STAT406- Methods of Statistical Learning Lecture 16

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Failing hard and failing often



Hey, it runs!

- (1) for (b in 1:B)
 - (a) Draw a bootstrap sample from the training data
 - (b) Grow a "random forest tree" as follows: for each terminal node:
 - (i) Randomly select m features
 - (ii) Pick the best split among these
 - (iii) Split the node into two children
 - (c) Repeat (b) to grow a (very very) large tree
- (2) Return the ensemble of trees $(T_b)_{1 \le b \le B}$

Given a new point x, for regression we use

$$\hat{f}(\mathbf{x}) = \frac{1}{B} \sum_{b=1}^{B} T_b(\mathbf{x})$$

For classification:

$$\hat{f}(\mathbf{x}) = \text{majority vote among} \left\{ T_b(\mathbf{x}), 1 \le b \le B \right\}$$

Q: why not average conditional prob's?

Out-of-bag error estimates

- Each bagged tree is trained on a bootstrap sample
- Predict the observations not in the bootstrap sample with that tree
- One will have "about" B/3 predictions for each point in the training set
- These can be used to estimate the prediction error (classification error rate) without having to use CV

Out-of-bag error estimates

- For each training observation (y_i, \mathbf{x}_i) , obtain a prediction using only those trees in which (y_i, \mathbf{x}_i) was **NOT** used
- In other words, let \mathcal{I}_i the set of trees (bootstrap samples) where (y_i, \mathbf{x}_i) does not appear, then

$$\hat{y}_i = \frac{1}{|\mathcal{I}_i|} \sum_{i \in \mathcal{I}} T_j(\mathbf{x}_i)$$

- This error estimate can be computed at the same time as the trees are being built
- When this error estimate is stabilized we can stop adding trees to the ensemble

Example

OOB example

- Feature ranking relative importance of each variable
- Given a single tree T, at each node t split we can compute the sum of reductions in sum of squares (or gini or deviance measures) m_t²
- We assign this squared measure m_t^2 to the variable (feature) used in the split

- To each feature, we assign the sum of "squared gains" attributed to it
- For the i-th variable X_i we have

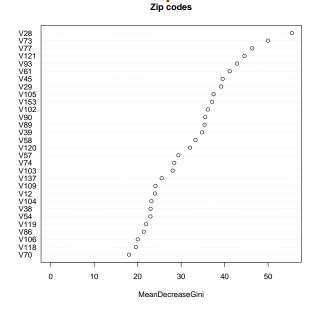
$$\mathcal{J}_i^2(T) = \begin{cases} m_t^2 & \text{if split involved } X_i \\ 0 & \text{otherwise} \end{cases}$$

For a random forest we use

$$\mathcal{J}_i^2 = \sum_T \mathcal{J}_i^2(T)$$

In other words, we sum (or average)
the importance of the variable across
the trees in the forest

Random Forest - plot



Ensembles

- Ensembles of classifiers
- Combine classifiers trained on the same (or similar [e.g. bootstrapped]) data
- Consensus is reached by (equally weighted) voting or averaged estimated probabilities.
- Bagging and Random Forests are examples of ensembles.

Boosting

- Originally proposed for classification
- Main idea: sequentially re-train a simple classifier assigning more importance to points that were previously misclassified

Boosting

- The end result is a weighted average of all the classifiers
- Interesting ideas:
 - Not all components of the ensemble are treated equally
 - Members of the ensemble use information about other members
 - The underlying loss function has a "margin" (unlike 0-1 losses)

Boosting - AdaBoost.M1

Algorithm. Data $(y_i, \mathbf{x_i})$, with $y_i \in \{-1, 1\}$

- Set initial weights $w_i = 1/n$, $1 \le i \le n$
- For i = 1, ..., K
- Build a classifier $T_{\mathbf{j}}(\mathbf{x})$ to the data using weights $w_{\mathbf{i}}$, $1 \le \mathbf{i} \le n$

Boosting - AdaBoost.M1

Let

$$e_{\mathbf{j}} = \sum_{\mathbf{i}=1}^{n} w_{\mathbf{i}} I(y_{\mathbf{i}} \neq T_{\mathbf{j}}(\mathbf{x}_{\mathbf{i}})) / \sum_{\ell=1}^{n} w_{\ell}$$

- Let $\alpha_{\mathbf{j}} = \log ((1 e_{\mathbf{j}})/e_{\mathbf{j}})$ and $w_{\mathbf{i}} = w_{\mathbf{i}} \exp (\alpha_{\mathbf{i}} I(y_{\mathbf{i}} \neq T_{\mathbf{i}}(\mathbf{x}_{\mathbf{i}}))), \mathbf{i} = 1, \dots, n$
- Final classifier:

$$T(\mathbf{x}) = \operatorname{sign}\left(\sum_{\mathbf{j}=1}^{K} \alpha_{\mathbf{j}} T_{\mathbf{j}}(\mathbf{x})\right)$$