732A99/TDDE01 Machine Learning

Lecture 1a Block 2: Ensemble Methods

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Contents

Literature

- Main source
  - Hastie, T., Tibshirani, R. and Friedman, J. *The Elements of Statistical Learning*. Springer, 2009. Sections 8.7, 10.1-10.5, 10.10.2 and 15.1-15.2.
- Additional source
  - Bishop, C. M. *Pattern Recognition and Machine Learning*. Springer, 2006. Sections 14.1-14.4.

Wisdom of Crowds

- "The collective knowledge of a diverse and independent body of people typically exceeds the knowledge of any single individual, and can be harnessed by voting".

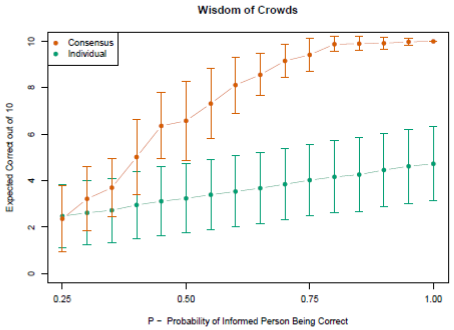
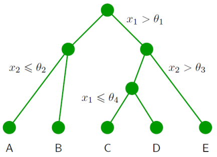
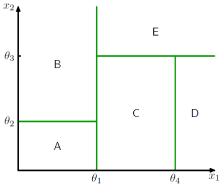


FIGURE 8.11. *Simulated academy awards voting.* 50 *members vote in* 10 *categories, each with* 4 *nominations. For any category, only* 15 *voters have some knowledge, represented by their probability of selecting the "correct" candidate in that category (so* $P = 0.25$ *means they have no knowledge). For each category, the* 15 *experts are chosen at random from the* 50*. Results show the expected correct (based on* 50 *simulations) for the consensus, as well as for the individuals. The error bars indicate one standard deviation. We see, for example, that if the* 15 *informed for a category have a* 50 % *chance of selecting the correct candidate, the consensus doubles the expected performance of an individual.*

Decision Trees

- A decision tree partitions the input space into rectangular regions. Each region has associated a predictor.





- The model in each region is typically a constant, specifically
  - the result of majority voting for classification, since the **best** classifier under the 0-1 loss function is $\arg\max_y p(y|x)$, and
  - the average for regression, since the **best** regression function under the squared error loss function is $E_{Y|x}[y]$.
- Decision tree construction: Greedy search for next split variable and threshold while enough data points in each leaf, and then typically pruning.
- Decision trees have many advantages (fast, interpretable, etc.) and two major disadvantages: **Low accuracy and high variance** with respect to the training data.
- These disadvantages make them good candidates for bagging, at the expense of compromising some of their advantages.

Bagging

- Boosting aggregation (bagging) is a technique to combine (weak) regressions and so produce a more accurate (committee) regression. It can also be applied to classification.
- Main steps:
  - Obtain B bootstrap samples of the original training data, i.e. draw B samples with replacement from the original data and of the same size as the original data.
  - Run the regression algorithm on each bootstrap sample b to obtain the regression $f^b(x)$.
  - Return the average of the regressions obtained, that is

$$f_{bag}(x) = \frac{1}{B} \sum_b f^b(x)$$

- Bagging (generalized) linear regressions is not particularly useful: The bagged regression will converge to the one learned from the original data as B increases.
- Then, it makes more sense to use bagging with non-linear regressions, e.g. decision trees.
- For classification, we can average the individual models by averaging their posterior class probabilities, or use majority voting.

