An introduction to random forests

Eric Debreuve / Team Morpheme

Institutions: University Nice Sophia Antipolis / CNRS / Inria
Labs: I3S / Inria CRI SA-M / iBV

Outline

▷ • Machine learning

• Decision tree

• Random forest
  • Bagging
  • Random decision trees

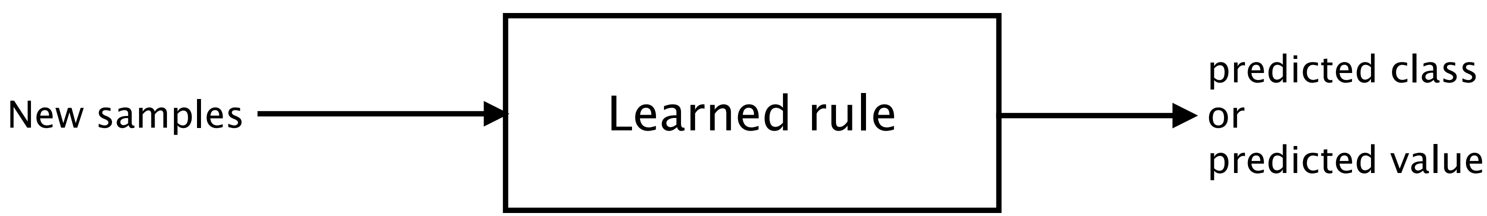
• Kernel-Induced Random Forest (KIRF)

• Byproducts
  • Out-of-bag error
  • Variable importance

Machine learning

- Learning/training: build a classification or regression rule from a set of samples

- Prediction: assign a class or value to new samples



(Un)Supervised learning

- Supervised
  - Learning set = { (sample [acquisition], class [expert]) }

- Unsupervised
  - Learning set = unlabeled samples

- Semi-supervised
  - Learning set = some labeled samples + many unlabeled samples

Ensemble learning

- Combining weak classifiers (of the same type)...
- ... in order to produce a strong classifier
  - Condition: diversity among the weak classifiers

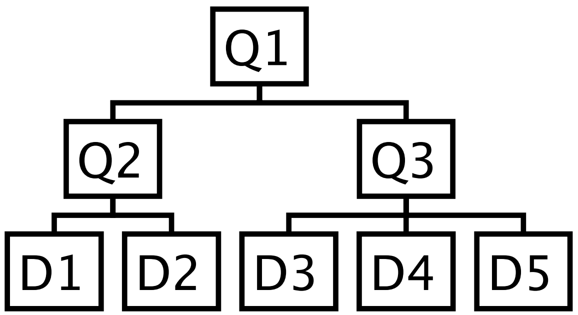
- Example: Boosting
  - Train each new weak classifier focusing on samples misclassified by previous ones

  - Popular implementation: AdaBoost
    - Weak classifiers: only need to be better than random guess

Outline

- Machine learning
- ▷ Decision tree
- Random forest
  - Bagging
  - Random decision trees
- Kernel-Induced Random Forest (KIRF)
- Byproducts
  - Out-of-bag error
  - Variable importance

Decision tree



- Root node
  - Entry point to a collection of data
- Inner nodes (among which the root node)
  - A question is asked about data
  - One child node per possible answer
- Leaf nodes
  - Correspond to the decision to take (or conclusion to make) if reached

- Example: CART – Classification and Regression Tree
  - Labeled sample
    - Vector of variable/feature values + class label

  - Binary decision tree
    - Top-down, greedy building…
    - … by recursively partitioning the feature space into hyper-rectangles

  - Similarity with weighted kNN

- Normally, pruning
  - To avoid over-fitting of learning data
  - To achieve a trade-off between prediction accuracy and complexity

Decision tree > CART > Building

- All labeled samples initially assigned to root node
- N ← root node
- With node N do
  - Find the feature F + threshold value T...
    - ... that split the samples assigned to N into 2 subsets S_{left} and S_{right}...
    - ... so as to maximize the label purity within these subsets

