Recitation 10

Trees, Bootstrap, Bagging, Random Forest, Adaboost

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CDS

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Announcement

- HW 5 is due on Friday night + HW 6 will be out and due in 2 weeks
- HW 4 grades by this weekend
- Midterm solutions

Agenda

1. Announcement
2. Trees
3. Bootstrap
4. Bagging
5. Boosting
6. Takeaways

Decision Trees

- Non-linear classifier that groups examples hierarchically to make predictions
- Each leaf node refers to a subset of data points and each split is based on a single feature

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- Non-linear classifier that groups examples hierarchically to make predictions
- Each leaf node refers to a subset of data points and each split is based on a single feature
- Finding the optimal tree is intractable $\rightarrow$ Greedy selection methods
- Prediction is an average over all points present in the current bucket i.e. $\hat{y}_i = \sum_{j=1}^{m} y_j | x_j$

Trees - Q1

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A. Given a fixed tree, if we split a leaf node we add a single leaf to the tree. Thus k splits corresponds to k + 1 leaves

Trees - Q2

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A. A tree of height k can have at most 2^k regions (leaves).

Trees - Q3

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A. A tree of height $\lceil \log_2(n) \rceil$ can put each example into its own bucket.

Trees - Q4

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A. A tree of height $\lceil \log_2(n) \rceil$ can differentiate each point based on the first feature. At each leaf, we can start a subtree for the second feature and so on. Therefore the required upper bound is $\lceil d \log_2(n) \rceil$

Misclassification error in a node

- Let's consider the multiclass classification case: $\mathcal{Y} = \{1, 2, \ldots, K\}$.
- Let node m represent region R_m, with N_m observations
- We denote the proportion of observations in R_m with class k by

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{\{i: x_i \in R_m\}} \mathbf{1}(y_i = k).$$

- We predict the majority class in node m:

$$k(m) = \arg\max_k \hat{p}_{mk}$$

Node Impurity Measures and Split Points

- Misclassification error

$$1 - \hat{p}_{mk(m)}.$$

- The Gini index encourages $\hat{p}_{mk}$ to be close to 0 or 1

$$\sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$

- Entropy / Information gain

$$-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}.$$

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- Suppose we have N_L points in R_L and N_R points in R_R.
- Let $Q(R_L)$ and $Q(R_R)$ be the node impurity measures for each node.
- We aim to find a split that minimizes the *weighted average of node impurities*:

$$\frac{N_L Q(R_L) + N_R Q(R_R)}{N_L + N_R}$$

Trees - Q5

Q. Suppose we are looking at a fixed node of a classification tree, and the class labels are, sorted by the first feature values,

$$4, 1, 0, 0, 1, 0, 2, 3, 3.$$

We are currently testing splitting the node into a left node containing $4, 1, 0, 0, 1, 0$ and a right node containing $2, 3, 3$. For each of the following impurity measures, give the value for the left and right parts, along with the total score for the split.

1. Gini index.
2. Entropy.

Trees - Q5

1. Gini:
   - Left: $3/6(3/6) + 2/6(4/6) + 1/6(5/6) = 22/36$
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   - Total: $6[-3/6 \log(3/6) - 2/6 \log(2/6) - 1/6 \log(1/6)] + 3[-1/3 \log(1/3) - 2/3 \log(2/3)]$.

Trees

- Interpretable and great at capturing non-linear boundaries
- With the caveat of a high chance of overfitting and high variance

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- But we don't have access to many data samples.
- A **bootstrap method** simulates B independent samples from P by taking B bootstrap samples from the sample $\mathcal{D}_n$.
- Turns out this works quite well
- We also now have B instances of any statistic (median, variance etc.) so we can calculate properties of this distribution

Bootstrap - Q6

Let $X_1, \ldots, X_{2n+1}$ be an i.i.d. sample from a distribution. To estimate the median of the distribution, you can compute the sample median of the data.

- How do we compute an estimate of the variance of the sample median?

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Let $X_1, \ldots, X_{2n+1}$ be an i.i.d. sample from a distribution. To estimate the median of the distribution, you can compute the sample median of the data.

- How do we compute an estimate of the variance of the sample median?
  - Draw B bootstrap samples $D^1, \ldots, D^B$ each of size $2n+1$. The samples are formed by drawing uniformly with replacement from the original data set $X_1, \ldots, X_{2n+1}$. We will make a total of $B(2n+1)$ draws.
  - For each D^i compute the corresponding median $\hat{m}_i$.
  - Compute the sample variance of the B medians $m_1, \ldots, m_B$.

