Machine Learning – Lecture 12

Randomized Trees, Forests, and Ferns

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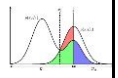
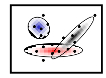
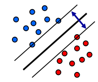
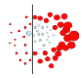
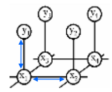
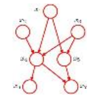
Course Outline

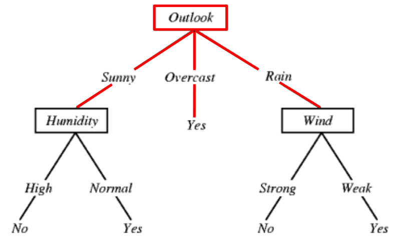
- Fundamentals (2 weeks)
  - Bayes Decision Theory
  - Probability Density Estimation
- Discriminative Approaches (5 weeks)
  - Linear Discriminant Functions
  - Statistical Learning Theory & SVMs
  - Ensemble Methods & Boosting
  - Randomized Trees, Forests & Ferns
- Generative Models (4 weeks)
  - Bayesian Networks
  - Markov Random Fields

Topics of This Lecture

- Decision Trees
- Randomized Decision Trees
  - Randomized attribute selection
- Random Forests
  - Bootstrap sampling
  - Ensemble of randomized trees
  - Posterior sum combination
  - Analysis
- Extremely randomized trees
  - Random attribute selection
- Ferns
  - Fern structure
  - Semi-Naïve Bayes combination
  - Applications

Recap: 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

Recap: 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?

This will be our focus!

CART – 2. Picking a Good Splitting Feature

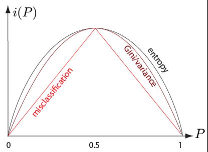
- Goal
  - Want a tree that is as simple/small as possible (Occam's razor).
  - But: Finding a minimal tree is an NP-hard optimization problem.
- Greedy top-down search
  - Efficient, but not guaranteed to find the smallest tree.
  - Seek a property T at each node N that makes the data in the child nodes as *pure* as possible.
  - For formal reasons more convenient to define *impurity* $i(N)$.
  - Several possible definitions explored.

Picking a Good Splitting Feature

- Goal
  - Select the query (=split) that decreases impurity the most

$$\triangle i(N) = i(N) - P_L i(N_L) - (1 - P_L) i(N_R)$$

fraction of points in left child node



- Impurity measures
  - Entropy impurity (information gain):

$$i(N) = -\sum_j p(\mathcal{C}_j|N) \log_2 p(\mathcal{C}_j|N)$$

  - Gini impurity:

$$i(N) = \sum_{i \neq j} p(\mathcal{C}_i|N) p(\mathcal{C}_j|N) = \frac{1}{2}\left[1 - \sum_j p^2(\mathcal{C}_j|N)\right]$$

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.
    - Cross-validation
    - Chi-square test
    - MDL
  - Postpruning: Grow the full tree, then remove subtrees that do not have sufficient evidence.
    - Merging nodes
    - Rule-based pruning
- In practice often preferable to apply post-pruning.

Recap: Decision Trees - Summary

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

Recap: Decision Trees - Summary

- 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.

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.

$$O(DN \log N)$$

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  - Ensemble of randomized trees
  - Posterior sum combination
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  - Random attribute selection
- Ferns
  - Fern structure
  - Semi-Naïve Bayes combination
  - Applications

Randomized Decision Trees (Amit & Geman 1997)

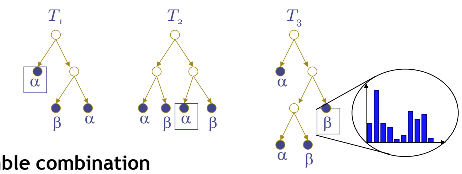
- Decision trees: main effort on finding good split
  - Training runtime: $O(DN^2 \log N)$
  - This is what takes most effort in practice.
  - Especially cumbersome with many attributes (large D).
- Idea: randomize attribute selection
  - No longer look for globally optimal split.
  - Instead randomly 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

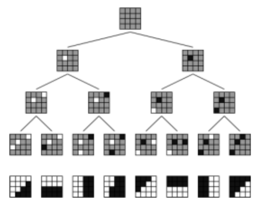


- Ensemble combination
  - Tree leaves (l,η) store posterior probabilities of the target classes. $p_{l,\eta}(\mathcal{C}|\mathbf{x})$
  - Combine the output of several trees by averaging their posteriors (Bayesian model combination)

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

Applications: Character Recognition

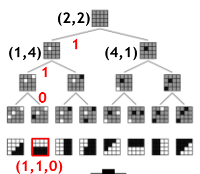
- Computer Vision: Optical character recognition
  - Classify small (14x20) images of hand-written characters/digits into one of 10 or 26 classes.
- Simple binary features
  - Tests for individual binary pixel values.
  - Organized in randomized tree.