  - Assign (F,T) to N

  - If S_{left} and S_{right} too small to be splitted
    - Attach child leaf nodes L_{left} and L_{right} to N
    - Tag the leaves with the most present label in S_{left} and S_{right}, resp.
  - else
    - Attach child nodes N_{left} and N_{right} to N
    - Assign S_{left} and S_{right} to them, resp.
    - Repeat procedure for $N = N_{left}$ and $N = N_{right}$

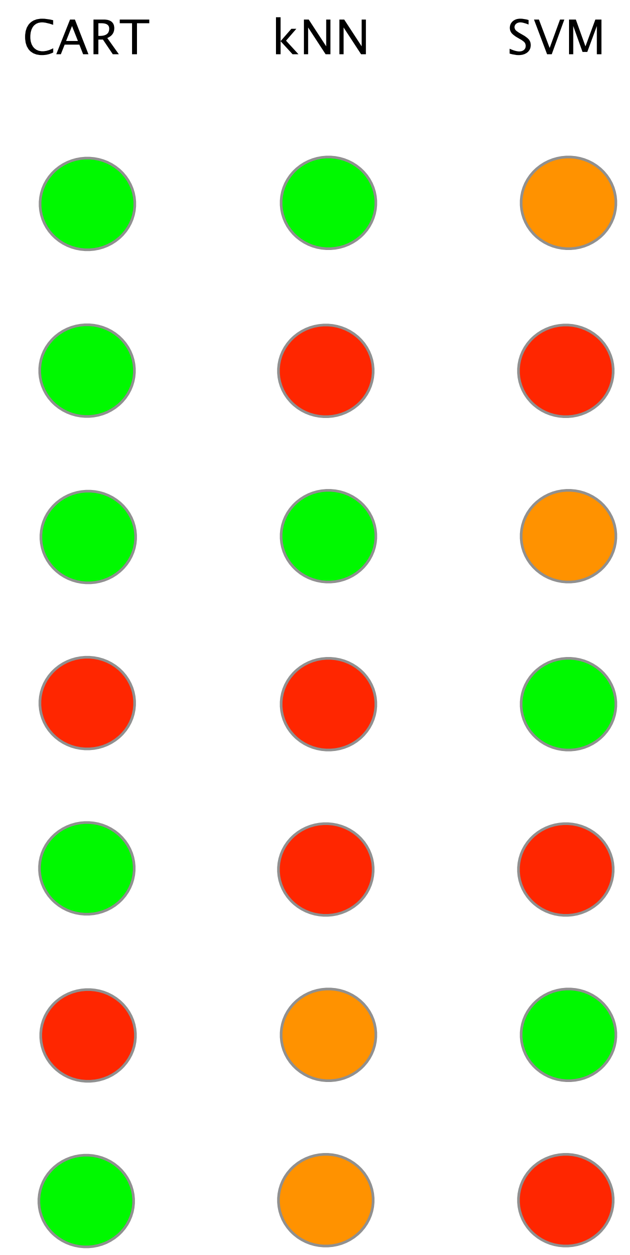
Decision tree > CART > Building > Purity

- (Im)Purity
  - Quality measure applied to each subset S_{left} and S_{right}
  - Combination of the measures (e.g., weighted average)

- Examples
  - Gini index = $\sum_{l=1}^{L} f_l (1 - f_l)$
  - Entropy = $-\sum_{l=1}^{L} f_l \log_2 f_l$
  - Misclassification error = $1 - \max_{l \in [1..L]} f_l$

Decision tree > CART > Properties

- Intrinsically multiclass
- Handles Apple and Orange features
- Robustness to outliers
- Works w/ "small" learning set
- Scalability (large learning set)
- Prediction accuracy
- Parameter tuning



