RWTH AACHEN UNIVERSITY

Machine Learning – Lecture 11

Random Forests

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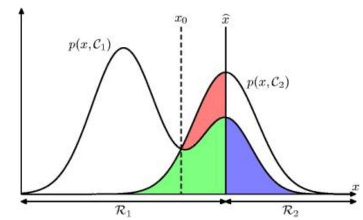
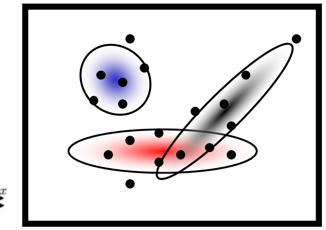
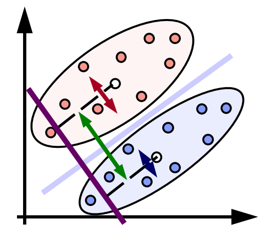
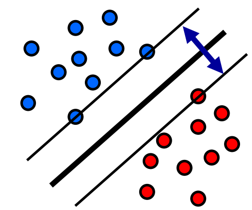
Course Outline

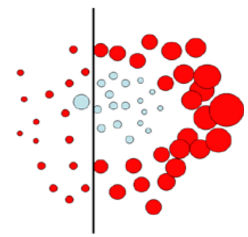
- Fundamentals
  - Bayes Decision Theory
  - Probability Density Estimation
- Classification Approaches
  - Linear Discriminants
  - Support Vector Machines
  - Ensemble Methods & Boosting
  - Random Forests
- Deep Learning
  - Foundations
  - Convolutional Neural Networks
  - Recurrent Neural Networks

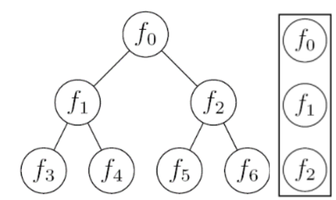


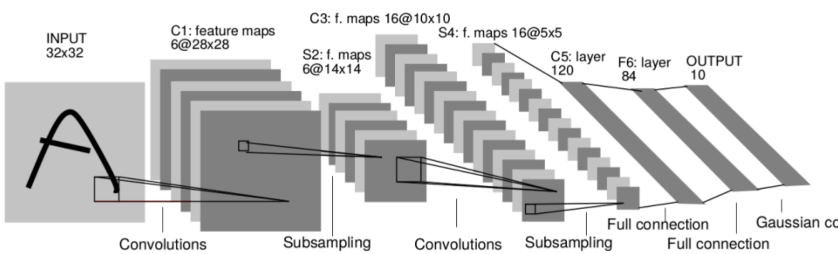












Recap: AdaBoost – "Adaptive Boosting"

- Main idea [Freund & Schapire, 1996]
  - Instead of resampling, reweight misclassified training examples.
    - Increase the chance of being selected in a sampled training set.
    - Or increase the misclassification cost when training on the full set.

- Components
  - $h_m(\mathbf{x})$: "weak" or base classifier
    - Condition: <50% training error over any distribution
  - $H(\mathbf{x})$: "strong" or final classifier

- AdaBoost:
  - Construct a strong classifier as a thresholded linear combination of the weighted weak classifiers:

$$H(\mathbf{x}) = sign\left(\sum_{m=1}^{M} \alpha_m h_m(\mathbf{x})\right)$$

Recap: AdaBoost – Algorithm

1. Initialization: Set $w_n^{(1)} = \frac{1}{N}$ for $n = 1,\ldots,N$.
2. For $m = 1,\ldots,M$ iterations
   a) Train a new weak classifier $h_m(\mathbf{x})$ using the current weighting coefficients $\mathbf{W}^{(m)}$ by minimizing the weighted error function

   $$J_m = \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)$$

   $$I(A) = \begin{cases} 1, & \text{if } A \text{ is true} \\ 0, & \text{else} \end{cases}$$

   b) Estimate the weighted error of this classifier on $\mathbf{X}$:

   $$\epsilon_m = \frac{\sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)}{\sum_{n=1}^{N} w_n^{(m)}}$$

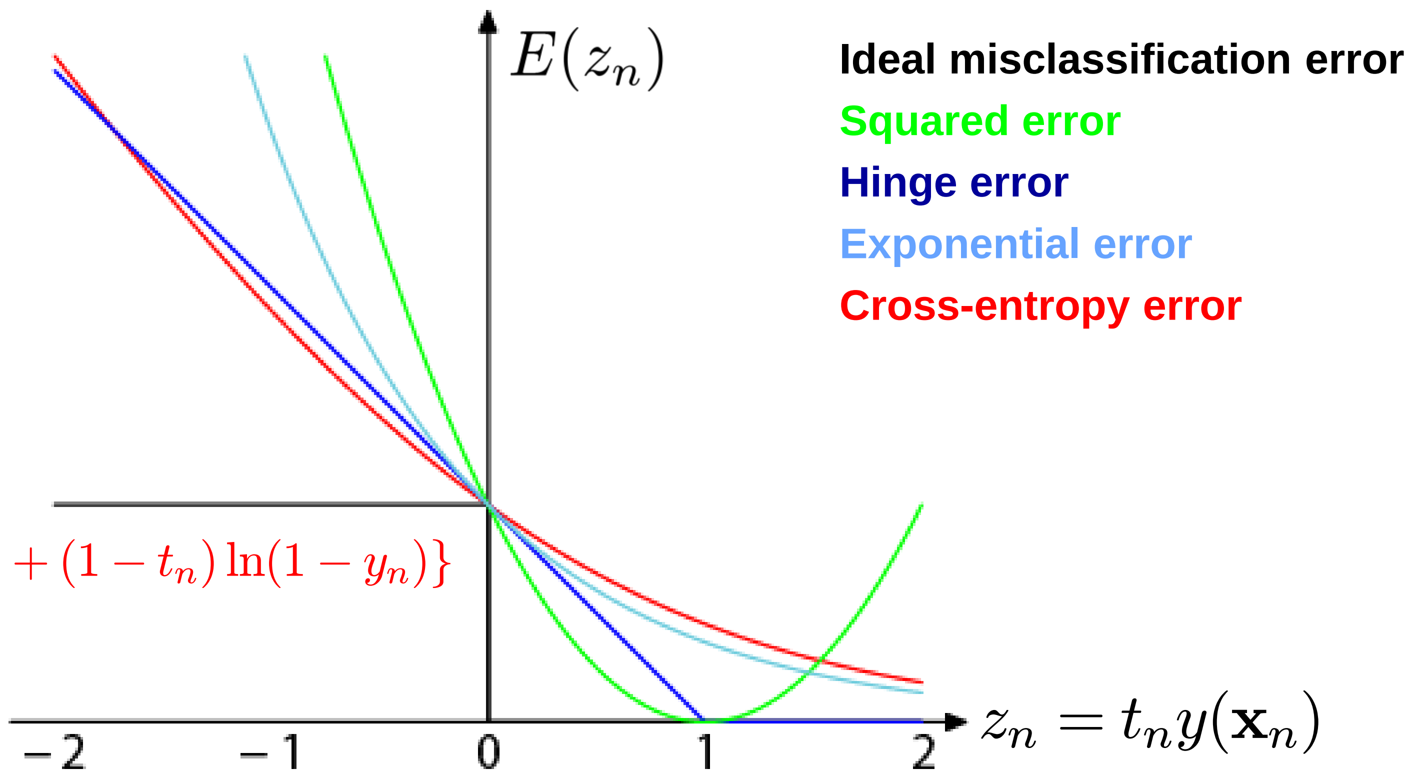
   c) Calculate a weighting coefficient for $h_m(\mathbf{x})$:

   $$\alpha_m = \ln\left\{\frac{1-\epsilon_m}{\epsilon_m}\right\}$$

   d) Update the weighting coefficients:

   $$w_n^{(m+1)} = w_n^{(m)} \exp\left\{\alpha_m I(h_m(\mathbf{x}_n) \neq t_n)\right\}$$

Recap: AdaBoost – Error Functions



$$E = -\sum \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

- “Cross-entropy error” used in Logistic Regression
  - Similar to exponential error for $z>0$.
  - Only grows linearly with large negative values of z.

  $\Rightarrow$ Make AdaBoost more robust by switching to this error function.