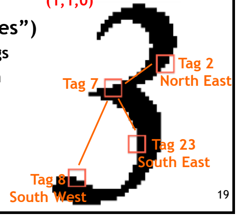
Y. Amit, D. Geman, Shape Quantization and Recognition with Randomized Trees, *Neural Computation*, Vol. 9(7), pp. 1545-1588, 1997.

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



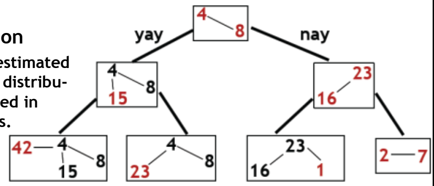
- Representation of digits ("Queries")
  - Specific spatial arrangements of tags
  - An image answers "yes" if any such structure is found anywhere
  - *How do we know which spatial arrangements to look for?*



Slide adapted from Jan Hosang

Applications: Character Recognition

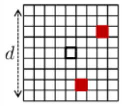
- Answer: Create a second-level decision tree!
  - Start with two tags connected by an arc
  - Search through extensions of confirmed queries (or rather through a subset of them, there are lots!)
  - Select query with best information gain
  - Recurse…
- Classification
  - Average estimated posterior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



Slide adapted from Jan Hosang

Applications: Fast Keypoint Detection

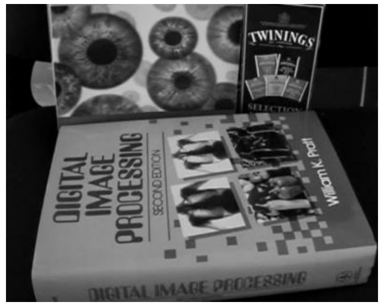
- Computer Vision: fast keypoint detection
  - Detect keypoints: small patches in the image used for matching
  - Classify into one of ~200 categories (visual words)
- Extremely simple features
  - E.g. pixel value in a color channel (CIELab)
  - E.g. sum of two points in the patch
  - E.g. difference 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

Machine Learning, Summer '16



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

Topics of This Lecture

Machine Learning, Summer '16

Random Forests (Breiman 2001)

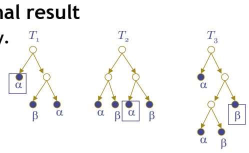
Machine Learning, Summer '16

- 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

Machine Learning, Summer '16

- 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)

Machine Learning, Summer '16

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

  ⇒ 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)

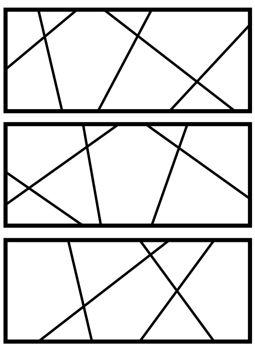
- Random attribute selection
  - For each node, randomly choose subset of K attributes on which the split is based (typically $K = \sqrt{N_f}$).
  - ⇒ Faster training procedure
    - Need to test only few attributes.
  - Minimizes inter-tree dependence
    - Reduce correlation between different trees.
- Each tree is grown to maximal size and is left unpruned
  - Trees are deliberately overfit
  - ⇒ 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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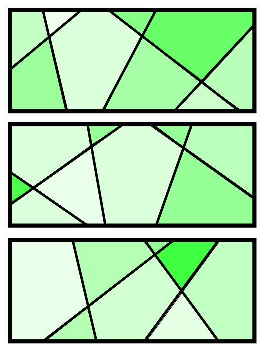
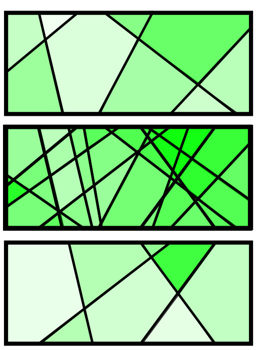


A Graphical Interpretation

Different trees induce different partitions on the data.

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



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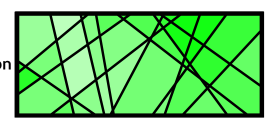

...which at the same time also better reflects the uncertainty due to the bootstrapped sampling.

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.