Outline

- Machine learning
- Decision tree
- ▷ Random forest
  - Bagging
  - Random decision trees
- Kernel-Induced Random Forest (KIRF)
- Byproducts
  - Out-of-bag error
  - Variable importance

Random forest

- Definition
  - Collection of unpruned CARTs
  - Rule to combine individual tree decisions

- Purpose
  - Improve prediction accuracy

- Principle
  - Encouraging diversity among the tree

- Solution: randomness
  - Bagging
  - Random decision trees (rCART)

Random forest > Bagging

- Bagging: Bootstrap aggregation

- Technique of ensemble learning...
    - ... to avoid over-fitting
        - Important since trees are unpruned
    - ... to improve stability and accuracy

- Two steps
    - Bootstrap sample set
    - Aggregation

Random forest > Bagging > Bootstrap

- L: original learning set composed of p samples

- Generate K learning sets L_k...
  - ... composed of q samples, $q \leq p$,...
  - ... obtained by uniform sampling with replacement from L
  - In consequences, L_k may contain repeated samples

- Random forest: q = p
  - Asymptotic proportion of unique samples in L_k = 100 (1 – 1/e) ~ 63%
  - → The remaining samples can be used for testing

Random forest > Bagging > Aggregation

- Learning
  - For each L_k, one classifier C_k (rCART) is learned

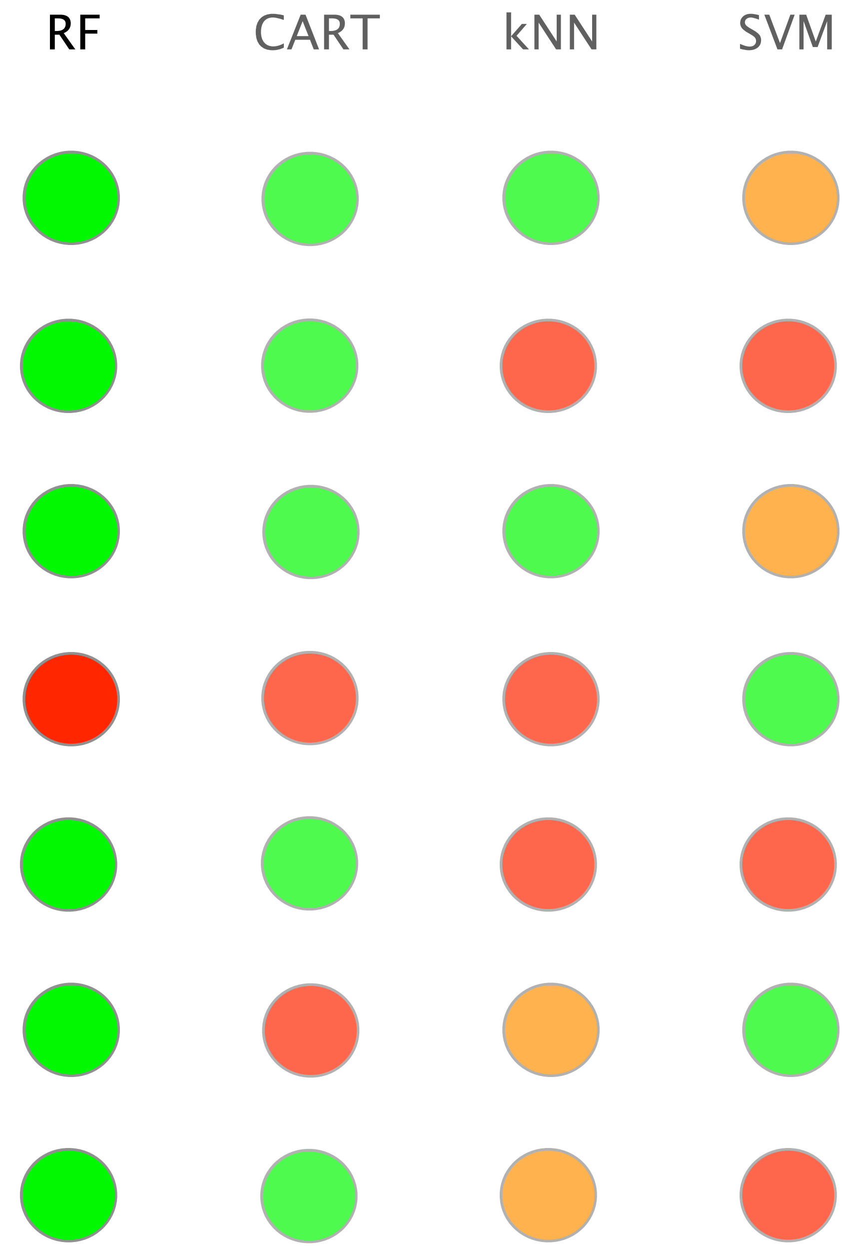
- Prediction
  - S: a new sample
  - Aggregation = majority vote among the K predictions/votes $C_k(S)$