  $\Rightarrow$ “GentleBoost”

Image source: Bishop, 2006

Topics of This Lecture

- Decision Trees
- Randomized Decision Trees
  - Randomized attribute selection
- Random Forests
  - Bootstrap sampling
  - Ensemble of randomized trees
  - Posterior sum combination
  - Analysis

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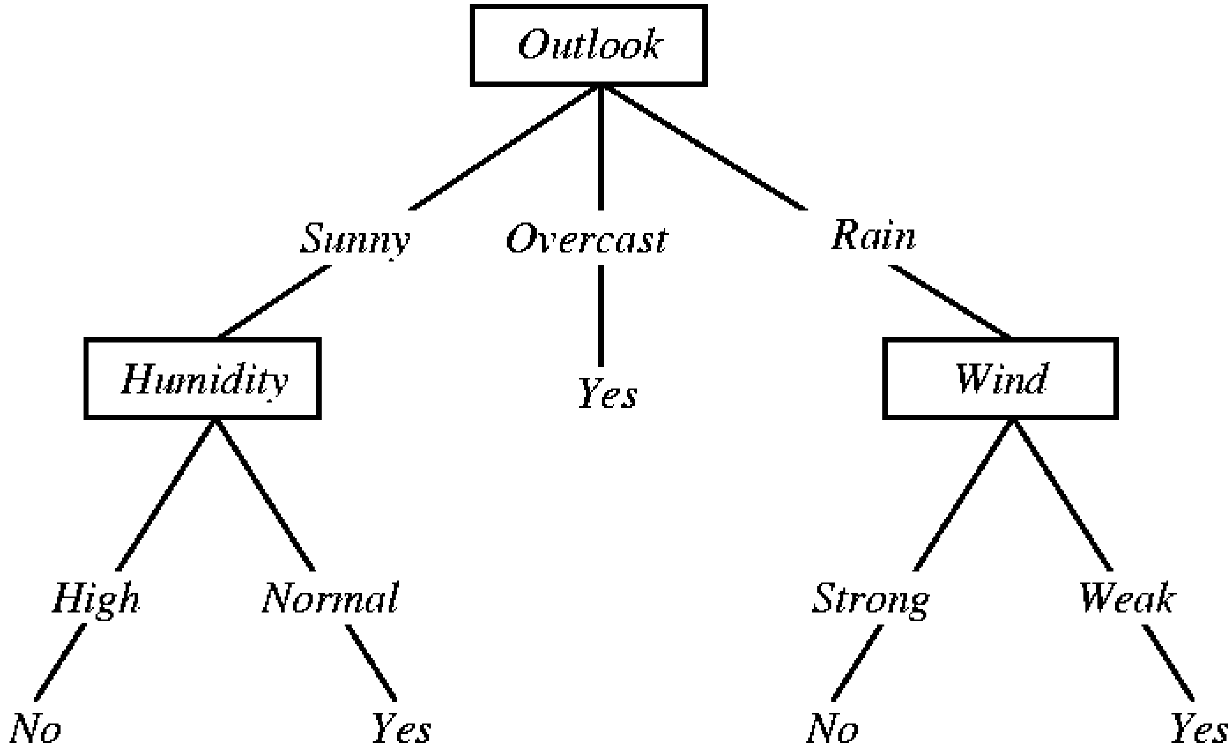
Decision Trees

- Very old technique
  - Origin in the 60s, might seem outdated.
- But…
  - Can be used for problems with nominal data
    - E.g. attributes color $\in$ {red, green, blue} or weather $\in$ {sunny, rainy}.
    - Discrete values, no notion of similarity or even ordering.
  - Interpretable results
    - Learned trees can be written as sets of if-then rules.
  - Methods developed for handling missing feature values.
  - Successfully applied to broad range of tasks
    - E.g. Medical diagnosis
    - E.g. Credit risk assessment of loan applicants
  - Some interesting novel developments building on top of them…

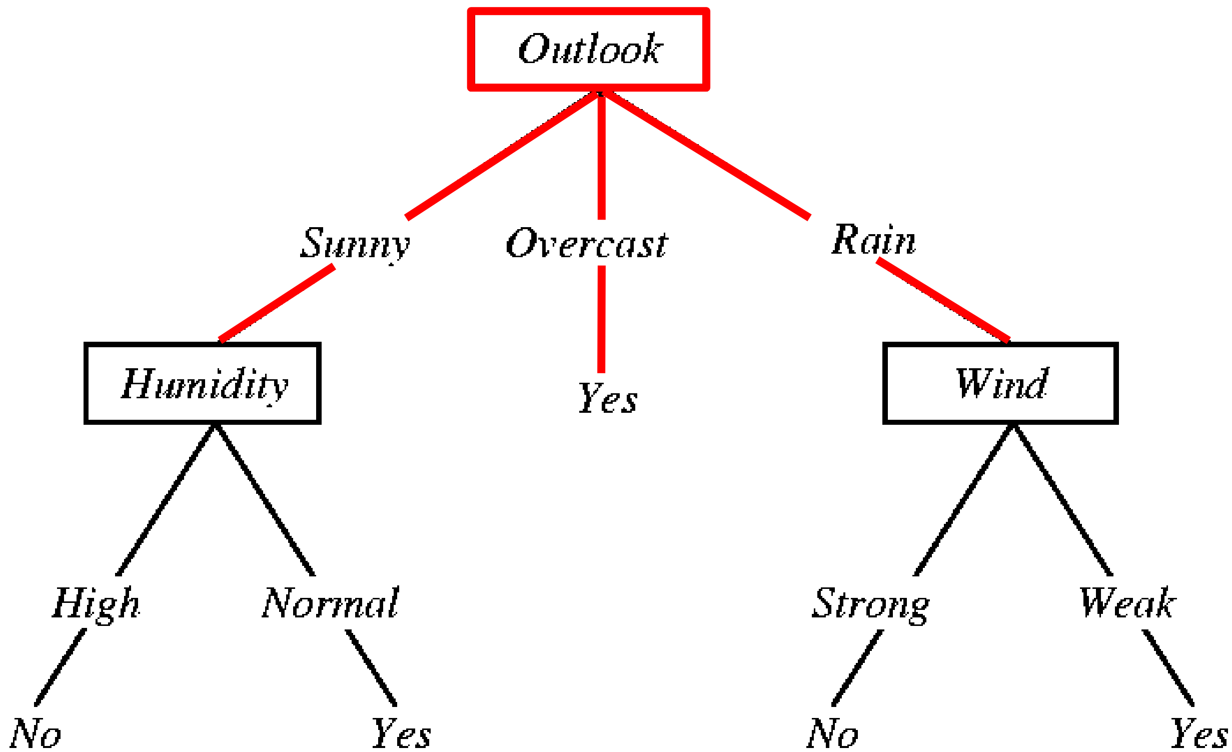
Decision Trees



- Example:
  - "Classify Saturday mornings according to whether they're suitable for playing tennis."

Image source: T. Mitchell, 1997

Decision Trees

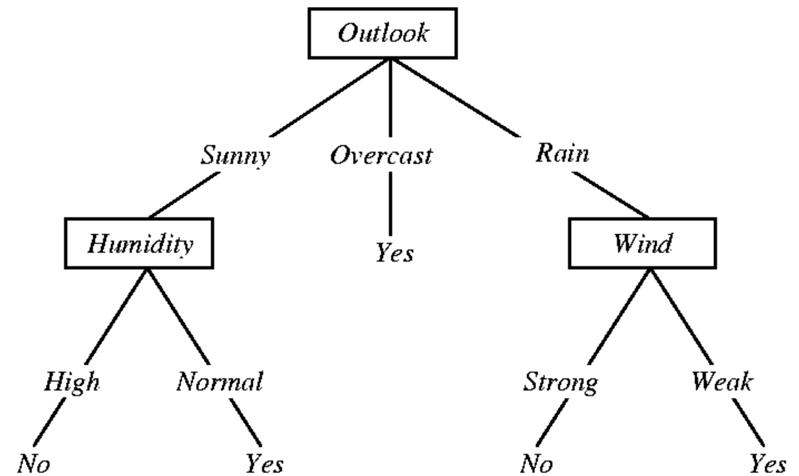


- Elements
  - Each node specifies a test for some attribute.
  - Each branch corresponds to a possible value of the attribute.

Image source: T. Mitchell, 1997

Decision Trees

- Assumption
  - Links must be mutually distinct and exhaustive
  - I.e. one and only one link will be followed at each step.