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- Recap: Random Forests
  - Bootstrap sampling
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- Extremely randomized trees
  - Random attribute selection
- Ferns
  - Fern structure
  - Semi-Naïve Bayes combination
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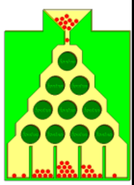
A Case Study in Deconstructivism…

- What we've done so far
  - Take the original decision tree idea.
  - Throw out all the complicated bits (pruning, etc.).
  - Learn on random subset of training data (bootstrapping/bagging).
  - Select splits based on random choice of candidate queries.
    - So as to maximize information gain.
    - Complexity: $O(KN^2 \log N)$
  - ⇒ Ensemble of weaker classifiers.
- How can we further simplify that?
  - Main effort still comes from selecting the optimal split (from reduced set of options)…
  - Simply choose a random query at each node.
    - Complexity: $O(N)$
  - ⇒ *Extremely randomized decision trees*

Extremely Randomized Decision Trees

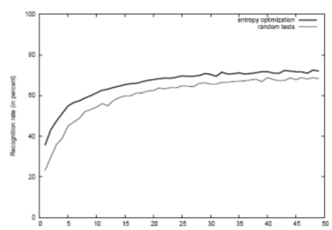
- Random queries at each node…
  - Tree gradually develops from a classifier to a flexible container structure.
  - Node queries define (randomly selected) structure.
  - Each leaf node stores posterior probabilities



- Learning (e.g. for keypoint detection)
  - Patches are "dropped down" the trees.
    - Only pairwise pixel comparisons at each node.
    - Directly update posterior distributions at leaves
  - ⇒ Very fast procedure, only few pixel-wise comparisons
  - ⇒ No need to store the original patches!

Image source: Wikipedia

Performance Comparison



Keypoint detection task

- Results
  - Almost equal performance for random tests when a sufficient number of trees is available (and much faster to train!).

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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- **Ferns**
  - Fern structure
  - Semi-Naïve Bayes combination
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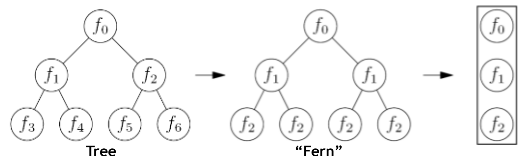
From Trees to Ferns...



- Observation
  - If we select the node queries randomly anyway, what is the point of choosing different ones for each node?
  - ⇒ Keep the same query for all nodes at a certain level.
  - This effectively enumerates all 2^M possible outcomes of the M tree queries.
  - Tree can be collapsed into a fern-like structure.

What Does This Mean?

- Interpretation of the decision tree
  - We model the class conditional probabilities of a large number of binary features (the node queries).
  - Notation
    - f_i : Binary feature
    - N_f: Total number of features in the model.
    - $\mathcal{C}_k$: Target class
  - Given $f_1,\ldots,f_{N_f}$, we want to select class $\mathcal{C}_k$ such that
    $$k = \arg\max_k p(\mathcal{C}_k|f_1,\ldots,f_{N_f})$$
  - Assuming a uniform prior over classes, this is the equal to
    $$k = \arg\max_k p(f_1,\ldots,f_{N_f}|\mathcal{C}_k)$$
  - Main issue: How do we model the joint distribution?

Modeling the Joint Distribution

- Full Joint
  - Model all correlations between features
    $$p(f_1,\ldots,f_{N_f}|\mathcal{C}_k)$$
  - ⇒ Model with 2^{N_f} parameters, not feasible to learn.
- Naïve Bayes classifier
  - Assumption: all features are independent.
    $$p(f_1,\ldots,f_{N_f}|\mathcal{C}_k) = \prod_{i=1}^{N_f} p(f_i|\mathcal{C}_k)$$
  - ⇒ Too simplistic, assumption does not really hold!
  - ⇒ Naïve Bayes model ignores correlation between features.

Modeling the Joint Distribution

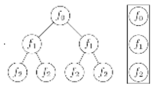
- Decision tree
  - Each path from the root to a leaf corresponds to a specific combination of feature outcomes, e.g.
    $$p_{leaf_m}(\mathcal{C}_k) = p(f_{m1}=1, f_{m2}=0,\ldots,f_{md}=1|\mathcal{C}_k)$$
  - Those path outcomes are independent, therefore
    $$p(f_1,\ldots,f_{N_f}|\mathcal{C}_k) \approx \prod_{m=1}^{M} p_{leaf_m}(\mathcal{C}_k)$$
  - But not all feature outcomes are represented here...