Random forest > Random decision tree

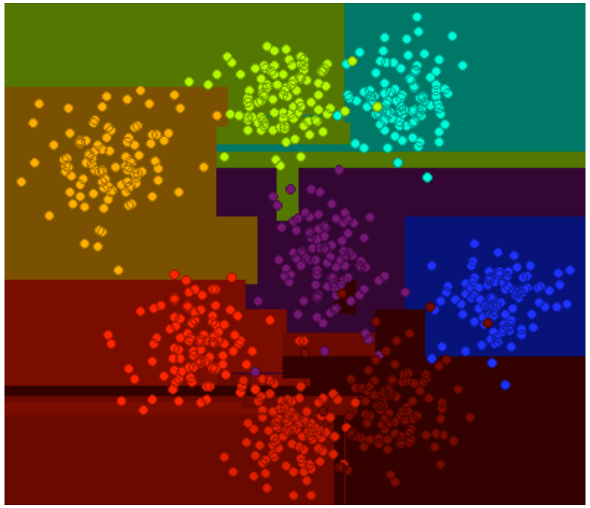
- All labeled samples initially assigned to root node
- N ← root node
- With node N do
  - Find the feature F among a random subset of features + threshold value T...
    - ... that split the samples assigned to N into 2 subsets S_{left} and S_{right}...
    - ... so as to maximize the label purity within these subsets
  - Assign (F,T) to N
  - If S_{left} and S_{right} too small to be splitted
    - Attach child leaf nodes L_{left} and L_{right} to N
    - Tag the leaves with the most present label in S_{left} and S_{right}, resp.
  - else
    - Attach child nodes N_{left} and N_{right} to N
    - Assign S_{left} and S_{right} to them, resp.
    - Repeat procedure for N = N_{left} and N = N_{right}
- Random subset of features
  - Random drawing repeated at each node
  - For D-dimensional samples, typical subset size = round(sqrt(D)) (also round(log2(x)))
  - → Increases diversity among the rCARTs + reduces computational load
- Typical purity: Gini index

Random forest > Properties

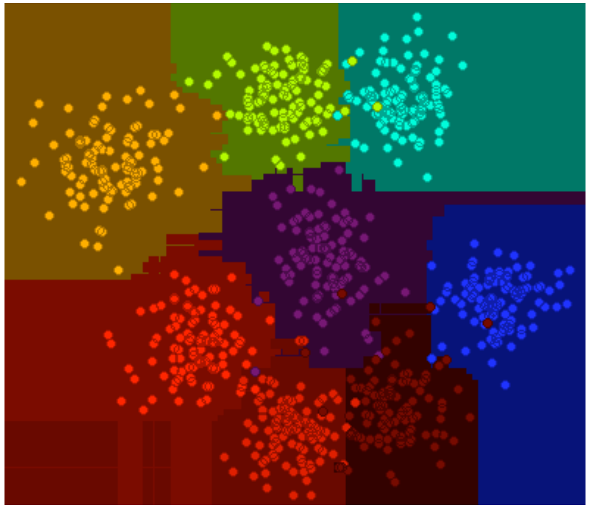
- Intrinsically multiclass
- Handles Apple and Orange features
- Robustness to outliers
- Works w/ "small" learning set
- Scalability (large learning set)
- Prediction accuracy
- Parameter tuning