- Interpretability
  - Information in a tree can then be rendered as logical expressions.
  - In our example:

$$
\begin{aligned}
&(Outlook = Sunny \wedge Humidity = Normal) \\
\vee\ &(Outlook = Overcast) \\
\vee\ &(Outlook = Rain \wedge Wind = Weak)
\end{aligned}
$$

Image source: T. Mitchell, 1997

Training Decision Trees

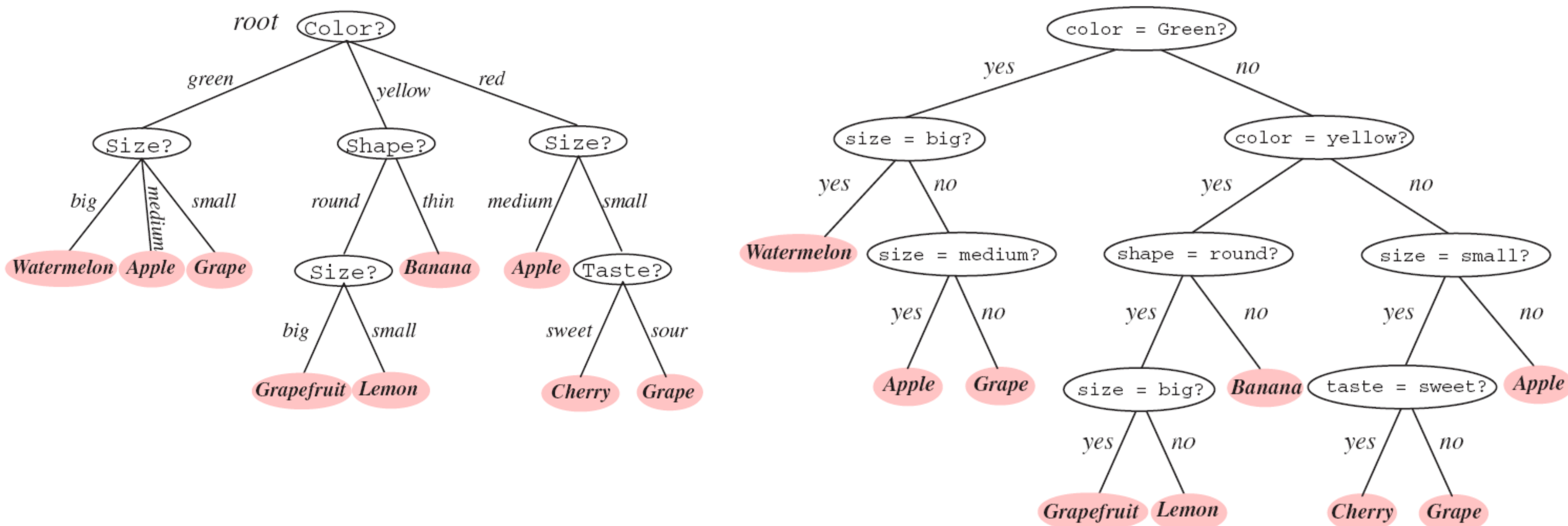
- Finding the optimal decision tree is NP-hard…
- Common procedure: Greedy top-down growing
  - Start at the root node.
  - Progressively split the training data into smaller and smaller subsets.
  - In each step, pick the *best attribute* to split the data.
  - If the resulting subsets are pure (only one label) or if no further attribute can be found that splits them, terminate the tree.
  - Else, recursively apply the procedure to the subsets.
- CART framework
  - Classification And Regression Trees (Breiman et al. 1993)
  - Formalization of the different design choices.

CART Framework

- Six general questions
  1. Binary or multi-valued problem?
     – I.e. how many splits should there be at each node?
  2. Which property should be tested at a node?
     – I.e. how to select the query attribute?
  3. When should a node be declared a leaf?
     – I.e. when to stop growing the tree?
  4. How can a grown tree be simplified or pruned?
     – Goal: reduce overfitting.
  5. How to deal with impure nodes?
     – I.e. when the data itself is ambiguous.
  6. How should missing attributes be handled?

CART – 1. Number of Splits

- Each multi-valued tree can be converted into an equivalent binary tree:



⇒ Only consider binary trees here…

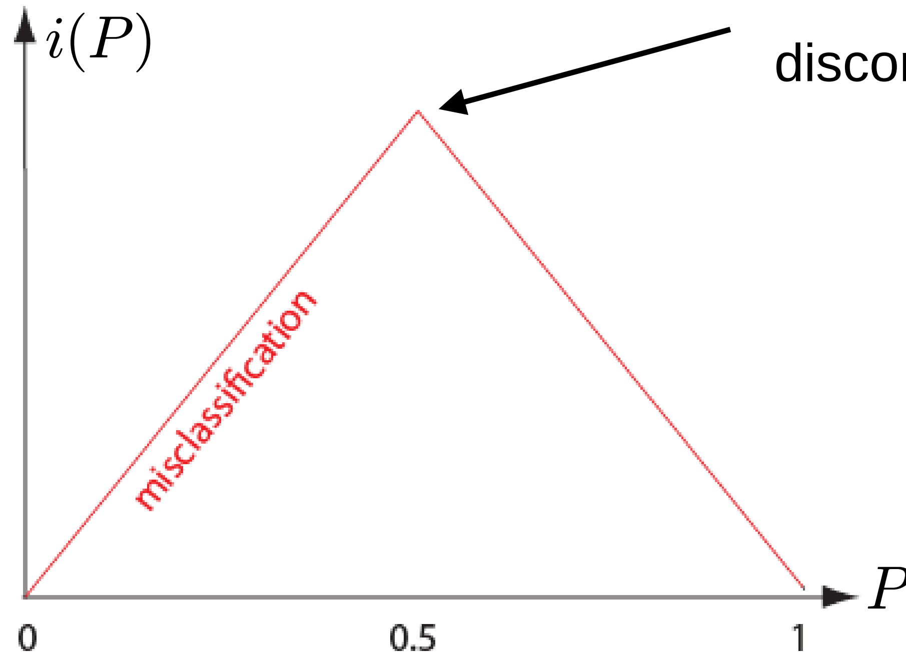
Image source: R.O. Duda, P.E. Hart, D.G. Stork, 2001

CART – 2. Picking a Good Splitting Feature

- Goal
  - Want a tree that is as simple/small as possible (Occam's razor).
  - But: Finding a minimal tree is an NP-hard optimization problem.

- Greedy top-down search
  - Efficient, but not guaranteed to find the smallest tree.
  - Seek a property T at each node s_j that makes the data in the child nodes as pure as possible.
  - For formal reasons more convenient to define impurity $i(s_j)$.
  - Several possible definitions explored.

CART – Impurity Measures



Problem:
discontinuous derivative!

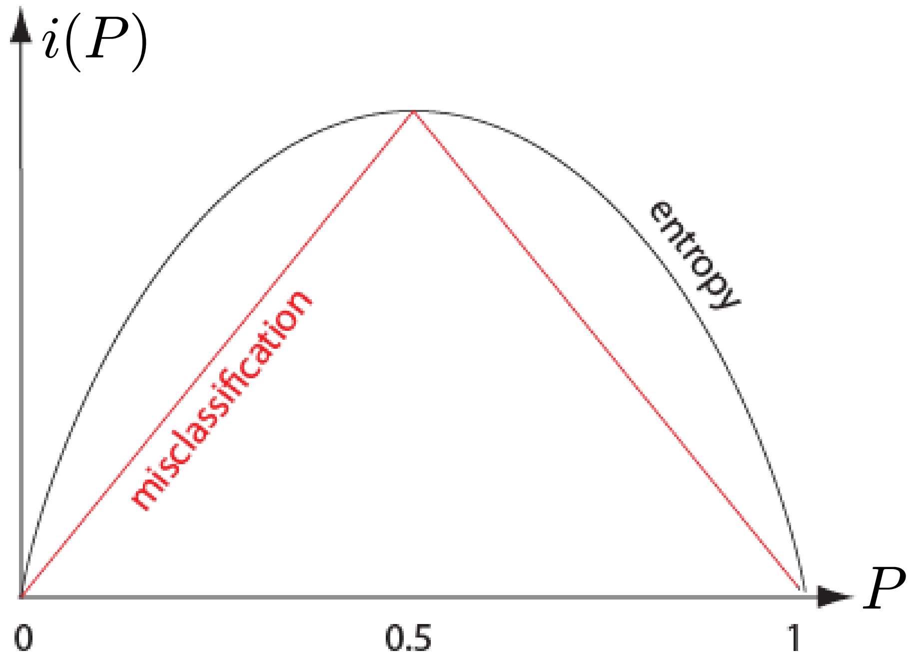
- Misclassification impurity

$$i(s_j) = 1 - \max_k \boxed{p(C_k|s_j)}$$

"Fraction of the training patterns in category $\mathcal{C}_k$ that end up in node s_j."