Bagging

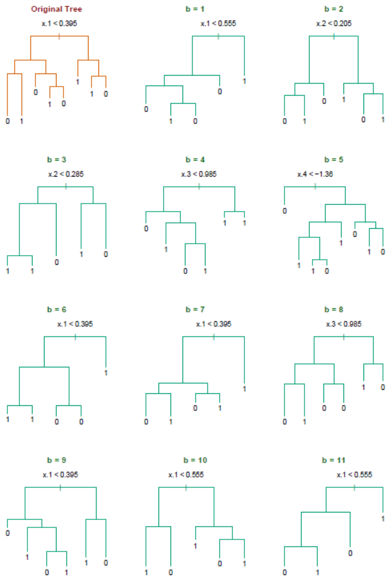


FIGURE 8.9. *Bagging trees on simulated dataset. The top left panel shows the original tree. Eleven trees grown on bootstrap samples are shown. For each tree, the top split is annotated.*

Bagging

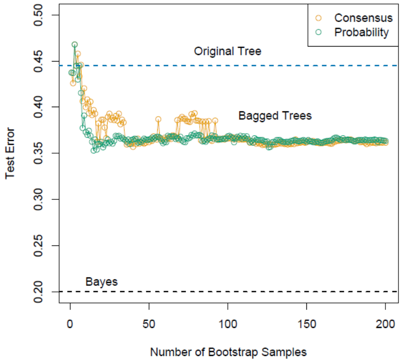


FIGURE 8.10. *Error curves for the bagging example of Figure 8.9. Shown is the test error of the original tree and bagged trees as a function of the number of bootstrap samples. The orange points correspond to the consensus vote, while the green points average the probabilities.*

Bagging

- Let $h(x)$ denote the true **regression**. Then, $f^b(x) = h(x) + \epsilon^b(x)$.
- The mean-squared error of $f^b(x)$ can be expressed as
$$E_X[(f^b(x) - h(x))^2] = E_X[\epsilon^b(x)^2]$$
- The mean-squared error of $f_{bag}(x)$ can be expressed as
$$E_X[(\frac{1}{B}\sum_b f^b(x) - h(x))^2] = E_X[(\frac{1}{B}\sum_b \epsilon^b(x))^2]$$
- **Assume** that the error terms $\epsilon^b(x)$ have zero mean and are uncorrelated, i.e. $E_X[\epsilon^b(x)] = 0$ and $E_X[\epsilon^b(x)\epsilon^{b'}(x)] = 0$. Then,
$$E_X[(\frac{1}{B}\sum_b f^b(x) - h(x))^2] = \frac{1}{B}\Big(\frac{1}{B}\sum_b E_X[\epsilon^b(x)^2]\Big)$$
which implies that bagging reduces the average error of the individual regressions by a factor of B.
- In practice, the reduction in error is less dramatic as the individual errors are correlated.
- At least, the bagged error is **never** larger than the average individual error:
$$\frac{1}{B}\sum_b E_X[\epsilon^b(x)^2] = E_X[\sum_b \frac{1}{B}\epsilon^b(x)^2] \geq E_X[(\frac{1}{B}\sum_b \epsilon^b(x))^2]$$
by Jensen's inequality, i.e. $\sum_i \lambda_i g(a_i) \geq g(\sum_i \lambda_i a_i)$.

Bagging

- Bagging also reduces the variance of the regression error with respect to the **training data** D:

$$var_D(error_{bag}(D)) = E_D[(error_{bag}(D) - E_D[error_{bag}(D)])^2]$$

  where $error_{bag}(D) = \frac{1}{B^2}\sum_b error^b(D)$.

- The reason is that the variance of the average of n **identically distributed** variables $X_1, \ldots, X_n$ with variance σ^2 and **non-negative** pairwise correlation ρ is

$$\begin{aligned} var\left(\frac{1}{n}\sum_i X_i\right) &= \frac{1}{n^2}\sum_i var(X_i) + \frac{2}{n^2}\sum_i\sum_{j>i} cov(X_i, X_j) \\ &= \frac{n\sigma^2}{n^2} + \frac{n(n-1)}{n^2}\rho\sigma^2 = \rho\sigma^2 + \frac{1-\rho}{n}\sigma^2 < \sigma^2 \end{aligned}$$

- Note that the errors are now assumed to be non-negatively correlated. Moreover, they are assumed to be identically distributed, which is not necessarily true in practice. In any case, this is another reason why bagging is used with high variance algorithms such as decision trees.

