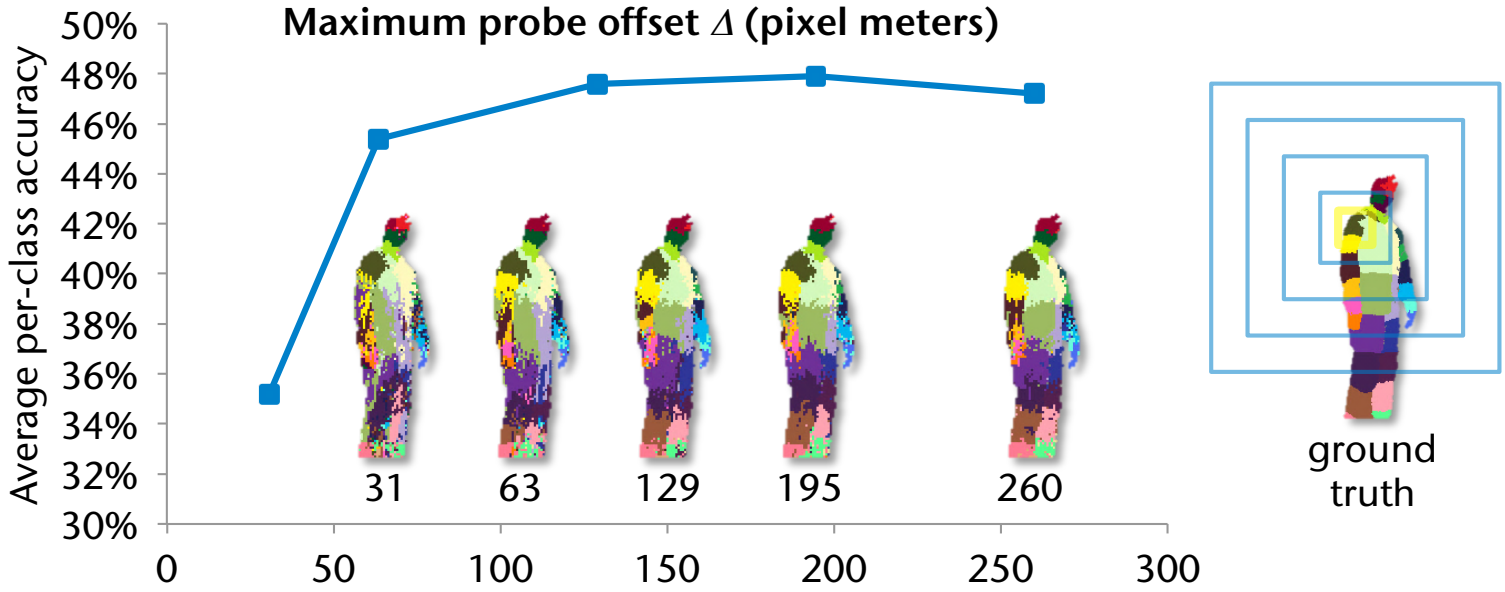
3 trees

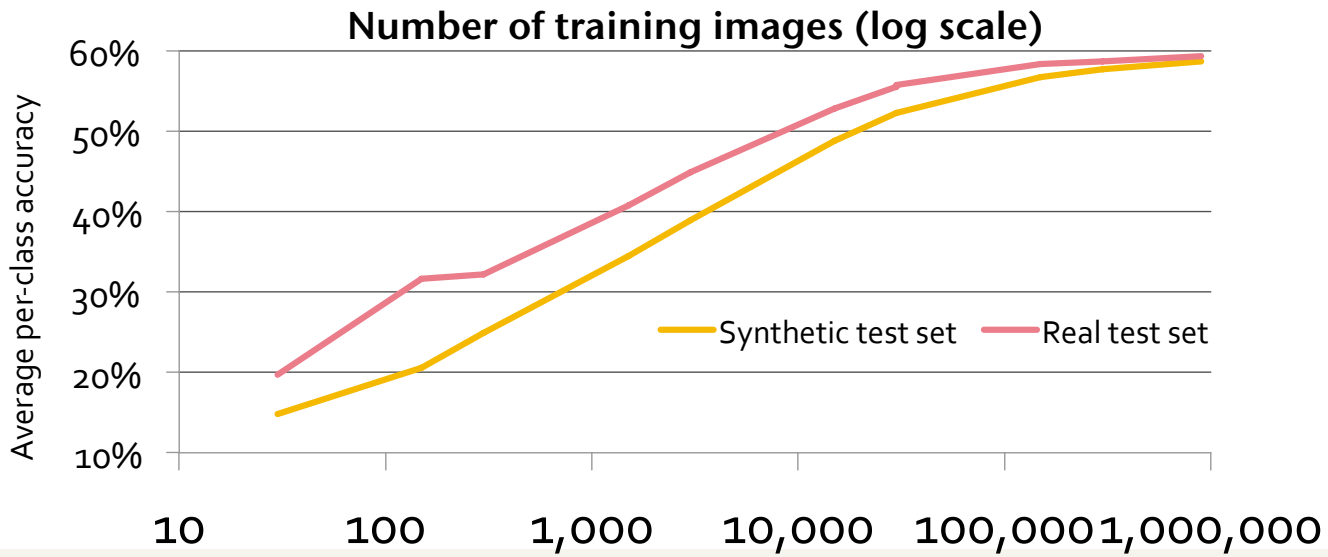
6 trees

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



More Parameters