Image source: R.O. Duda, P.E. Hart, D.G. Stork, 2001

CART – Impurity Measures



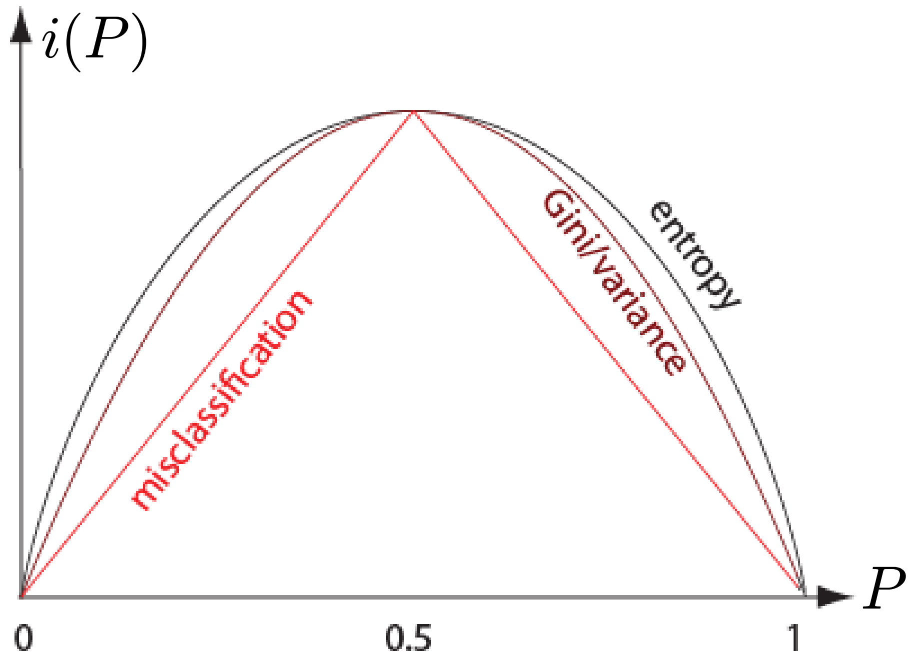
- Entropy impurity

$$i(s_j) = -\sum_k p(C_k|s_j)\log_2 p(C_k|s_j)$$

"Reduction in entropy = gain in information."

Image source: R.O. Duda, P.E. Hart, D.G. Stork, 2001

CART – Impurity Measures



- Gini impurity (variance impurity)

$$i(s_j) = \sum_{k \neq l} p(C_k|s_j)\, p(C_l|s_j)$$

$$= \frac{1}{2}\left[1 - \sum_k p^2(C_k|s_j)\right]$$

"Expected error rate at node s_j if the category label is selected randomly."

Image source: R.O. Duda, P.E. Hart, D.G. Stork, 2001

CART – Impurity Measures

- Which impurity measure should we choose?
  - Some problems with misclassification impurity.
    - Discontinuous derivative.

    $\Rightarrow$ Problems when searching over continuous parameter space.
    - Sometimes misclassification impurity does not decrease when Gini impurity would.
  - Both entropy impurity and Gini impurity perform well.
    - No big difference in terms of classifier performance.
    - In practice, stopping criterion and pruning method are often more important.

CART – 2. Picking a Good Splitting Feature

- Application
  - Select the query that decreases impurity the most

$$\Delta i(s_j) = i(s_j) - P_L i(s_{j,L}) - (1 - P_L) i(s_{j,R})$$

$P_L =$ fraction of points at left child node $s_{j,L}$

- Multiway generalization (gain ratio impurity):
  - Maximize

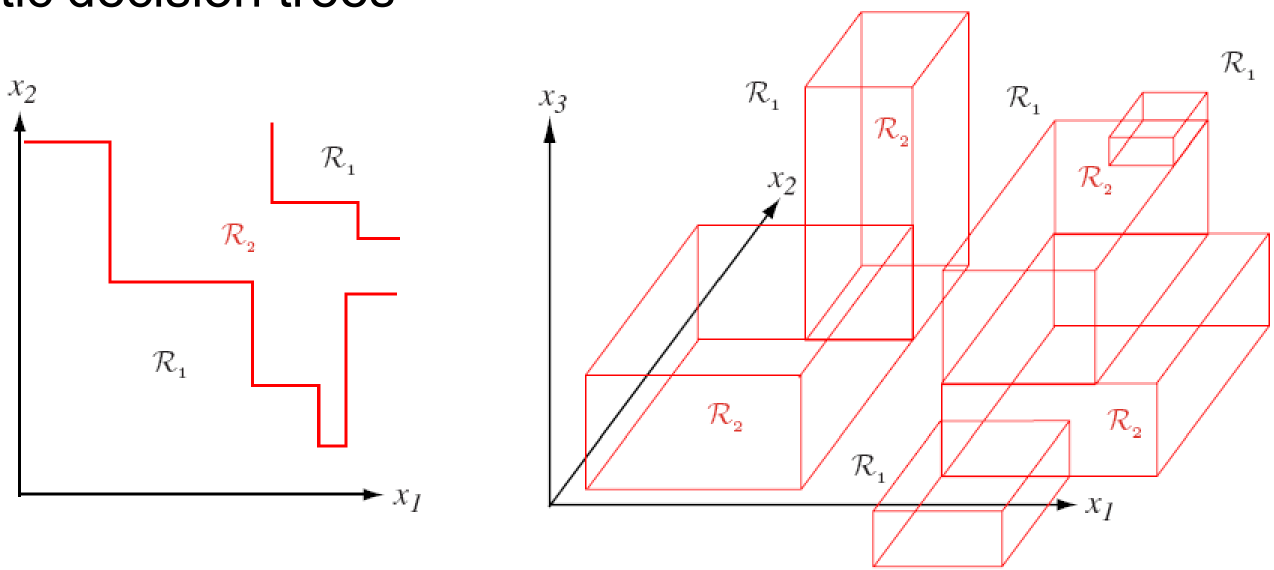
$$\Delta i(s_j) = \frac{1}{Z}\left(i(s_j) - \sum_{m=1}^{M} P_m i(s_{j,m}) \right)$$

  - where the normalization factor ensures that large K are not inherently favored:

$$Z = -\sum_{m=1}^{M} P_m \log_2 P_m$$

CART – Picking a Good Splitting Feature

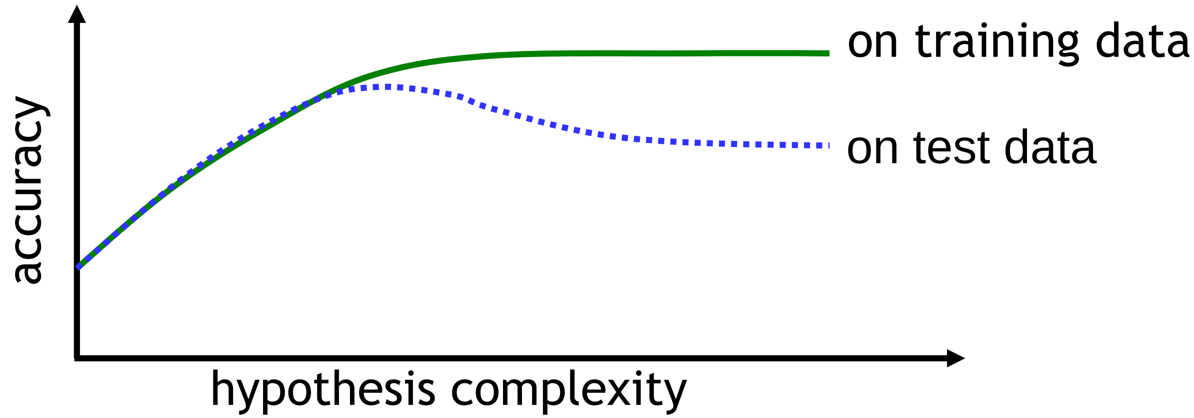
- For efficiency, splits are often based on a single feature
  - "Monothetic decision trees"



- Evaluating candidate splits
  - Nominal attributes: exhaustive search over all possibilities.
  - Real-valued attributes: only need to consider changes in label.
    - Order all data points based on attribute x_i.
    - Only need to test candidate splits where *label*(x_i) ≠ *label*(x_{i+1}).