Modeling the Joint Distribution

- Ferns
  - A fern F is defined as a set of S binary features $\{f_l,\ldots,f_{l+S}\}$.
  - M: number of ferns, $N_f = S \cdot M$.
  - This represents a compromise:
    $$p(f_1,\ldots,f_{N_f}|\mathcal{C}_k) \approx \prod_{j=1}^{M} p(F_j|\mathcal{C}_k)$$
    $$= \underbrace{p(f_1,\ldots,f_S|\mathcal{C}_k)}_{\text{Full joint inside fern}} \cdot p(f_{S+1},\ldots,f_{2S}|\mathcal{C}_k) \cdot \ldots$$
    Naïve Bayes between ferns
  - ⇒ Model with $M \cdot 2^S$ parameters (“Semi-Naïve”).
  - ⇒ Flexible solution that allows complexity/performance tuning.

Modeling the Joint Distribution

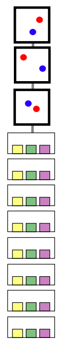
- Ferns
  - Ferns are thus semi-naïve Bayes classifiers.
  - They assume independence between sets of features (between the ferns)…
  - …and enumerate all possible outcomes inside each set.



- Interpretation
  - Combine the tests $f_l, \ldots, f_{l+S}$ into a binary number.
  - Update the "fern leaf" corresponding to that number.

0
0 → Update leaf 100_2 = 4
1

Ferns - Training

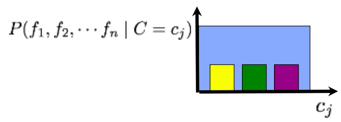


The tests compare the intensities of two pixels around the keypoint:

$$f_i = \begin{cases} 1 & \text{if } I(m_{i,1}) \le I(m_{i,2}) \\ 0 & \text{otherwise} \end{cases}$$

Invariant to lighting change by any raising function.

Posterior probabilities:



Ferns - Training

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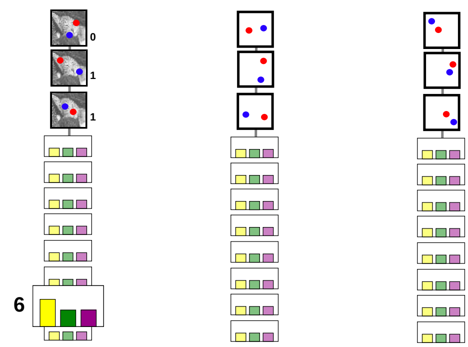
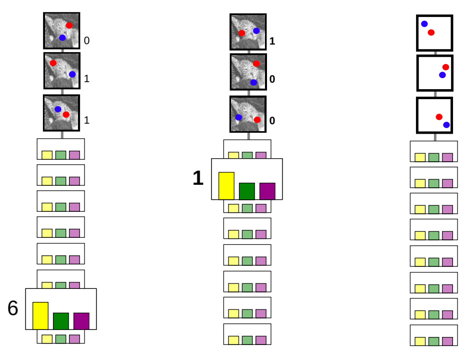
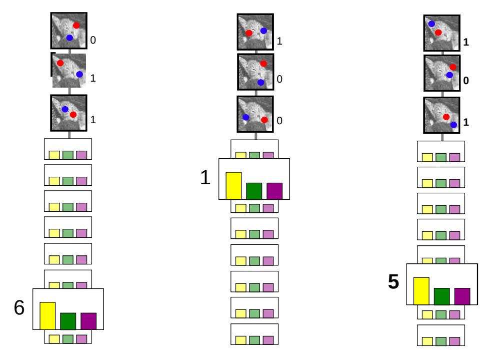