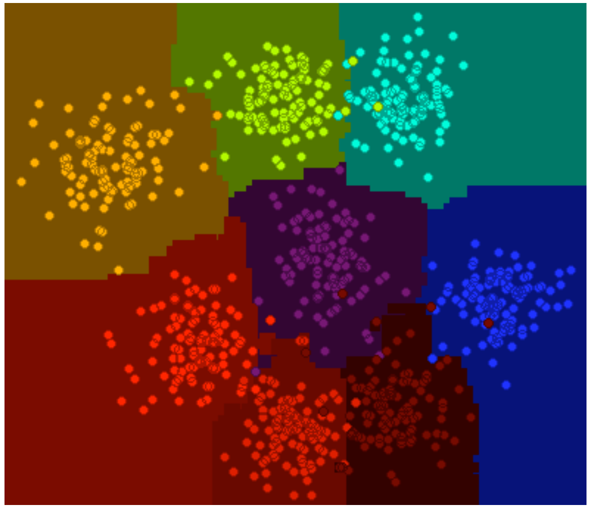
Random forest > Illustration



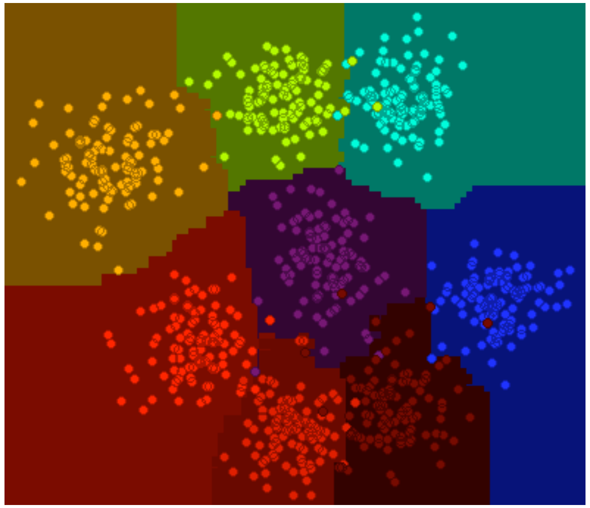
1 rCART



10 rCARTs



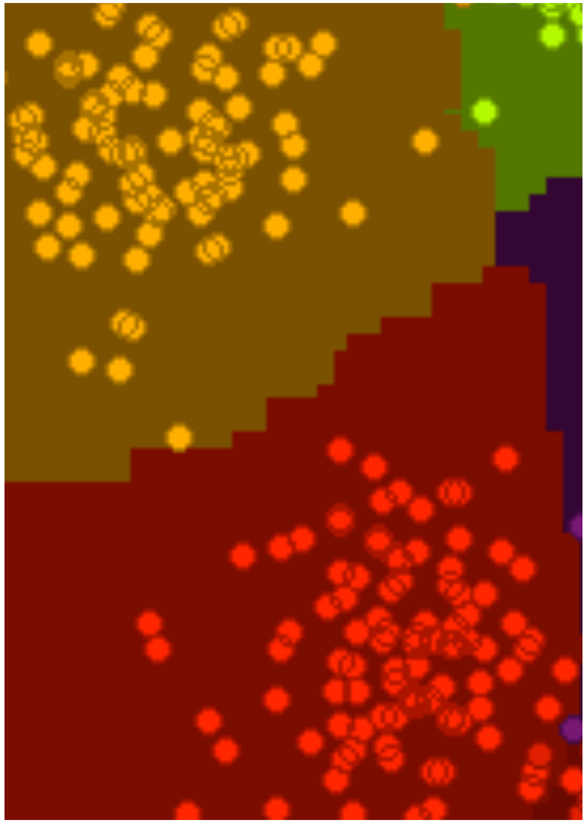
100 rCARTs



500 rCARTs

Random forest > Limitations

- Oblique/curved frontiers
  - Staircase effect
  - Many pieces of hyperplanes



- Fundamentally discrete
  - Functional data? (Example: curves)

Outline

- Machine learning
- Decision tree
- Random forest
  - Bagging
  - Random decision trees
- ▷ Kernel-Induced Random Forest (KIRF)
- Byproducts
  - Out-of-bag error
  - Variable importance

Kernel-Induced Random Forest (KIRF)

- Random forest
  - Sample S is a vector
  - Features of S = components of S

- Kernel-induced features