CART – 3. When to Stop Splitting

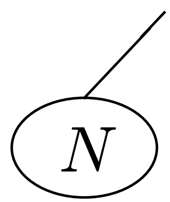
- Problem: Overfitting
  - Learning a tree that classifies the training data perfectly may not lead to the tree with the best generalization to unseen data.
  - Reasons
    - Noise or errors in the training data.
    - Poor decisions towards the leaves of the tree that are based on very little data.
- Typical behavior



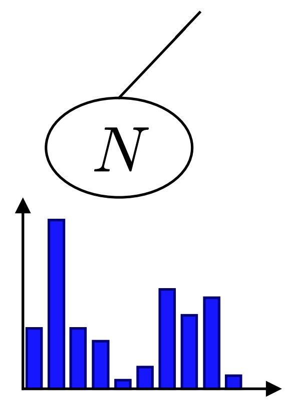
Slide adapted from Raymond Mooney

CART – Overfitting Prevention (Pruning)

- Two basic approaches for decision trees
  - Prepruning: Stop growing tree as some point during top-down construction when there is no longer sufficient data to make reliable decisions.
  - Postpruning: Grow the full tree, then remove subtrees that do not have sufficient evidence.
- Label leaf resulting from pruning with the majority class of the remaining data, or a class probability distribution.



$$\mathcal{C}_N = \arg\max_k p(\mathcal{C}_k|N)$$



$p(\mathcal{C}_k|N)$

Decision Trees – Computational Complexity

- Given
  - Data points $\{\mathbf{x}_1,\ldots,\mathbf{x}_N\}$
  - Dimensionality D

- Complexity
  - Storage: $O(N)$
  - Test runtime: $O(\log N)$
  - Training runtime: $O(DN^2 \log N)$
    - Most expensive part.
    - Critical step: selecting the optimal splitting point.
    - Need to check D dimensions, for each need to sort N data points.

$$O(DN \log N)$$

Summary: Decision Trees

- Properties
  - Simple learning procedure, fast evaluation.
  - Can be applied to metric, nominal, or mixed data.
  - Often yield interpretable results.

Summary: Decision Trees

- Limitations
  - Often produce noisy (bushy) or weak (stunted) classifiers.
  - Do not generalize too well.
  - Training data fragmentation:
    - As tree progresses, splits are selected based on less and less data.
  - Overtraining and undertraining:
    - Deep trees: fit the training data well, will not generalize well to new test data.
    - Shallow trees: not sufficiently refined.
  - Stability
    - Trees can be very sensitive to details of the training points.
    - If a single data point is only slightly shifted, a radically different tree may come out!

    $\Rightarrow$ Result of discrete and greedy learning procedure.
  - Expensive learning step
    - Mostly due to costly selection of optimal split.

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- Decision Trees
- Randomized Decision Trees
  - Randomized attribute selection
- Random Forests
  - Bootstrap sampling
  - Ensemble of randomized trees
  - Posterior sum combination
  - Analysis

Randomized Decision Trees (Amit & Geman 1997)

- Decision trees: main effort on finding good split
  - Training runtime: $O(DN^2 \log N)$
  - This is what takes most effort in practice.
  - Especially cumbersome with many attributes (large D).
- Idea: randomize attribute selection
  - No longer look for globally optimal split.
  - Instead randomly use subset of K attributes on which to base the split.
  - Choose best splitting attribute e.g. by maximizing the information gain (= reducing entropy):

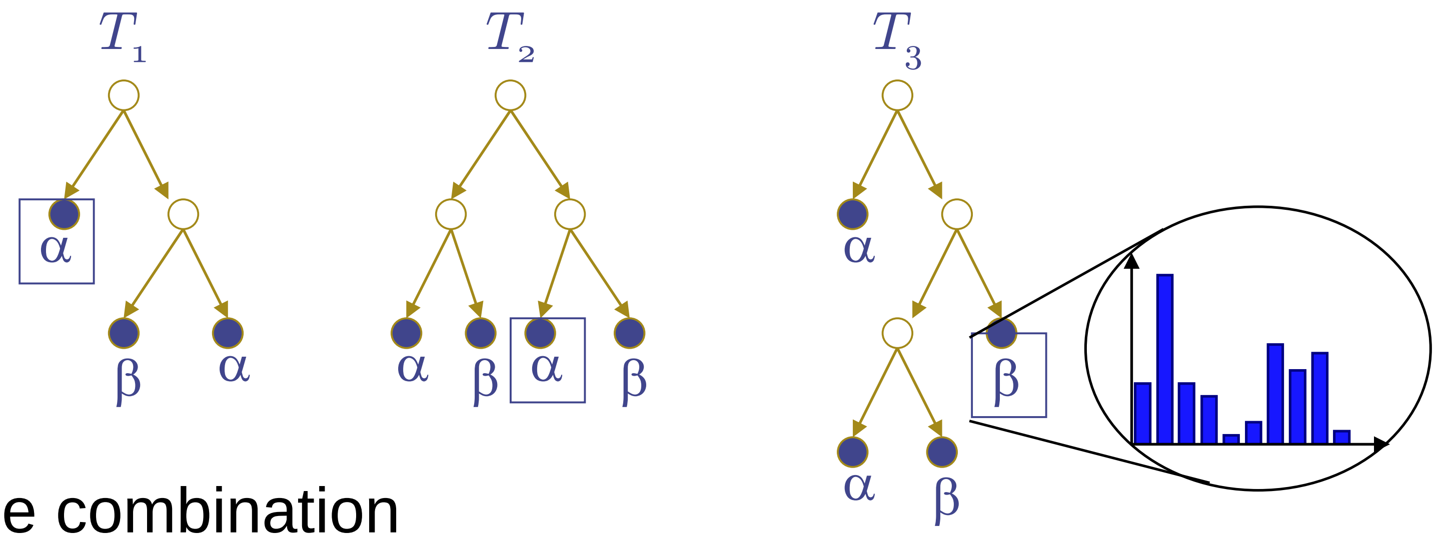
$$\triangle E = \sum_{k=1}^{K} \frac{|S_k|}{|S|} \sum_{j=1}^{N} p_j \log_2(p_j)$$

Randomized Decision Trees

- Randomized splitting
  - Faster training: $O(KN^2 \log N)$ with $K \ll D$
  - Use very simple binary feature tests.
  - Typical choice
    - $K = 10$ for root node.
    - $K = 100d$ for node at level d.

- Effect of random split
  - Of course, the tree is no longer as powerful as a single classifier…
  - But we can compensate by building several trees.

Ensemble Combination



- Ensemble combination
  - Tree leaves (l,η) store posterior probabilities of the target classes.

$$p_{l,\eta}(\mathcal{C}|\mathbf{x})$$

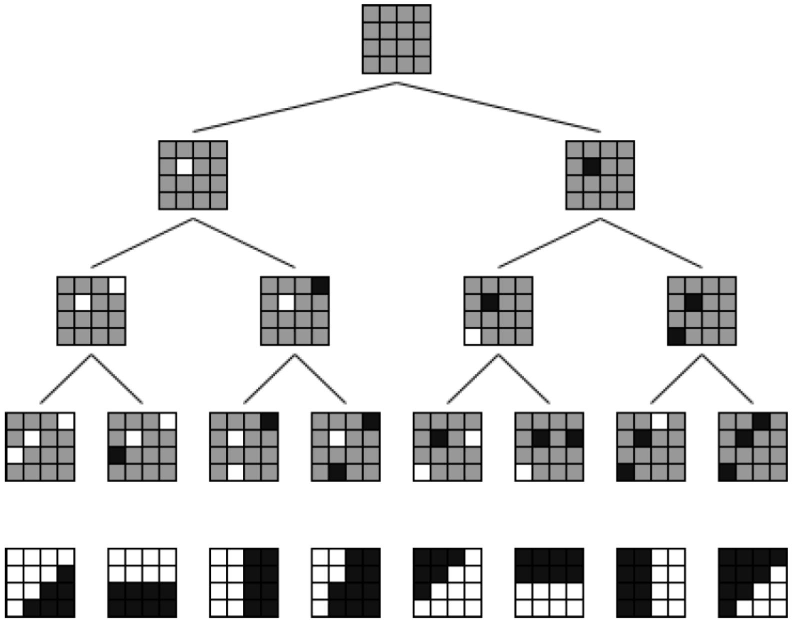
  - Combine the output of several trees by averaging their posteriors (Bayesian model combination)

$$p(\mathcal{C}|\mathbf{x}) = \frac{1}{L}\sum_{l=1}^{L} p_{l,\eta}(\mathcal{C}|\mathbf{x})$$

Applications: Character Recognition

- Computer Vision: Optical character recognition
  - Classify small (14x20) images of hand-written characters/digits into one of 10 or 26 classes.

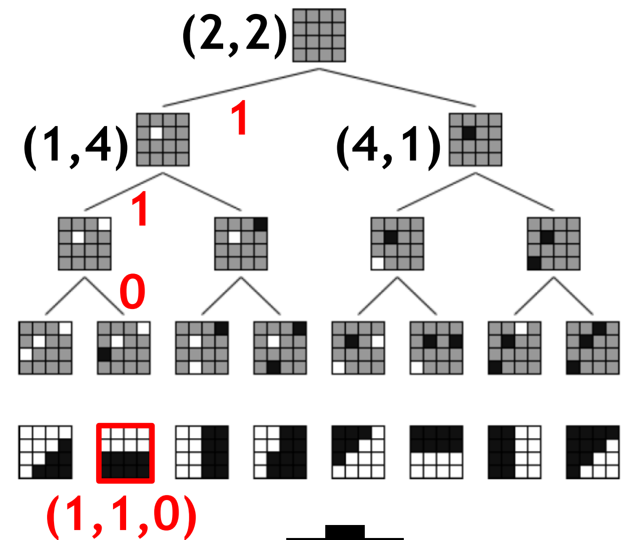
- Simple binary features
  - Tests for individual binary pixel values.
  - Organized in randomized tree.