Bagging

- Unlike for regression, bagging for **classification** can hurt performance:
  - Consider the 0-1 loss function, and assume that the true class is $Y = 1$ for all x. Consider some independent classifiers that predict $Y = 0$ with probability 0.6 for all x. Then, the error rate is 0.6 for any individual classifier, but it is 1 for the majority voting classifier.
- However, bagging can improve **independent** weak classifiers with error rate $e < 0.5$.
  - Consider the 0-1 loss function, and the majority voting classifier. This classifier returns the true label with probability $p(S > B/2)$ where $S \sim Binomial(B, 1 - e)$. Moreover, $p(S > B/2) \to 1$ as B grows large.

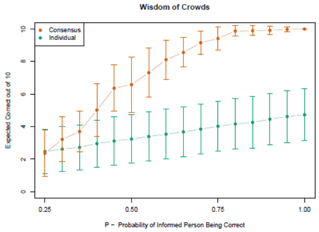


FIGURE 8.11. *Simulated academy awards voting. 50 members vote in 10 categories, each with 4 nominations. For any category, only 15 voters have some knowledge, represented by their probability of selecting the "correct" candidate in that category (so $P = 0.25$ means they have no knowledge). For each category, the 15 experts are chosen at random from the 50. Results show the expected correct (based on 50 simulations) for the consensus, as well as for the individuals. The error bars indicate one standard deviation. We see, for example, that if the 15 informed for a category have a 50% chance of selecting the correct candidate, the consensus doubles the expected performance of an individual.*

Bagging

- Bagging also reduces the variance (a.k.a. **instability**) of the (classification or regression) predictor with respect to the **training data** D:

$$var_D(f_{bag}(x;D)) = E_D[(f_{bag}(x;D) - E_D[f_{bag}(x;D)])^2]$$

  where $f_{bag}(x;D) = \frac{1}{B}\sum_b f^b(x;D)$.

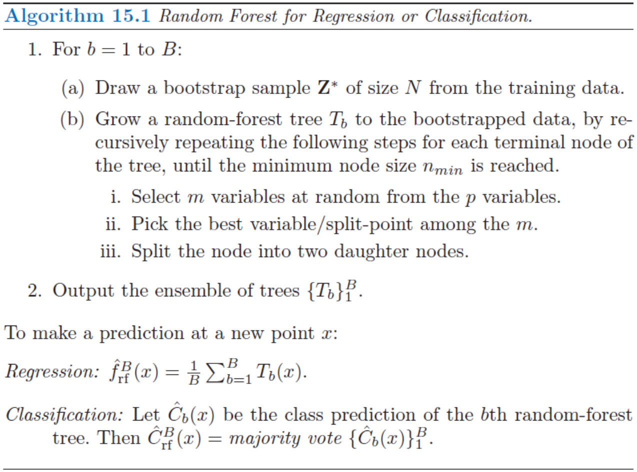
- The reason is that the variance of the average of n **identically distributed** variables $X_1, \dots, X_n$ with variance σ^2 and **non-negative** pairwise correlation ρ is

$$\begin{aligned} var\left(\frac{1}{n}\sum_i X_i\right) &= \frac{1}{n^2}\sum_i var(X_i) + \frac{2}{n^2}\sum_i \sum_{j>i} cov(X_i, X_j) \\ &= \frac{n\sigma^2}{n^2} + \frac{n(n-1)}{n^2}\rho\sigma^2 = \rho\sigma^2 + \frac{1-\rho}{n}\sigma^2 < \sigma^2 \end{aligned}$$

- Note that the predictors are assumed to be non-negatively correlated. Moreover, they are assumed to be identically distributed, which is not necessarily true in practice. In any case, this is another reason why bagging is used with high variance algorithms such as decision trees.