  - Learning set L = { S_i, $i \in [1..N]$ }

  - Kernel K(x,y)
    - Features of sample S = { $K_i(S) = K(S_i, S)$, $i \in [1..N]$ }
    - Samples S and S_i can be vectors or functional data

Kernel > Kernel trick

- Kernel trick
  - Maps samples into an inner product space...
  - ... usually of higher dimension (possibly infinite)...
  - ... in which classification (or regression) is easier
    - Typically linear

- Kernel K(x,y)
  - Symmetric
  - Positive semi-definite (Mercer's condition):

$$\int\int f(x)\,K(x,y)\,f(y)\,dxdy \geq 0$$

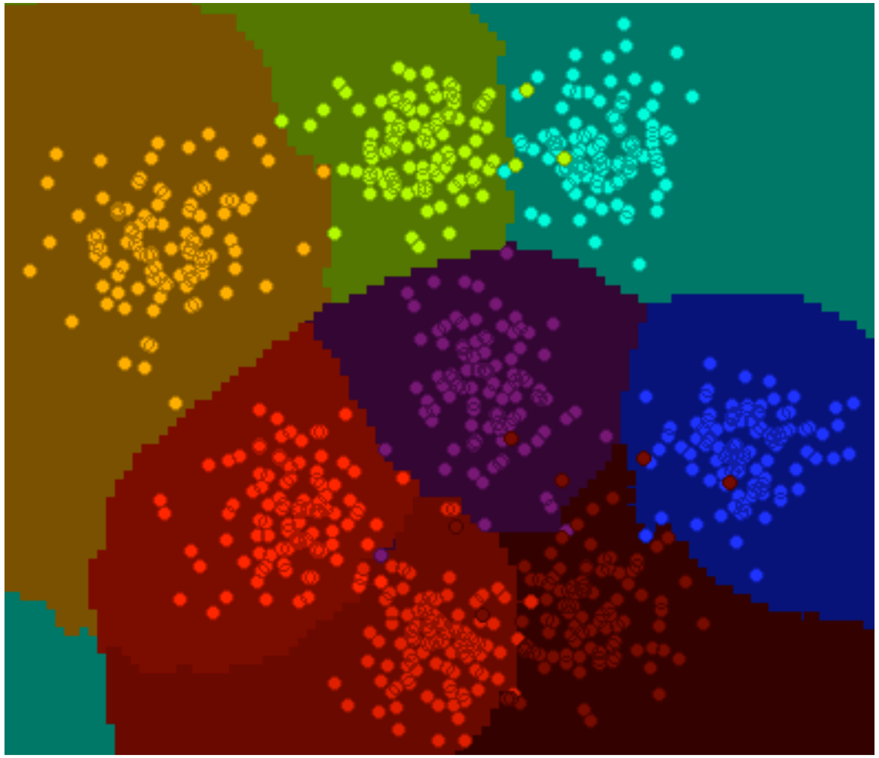
  - $K(x,y) = \langle \varphi(x), \varphi(y) \rangle$
    - Note: mapping needs not to be known (might not even have an explicit representation; e.g., Gaussian kernel)