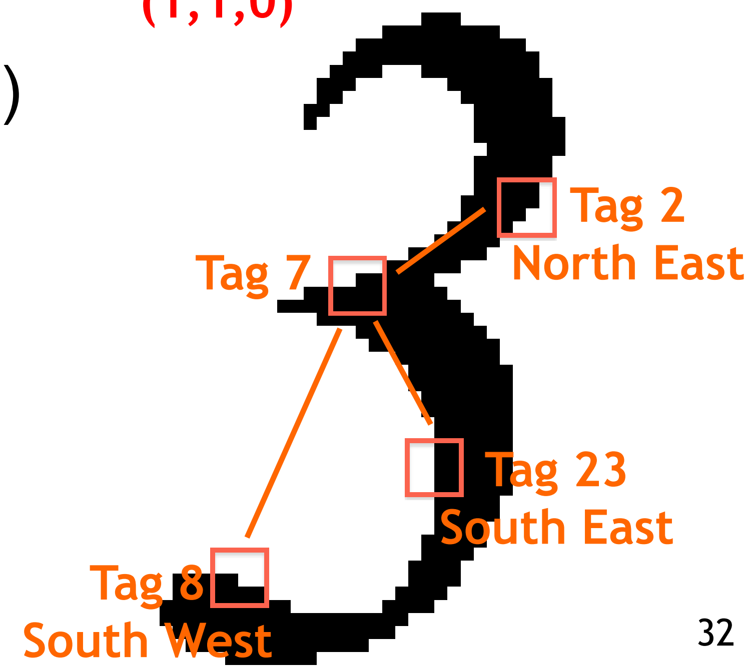
Y. Amit, D. Geman, Shape Quantization and Recognition with Randomized Trees, *Neural Computation*, Vol. 9(7), pp. 1545-1588, 1997.

Applications: Character Recognition

- Image patches ("Tags")
  - Randomly sampled 4×4 patches
  - Construct a randomized tree based on binary single-pixel tests
  - Each leaf node corresponds to a "patch class" and produces a tag



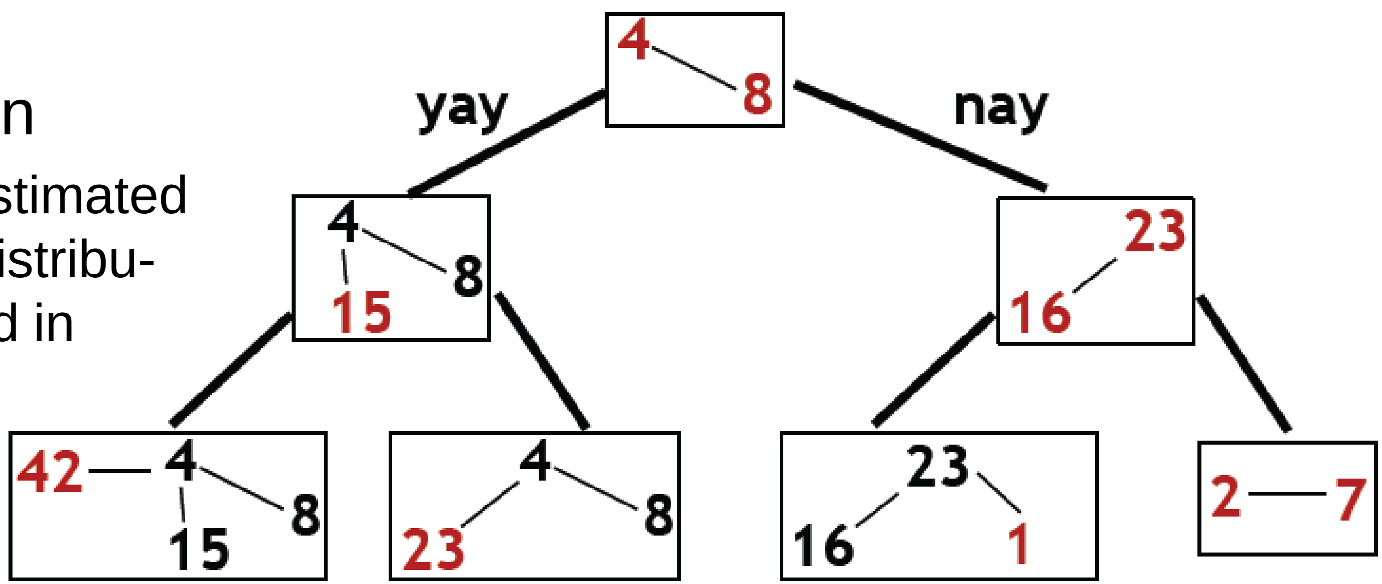
- Representation of digits ("Queries")
  - Specific spatial arrangements of tags
  - An image answers "yes" if any such structure is found anywhere
  - *How do we know which spatial arrangements to look for?*



Applications: Character Recognition

- Answer: Create a second-level decision tree!
  - Start with two tags connected by an arc
  - Search through extensions of confirmed queries (or rather through a subset of them, there are lots!)
  - Select query with best information gain
  - Recurse…

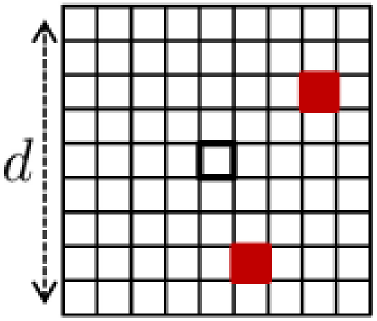
- Classification
  - Average estimated posterior distributions stored in the leaves.



Applications: Fast Keypoint Detection

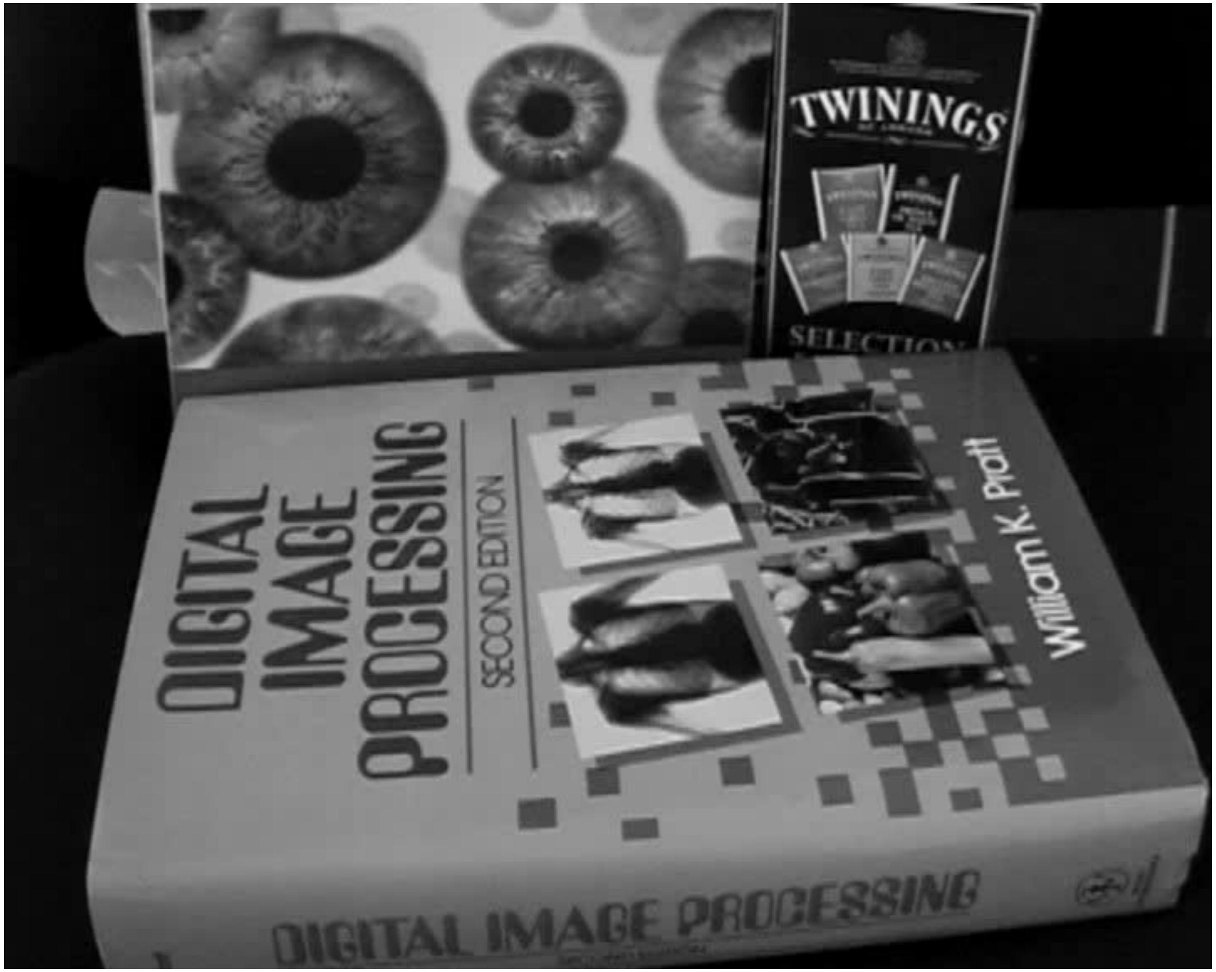
- Computer Vision: fast keypoint detection
  - Detect keypoints: small patches in the image used for matching
  - Classify into one of ~200 categories (visual words)