Random Forests

- Random forest = decision trees + bagging + **decorrelation**.



Algorithm 15.1 *Random Forest for Regression or Classification.*

```
1. For $b = 1$ to $B$:
    (a) Draw a bootstrap sample $\mathbf{Z}^*$ of size $N$ from the training data.
    (b) Grow a random-forest tree $T_b$ to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size $n_{min}$ is reached.
        i. Select $m$ variables at random from the $p$ variables.
        ii. Pick the best variable/split-point among the $m$.
        iii. Split the node into two daughter nodes.
2. Output the ensemble of trees $\{T_b\}_1^B$.
```

To make a prediction at a new point x:

Regression: $\hat{f}_{\text{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$.

Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}_{\text{rf}}^B(x) = \textit{majority vote}\ \{\hat{C}_b(x)\}_1^B$.

- Note that step 1ai aims to decorrelate the individual decision trees.

Random Forests

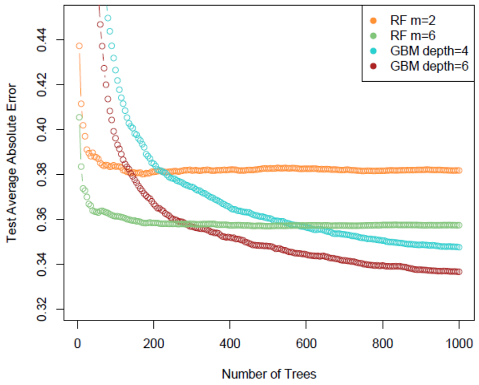
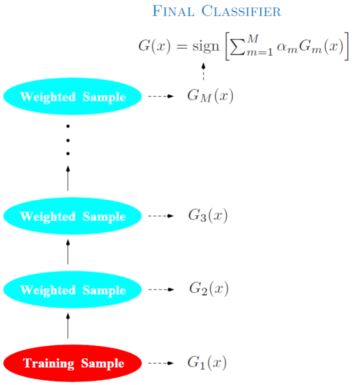


FIGURE 15.3. *Random forests compared to gradient boosting on the California housing data. The curves represent mean absolute error on the test data as a function of the number of trees in the models. Two random forests are shown, with* $m = 2$ *and* $m = 6$*. The two gradient boosted models use a shrinkage parameter* $\nu = 0.05$ *in (10.41), and have interaction depths of* 4 *and* 6*. The boosted models outperform random forests.*

Boosting

- Boosting is a technique to combine (weak) classifiers and so produce a more accurate (committee) classifier. It can also be applied to regression.
- Main steps:
  - Run the classification algorithm on the original/modified training data.
  - **Modify** the training data by giving
    - **more** weight to the **erroneously** classified points, and
    - **less** weight to the **correctly** classified points.
  - Iterate through the previous steps a number of times.
  - Return a weighted average of the classifiers obtained.



AdaBoost

Algorithm 10.1 *AdaBoost.M1.*

```
1. Initialize the observation weights $w_i = 1/N,\ i = 1, 2, \ldots, N$.
2. For $m = 1$ to $M$:
    (a) Fit a classifier $G_m(x)$ to the training data using weights $w_i$.
    (b) Compute
        $$\text{err}_m = \frac{\sum_{i=1}^{N} w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}.$$
    (c) Compute $\alpha_m = \log((1 - \text{err}_m)/\text{err}_m)$.
    (d) Set $w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq G_m(x_i))],\ i = 1, 2, \ldots, N$.
3. Output $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.
```