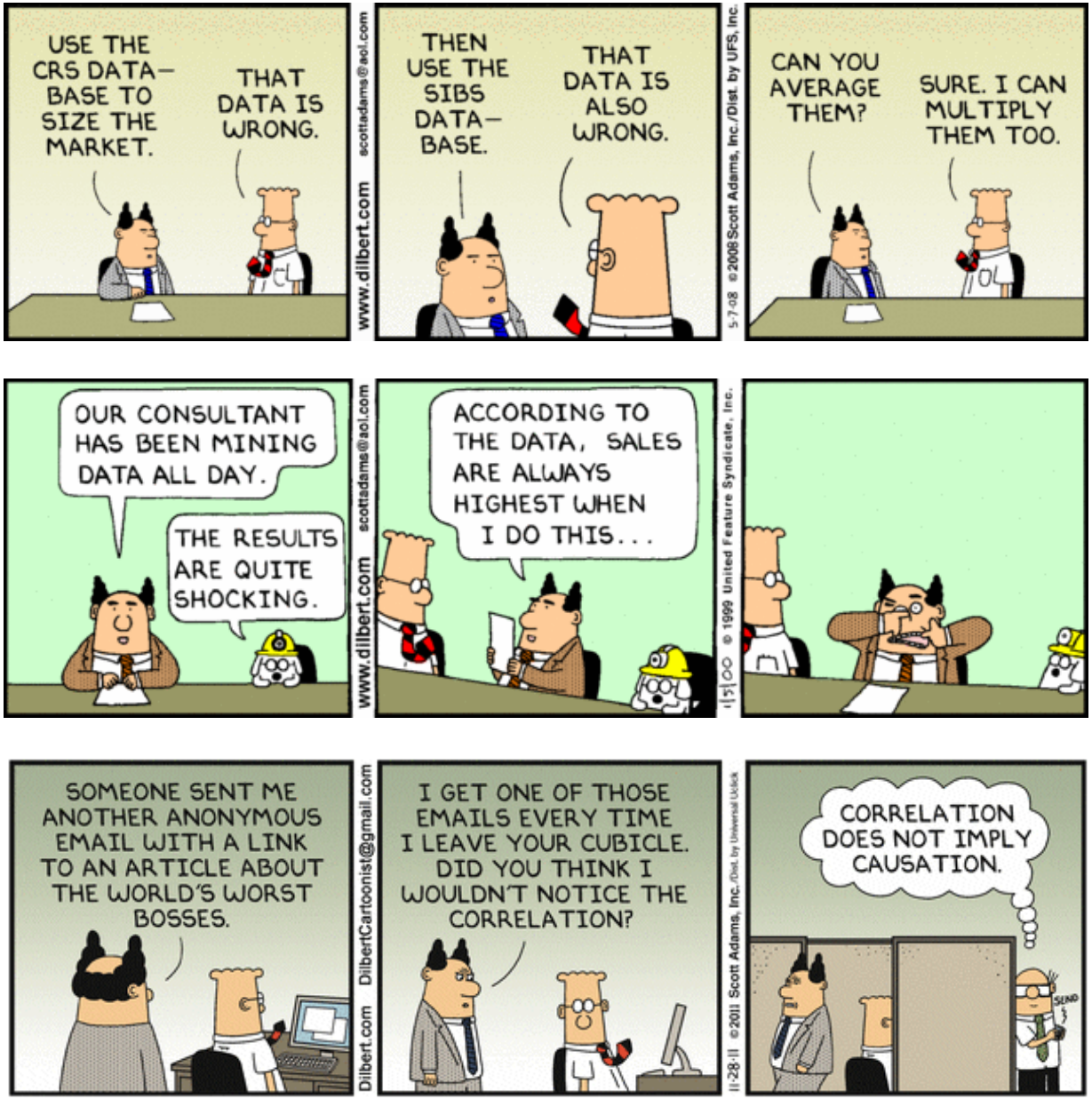




Video

Input depth image (bg removed)

Inferred body parts posterior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