- Extremely simple features
  - E.g. pixel value in a color channel (CIELab)
  - E.g. sum of two points in the patch
  - E.g. difference of two points in the patch
  - E.g. absolute difference of two points



- Create forest of randomized decision trees
  - Each leaf node contains probability distribution over 200 classes
  - Can be updated and re-normalized incrementally.

Application: Fast Keypoint Detection



M. Ozuysal, V. Lepetit, F. Fleuret, P. Fua, [Feature Harvesting for Tracking-by-Detection](). In *ECCV'06*, 2006.

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  - Bootstrap sampling
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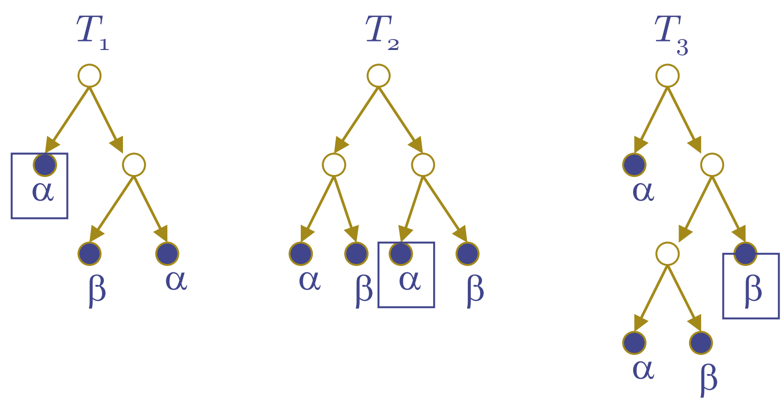
Random Forests (Breiman 2001)

- General ensemble method
  - Idea: Create ensemble of many (very simple) trees.
- Empirically very good results
  - Often as good as SVMs (and sometimes better)!
  - Often as good as Boosting (and sometimes better)!
- Standard decision trees: main effort on finding good split
  - Random Forests trees put very little effort in this.
  - CART algorithm with Gini coefficient, no pruning.
  - Each split is only made based on a random subset of the available attributes.
  - Trees are grown fully (important!).
- Main secret
  - Injecting the "right kind of randomness".

Random Forests – Algorithmic Goals

- Create many trees (50 – 1,000)
- Inject randomness into trees such that
  - Each tree has maximal strength
    - I.e. a fairly good model on its own
  - Each tree has minimum correlation with the other trees.
    - I.e. the errors tend to cancel out.
- Ensemble of trees votes for final result
  - Simple majority vote for category.



  - Alternative (Friedman)
    - Optimally reweight the trees via regularized regression (lasso).

Random Forests – Injecting Randomness (1)

- Bootstrap sampling process
  - Select a training set by choosing N times with replacement from all N available training examples.

  $\Rightarrow$ On average, each tree is grown on only ~63% of the original training data.
  - Remaining 37% “out-of-bag” (OOB) data used for validation.
    - Provides ongoing assessment of model performance in the current tree.
    - Allows fitting to small data sets without explicitly holding back any data for testing.
    - Error estimate is unbiased and behaves as if we had an independent test sample of the same size as the training sample.

Random Forests – Injecting Randomness (2)

- Random attribute selection
  - For each node, randomly choose subset of K attributes on which the split is based (typically $K = \sqrt{N_f}$).

  $\Rightarrow$ Faster training procedure
    - Need to test only few attributes.
  - Minimizes inter-tree dependence
    - Reduce correlation between different trees.

- Each tree is grown to maximal size and is left unpruned
  - Trees are deliberately overfit

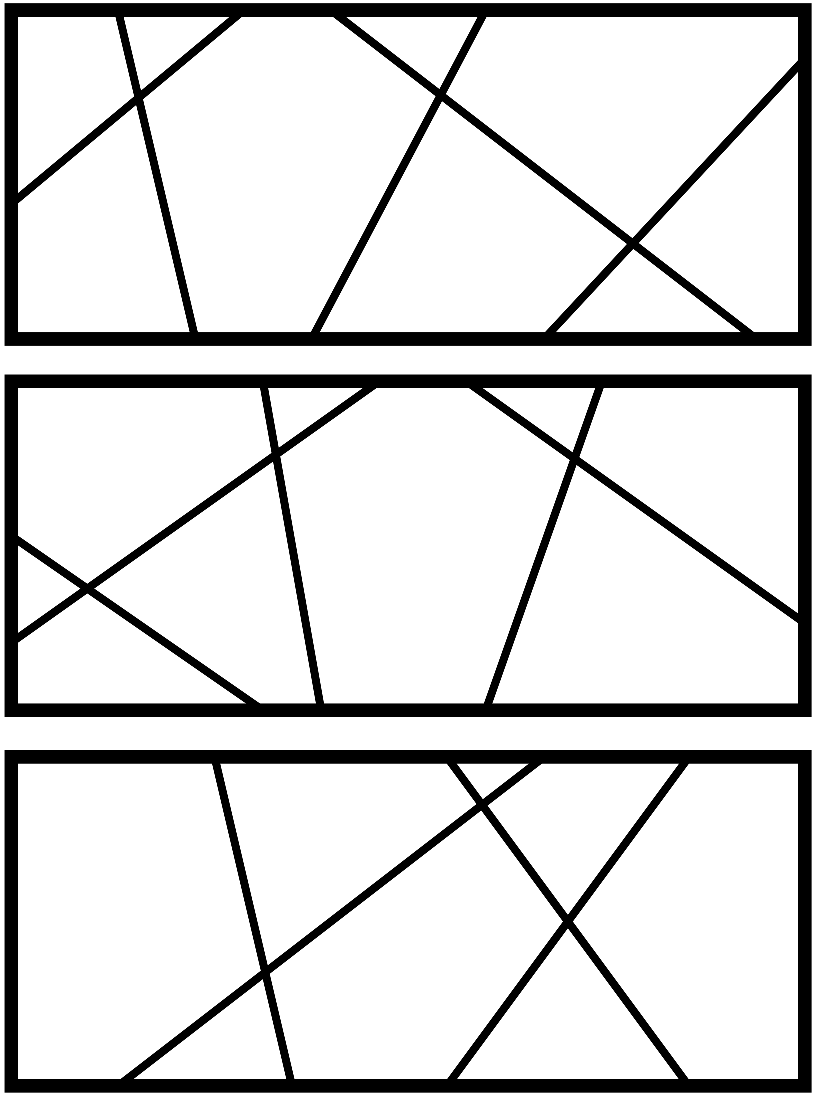
  $\Rightarrow$ Become some form of nearest-neighbor predictor.

Bet You're Asking…

How can this possibly *ever* work???

A Graphical Interpretation

Different trees induce different partitions on the data.