AdaBoost

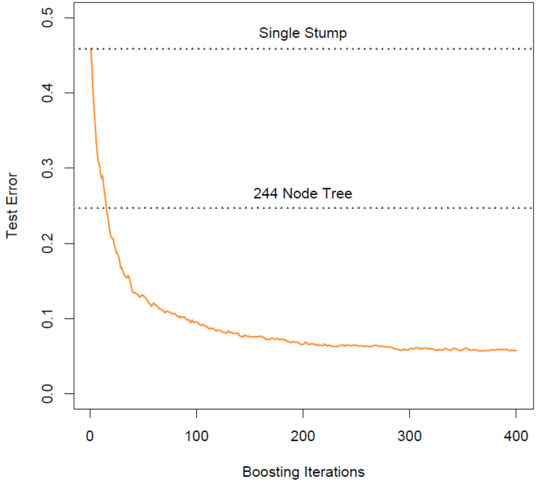


FIGURE 10.2. *Simulated data (10.2): test error rate for boosting with stumps, as a function of the number of iterations. Also shown are the test error rate for a single stump, and a 244-node classification tree.*

Forward Stagewise Additive Modeling

- Boosting can be seen as fitting an additive expansion of a set of basis functions. That is, the boosted classifier

$$G(x) = \sum_m \alpha_m G_m(x)$$

can be rewritten as

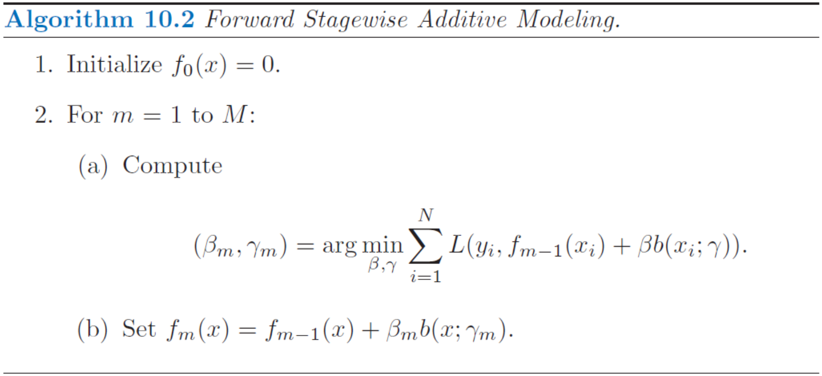
$$f(x) = \sum_m \beta_m b(x; \gamma_m)$$

and the aim of boosting can be rephrased as minimizing a loss function over the training data $\{x_i, y_i\}$, that is

$$\min_{\{\beta_m, \gamma_m\}} \sum_i L(y_i, \sum_m \beta_m b(x_i; \gamma_m))$$

- The problem above is challenging for most loss functions and basis functions. Heuristic solution: Add the basis functions one at a time.

Forward Stagewise Additive Modeling



Algorithm 10.2 *Forward Stagewise Additive Modeling.*

```
1. Initialize $f_0(x) = 0$.
2. For $m = 1$ to $M$:
    (a) Compute
        $$(\beta_m, \gamma_m) = \arg\min_{\beta,\gamma} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)).$$
    (b) Set $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$.
```

AdaBoost

- It can be shown that AdaBoost is equivalent to forward stagewise additive modeling with **exponential loss function**, that is

$$L(y, f(x)) = \exp(-yf(x))$$

- In each step of forward stagewise additive modeling, we have to solve

$$\begin{aligned}(\beta_m, \gamma_m) &= \arg\min_{\beta,\gamma} \sum_i \exp[-y_i(f_{m-1}(x_i) + \beta b(x_i;\gamma))] \\ &= \arg\min_{\beta,\gamma} \sum_i w_i^{(m)} \exp(-y_i \beta b(x_i;\gamma))\end{aligned}$$

where $w_i^{(m)} = exp(-y_i f_{m-1}(x_i))$ are the instance weights in AdaBoost.

- Note that

$$\sum_i w_i^{(m)} \exp(-y_i \beta b(x_i;\gamma)) = \exp(-\beta) \sum_{y_i = b(x_i;\gamma)} w_i^{(m)} + \exp(\beta) \sum_{y_i \neq b(x_i;\gamma)} w_i^{(m)}$$

and, thus, for any given $\beta > 0$

$$\gamma_m = \arg\min_{\gamma} \sum_i w_i^{(m)} I(y_i \neq b(x_i;\gamma))$$

which is what step 2a of AdaBoost does.