Kernel > Examples

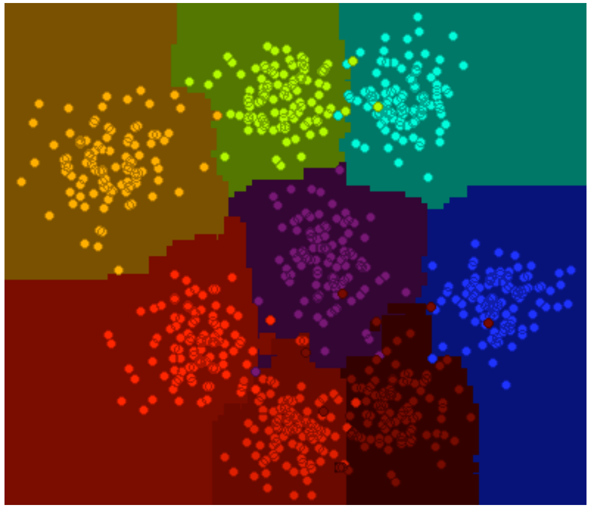
- Polynomial (homogeneous): $K(x, y) = (x \cdot y)^d$
- Polynomial (inhomogeneous): $K(x, y) = (x \cdot y + 1)^d$
- Hyperbolic tangent: $K(x, y) = \tanh(\alpha x \cdot y + \beta)$
- Gaussian: $K(x, y) = \exp(-\gamma |x - y|^2)$
  - Function of the distance between samples
  - Straightforward application to functional data of a metric space
    - E.g., curves

KIRF > Illustration

- Gaussian kernel
  - Some similarity with vantage-point tree



KIRF w/ 100 rCARTs



Reminder: RF w/ 100 rCARTs

KIRF > Limitations

- Which kernel?
  - Which kernel parameters?

- No “orange and apple” handling anymore
  - ($x \cdot y$ or $(x - y)^2$)

- Computational load (kernel evaluations)
  - Especially during learning

- Needs to store samples
  - (Instead of feature indices in Random forest)

Outline

- Machine learning
- Decision tree
- Random forest
  - Bagging
  - Random decision trees
- Kernel-Induced Random Forest (KIRF)
- ▷ Byproducts
  - Out-of-bag error
  - Variable importance

Byproduct > Reminder

- To grow one rCART
  - Bootstrap sample set from learning set L
  - Remaining samples
    - Called out-of-bag samples
    - Can be used for testing

- Two points of view
  - For one rCART, out-of-bag samples = L \ Bootstrap samples
    - Used for variable importance

  - For one sample S of L, set of rCARTs for which S was out-of-bag
    - Used for out-of-bag error

Byproduct > Out-of-bag error

- For each sample S of the learning set
  - Look for all the rCARTs for which S was out-of-bag
  - Build the corresponding sub-forest
  - Predict the class of S with it
  - Error = is prediction correct?
- Out-of-bag error = average over all samples of S
  - Note: predictions not made using the whole forest...
  - ... but with some aggregation
- Provides an estimation of the generalization error
  - Can be used to decide when to stop adding trees to the forest

Byproduct > Variable importance

- For each rCART
  - Compute out-of-bag error $OOB_{original}$
    - Fraction of misclassified out-of-bag samples
  - Consider the i[th] feature/variable of the samples
  - Randomly permute its values among the out-of-bag samples
  - Re-compute out-of-bag error $OOB_{permutation}$
  - rCART-level importance(i) = $OOB_{permutation} - OOB_{original}$
- Variable importance(i) = average over all rCARTs
  - Note: rCART-based errors (no aggregation)
    - Avoid attenuation of individual errors

An introduction to random forests

Thank you for your attention