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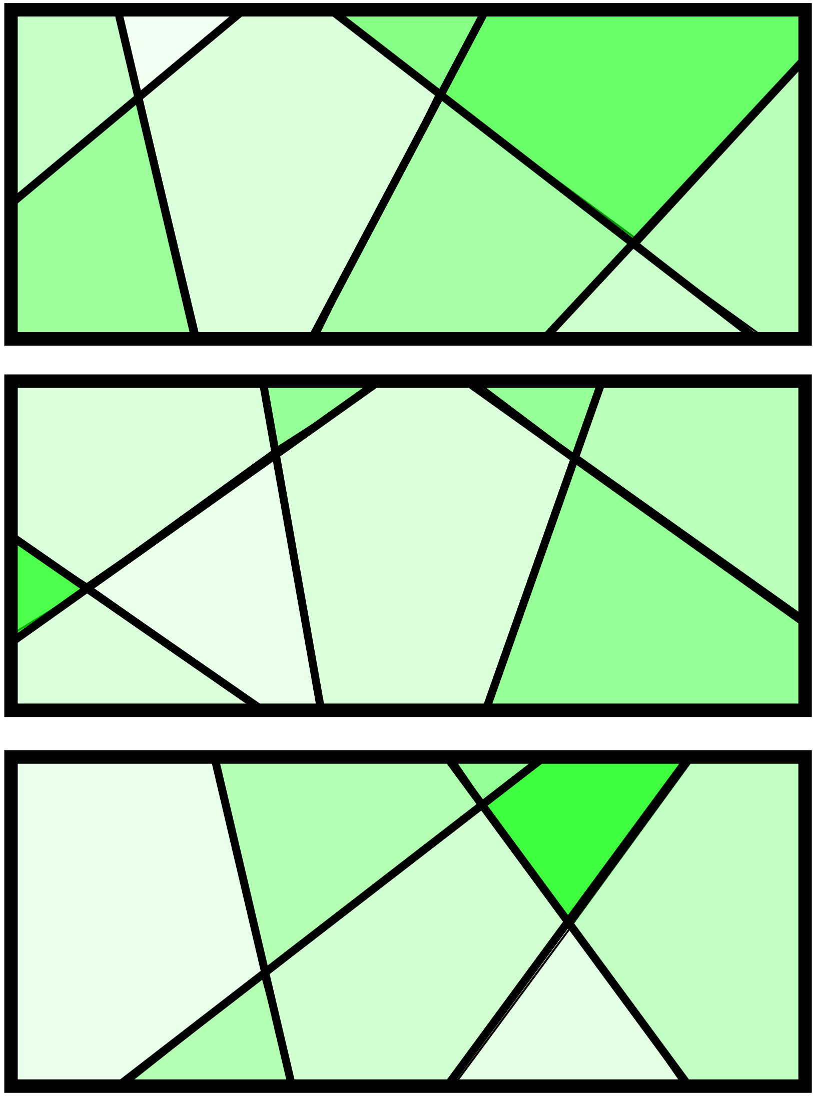
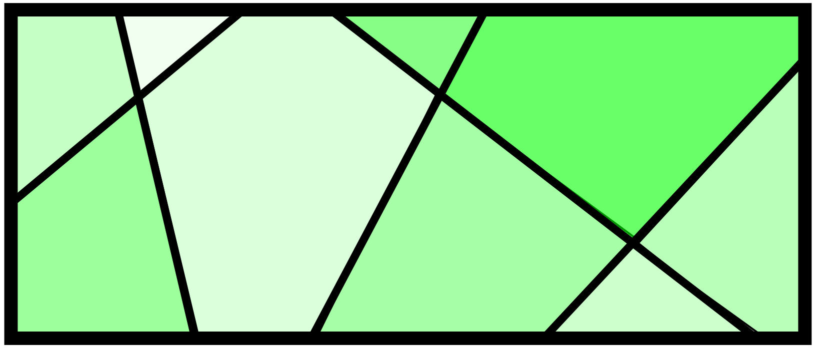
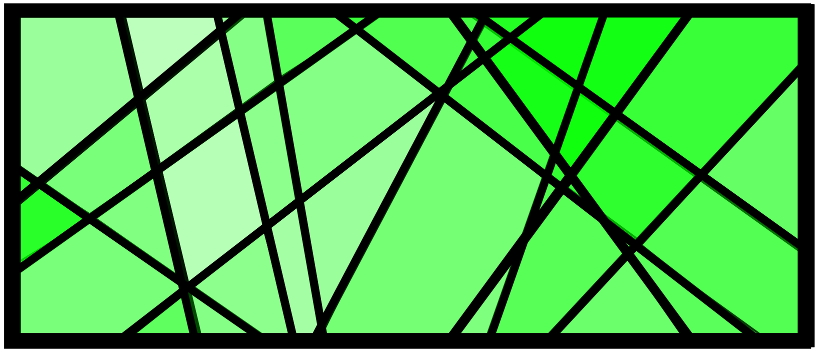


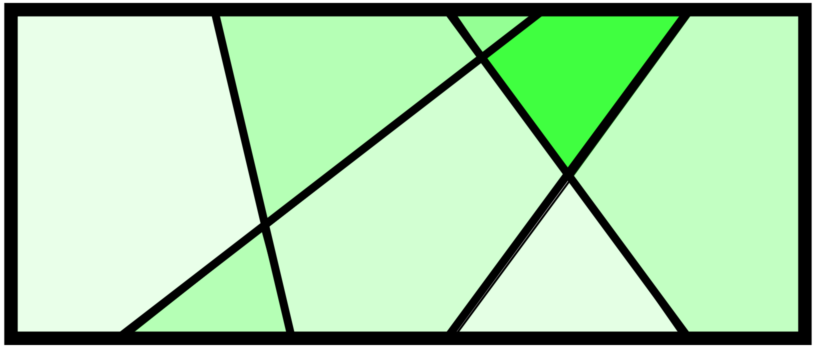
A Graphical Interpretation

Different trees induce different partitions on the data.



By combining them, we obtain a finer subdivision of the feature space…





Slide credit: Vincent Lepetit

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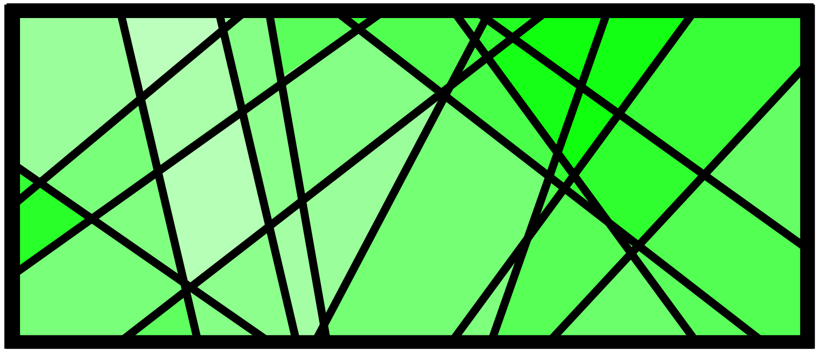


…which at the same time also better reflects the uncertainty due to the bootstrapped sampling.

Summary: Random Forests

- Properties
  - Very simple algorithm.
  - Resistant to overfitting – generalizes well to new data.
  - Faster training
  - Extensions available for clustering, distance learning, etc.

- Limitations
  - Memory consumption
    - Decision tree construction uses much more memory.
  - Well-suited for problems with little training data
    - Little performance gain when training data is really large.

You Can Try It At Home…

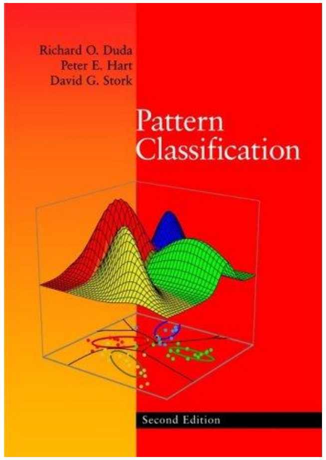
- Free implementations available
  - Original RF implementation by Breiman & Cutler
    - http://www.stat.berkeley.edu/users/breiman/RandomForests/
    - Papers, documentation, and code…
    - …in Fortran 77.
  - But also newer version available in Fortran 90!
    - http://www.irb.hr/en/research/projects/it/2004/2004-111/
  - Fast Random Forest implementation for Java (Weka)
    - http://code.google.com/p/fast-random-forest/

L. Breiman, Random Forests, *Machine Learning*, Vol. 45(1), pp. 5-32, 2001.

References and Further Reading

- More information on Decision Trees can be found in Chapters 8.2-8.4 of Duda & Hart.

R.O. Duda, P.E. Hart, D.G. Stork
Pattern Classification
2nd Ed., Wiley-Interscience, 2000



- The original papers for Randomized Trees
  - Y. Amit, D. Geman, Shape Quantization and Recognition with Randomized Trees, *Neural Computation*, Vol. 9(7), pp. 1545-1588, 1997.
  - V. Lepetit, P. Fua, Keypoint Recognition using Randomized Trees, *IEEE Trans. Pattern Analysis and Machine Intelligence*, Vol. 28(9), pp. 1465—1479, 2006.
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