- Now, solving for β results in $\beta_m = (1/2)\log((1 - err_m)/err_m)$.
- Finally, take $\alpha_m = 2\beta_m$ and note that

$$w_i^{(m+1)} = exp(-y_i[f_{m-1}(x_i) + \beta_m b(x_i;\gamma_m)]) = w_i^m exp(\alpha_m I(y_i \neq b(x_i;\gamma_m))) exp(-\beta_m)$$

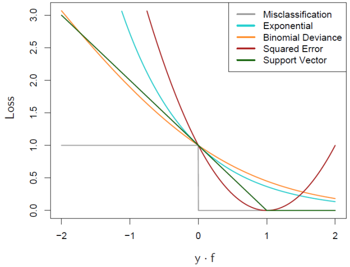
which, after dropping $exp(-\beta_m)$ as it multiplies all weights, is steps 2b-d.

AdaBoost

- It can be shown that the population minimizer of the exponential loss function is

$$\arg\min_{f(x)} E_{Y|x}[exp(-yf(x))] = \frac{1}{2}\log\frac{p(Y=+1|x)}{p(Y=-1|x)}$$

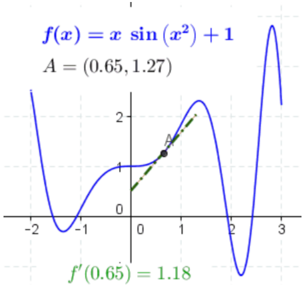
- Since AdaBoost's output is an approximation to the population minimizer, it makes sense to use the sign as the classification rule in step 3.
- Note that the exponential loss is an upper bound on the 0-1 loss.

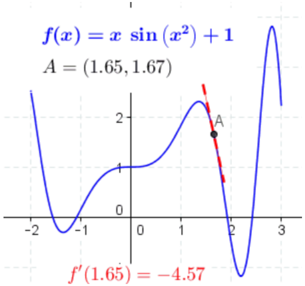


- Moreover, the exponential loss for a misclassified point increases exponentially with its margin $yf(x)$. This may make the performance of AdaBoost to degrade in settings with **wrongly labeled points**: AdaBoost may try to classify them correctly at the expense of other misclassified points that are correctly labeled.

Gradient Boosting

- For some loss functions and/or basis functions, forward stagewise additive modeling can be cumbersome. In those cases, gradient boosting may be the solution.
- Recall that $f'(x) = \lim_{h \to 0} \frac{f(x+h)-f(x)}{h}$





- Recall that the gradient is a vector whose components are the partial derivatives.

Gradient Boosting

```
Gradient Boosting

1.  Initialize $f_0(x) = \arg\min_\gamma \sum_i L(y_i, b(x_i;\gamma))$
2.  For $m = 1$ to $M$:
    (a) Compute the gradient residual $r_{im} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f(x)=f_{m-1}(x)}$
    (b) $\gamma_m = \arg\min_\gamma \sum_i (r_{im} - b(x_i;\gamma))^2$
    (c) $\beta_m = \arg\min_\beta \sum_i L(y_i, f_{m-1}(x_i) + \beta b(x_i;\gamma_m))$
    (d) $f_m(x) = f_{m-1}(x) + \beta_m b(x;\gamma_m)$
```

- Step 2b approximates the gradient residuals with the least squares basis function.
- Step 2a is easy in some cases, e.g. if $L(y, f(x)) = \frac{1}{2}(y - f(x))^2$ then

$$\frac{\partial L(y, f(x))}{\partial f(x)} = y - f(x)$$

Summary

- Bagging: Combines weak predictors to reduce error and variance.
- Random forest = decision trees + bagging + decorrelation.
- AdaBoost: Combination of weak predictors under exponential loss.
- Gradient boosting: Extension to arbitrary loss functions.
- How many individual models in bagging, boosting and random forest ? (Nested) cross-validation.