Bagging: Bootstrap Aggregation

- We draw B bootstrap samples $D^1, \ldots, D^B$ from original data $\mathcal{D}$
- Let $\hat{f}_1, \hat{f}_2, \ldots, \hat{f}_B$ be the prediction functions resulting from training on $D^1, \ldots, D^B$, respectively
- The **bagged prediction function** is a *combination* of these:

$$\hat{f}_{\text{avg}}(x) = \text{Combine}\left(\hat{f}_1(x), \hat{f}_2(x), \ldots, \hat{f}_B(x)\right)$$

- You reduce variance in prediction and incur a cost on interpretability

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$$\text{Var}(\hat{f}_{\text{avg}}(x)) = \text{Var}\left(\frac{1}{B}\sum_{b=1}^{B}\hat{f}_b(x)\right) = \frac{1}{B^2}\text{Var}\left(\sum_{b=1}^{B}\hat{f}_b(x)\right)$$

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  Assuming the various f_i are independent prediction functions.

  So $\frac{1}{B^2}\text{Var}\left(\sum_{b=1}^{B}\hat{f}_b(x)\right) = \frac{1}{B^2}B * \text{Var}\left(\hat{f}_1(x)\right) = \frac{1}{B}\text{Var}\left(\hat{f}_1(x)\right)$

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- A bootstrap sample from $\mathcal{D}_n = (x_1, \ldots, x_n)$ is a sample of size n drawn with replacement from $\mathcal{D}_n$. So there can be overlaps between bootstrap samples.

Bagging - Q9

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$$\text{Var}\left(\frac{1}{B}\sum_{b=1}^{B}\hat{f}_b\right) \tag{1}$$

$$= \frac{1}{B^2}\left[(B * \text{Var}(\hat{f}_1(x)) + B(B-1) * \text{Cov}(\hat{f}_1(x), \hat{f}_2(x))\right] \tag{2}$$

$$= \frac{1}{B}\sigma^2 + \frac{B-1}{B}\rho^2 \tag{3}$$

Bagging/RF - Q10

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We randomly sample features when building trees to reduce the covariance between trees.

Boosting

- Why train the different estimators independently?
- We can do better by making them target the mistakes of one-another

Adaboost Algorithm

Given training set $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.

1. Initialize observation weights $w_i = 1,\ i = 1, 2, \ldots, n$.

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3. Ouptut $G(x) = \text{sign}[\sum_{m=1}^{M} \alpha_m G_m(x)]$.

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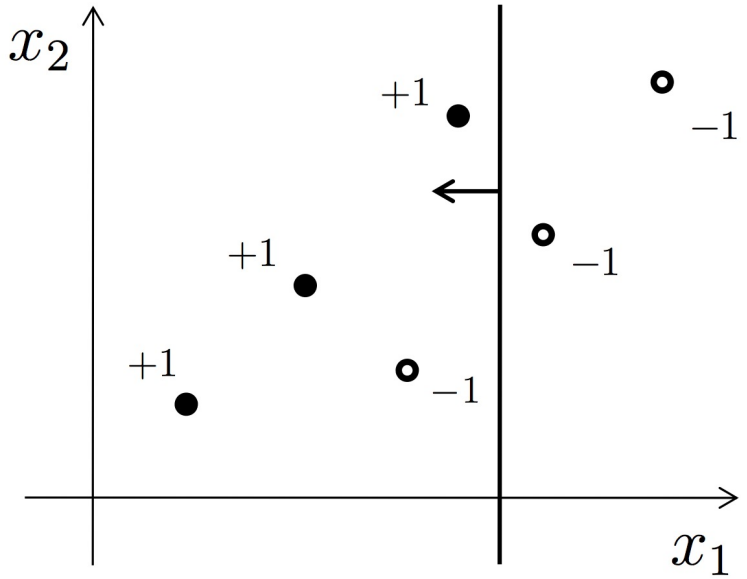
Adaboost - Q12

Consider building an ensemble of decision stumps Gm with the AdaBoost algorithm. $f(x) = \text{sign}\left(\sum_{m=1}^{M} \alpha_m G_m(x)\right)$ displays a few labeled point in two dimensions as well as the first stump we have chosen. A stump predicts binary ± 1 values, and depends only on one coordinate value (the split point). The little arrow in the figure is the normal to the stump decision boundary indicating the positive side where the stump predicts $+1$. All the points start with uniform weights.



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- Will the second stump receive higher coefficient in the ensemble than the first? In other words, will $\alpha_2 > \alpha_1$? Briefly explain your answer. (no calculation should be necessary).

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- Will the second stump receive higher coefficient in the ensemble than the first? In other words, will $\alpha_2 > \alpha_1$? Briefly explain your answer. (no calculation should be necessary). (sol.) $\alpha_2 > \alpha_1$ because the point that the second stump misclassifies will have a smaller relative weight since it is classified correctly by the first stump.

Takeaways

- Trees are an interpretable, non-linear classifier
- To reduce variance, we can run bagging/random forest instead of relying on a single tree
- (Potentially) Better than training the predictors independently we can make them correct each other with boosting