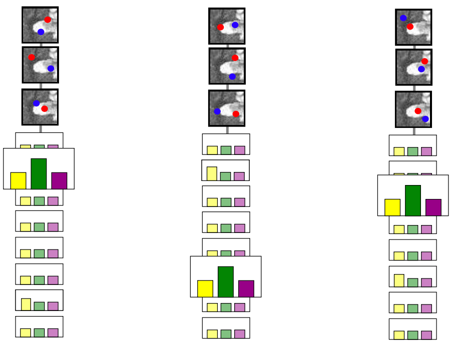
Ferns - Training



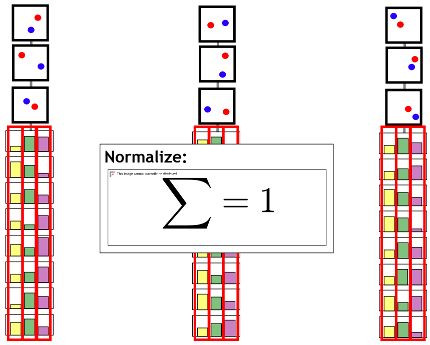
Ferns - Training



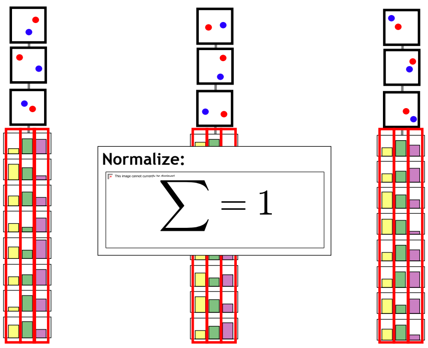
Ferns - Training



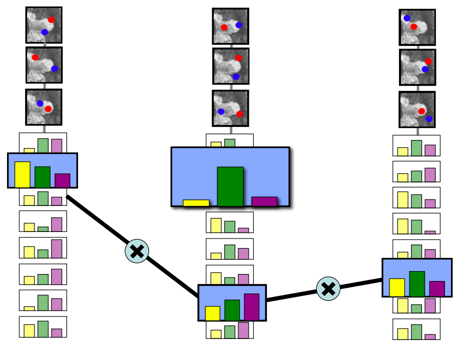
Ferns - Training Results



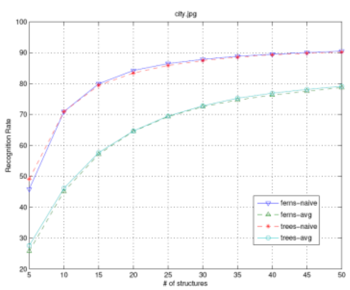
Ferns - Training Results



Ferns - Recognition



Performance Comparison



- **Results**
  - Ferns perform as well as randomized trees (but are much faster)
  - Naïve Bayes combination better than averaging posteriors.

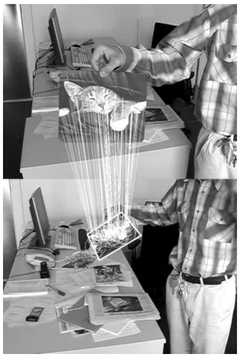
Keypoint Recognition in 10 Lines of Code

```
for(int i = 0; i < H; i++) P[i ] = 0.;
for(int k = 0; k < M; k++) {
  int index = 0, * d = D + k * 2 * S;
  for(int j = 0; j < S; j++) {
    index <<= 1;
    if (*(K + d[0]) < *(K + d[1]))
      index++;
    d += 2;
  }
  p = PF + k * shift2 + index * shift1;
  for(int i = 0; i < H; i++) P[i] += p[i];
}
```

- **Properties**
  - Very simple to implement;
  - (Almost) no parameters to tune;
  - Very fast.

M. Ozuysal, M. Calonder, V. Lepetit, P. Fua, Fast Keypoint Recognition using Random Ferns. In *IEEE. Trans. Pattern Analysis and Machine Intelligence*, 2009.

Application: Keypoint Matching with Ferns

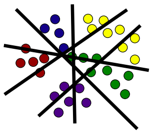


Application: Mobile Augmented Reality

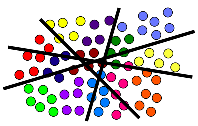
D. Wagner, G. Reitmayr, A. Mulloni, T. Drummond, D. Schmalstieg, Pose Tracking from Natural Features on Mobile Phones. In *ISMAR 2008*.

Practical Issues - Selecting the Tests

- For a small number of classes
  - We can try several tests.
  - Retain the best one according to some criterion.
    - E.g. entropy, Gini



- When the number of classes is large
  - Any test does a decent job.



Slide credit: Vincent Lepetit

Summary

- We started from full decision trees…
  - Successively simplified the classifiers…
- …and ended up with very simple randomized versions
  - Ensemble methods: Combination of many simple classifiers
  - Good overall performance
  - Very fast to train and to evaluate
- Common limitations of Randomized Trees and Ferns?
  - Need large amounts of training data!
    - In order to fill the many probability distributions at the leaves.
  - Memory consumption!
    - Linear in the number of trees.
    - Exponential in the tree depth.
    - Linear in the number of classes (histogram at each leaf!)

References and Further Reading

- 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.
- The original paper for Random Forests:
  - L. Breiman, Random Forests, *Machine Learning*, Vol. 45(1), pp. 5-32, 2001.
- The papers for Ferns:
  - M. Ozuysal, M. Calonder, V. Lepetit, P. Fua, Fast Keypoint Recognition using Random Ferns. In *IEEE. Trans. Pattern Analysis and Machine Intelligence*, 2009.
  - D. Wagner, G. Reitmayr, A. Mulloni, T. Drummond, D. Schmalstieg, Pose Tracking from Natural Features on Mobile Phones. In *ISMAR 2008*.