Lecture 9: Tree-Based Methods and Ensembling Methods

Readings: ESL (Ch. 9.2-10, 15), ISL (Ch. 8), Bach (Ch. 10); code

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Outline

1. Tree-Based Methods
2. Ensembling Methods
3. Parallel Ensembles: Bagging and Random Forest
4. Sequential Ensembles: Boosting and AdaBoost
5. Comparison & Summary
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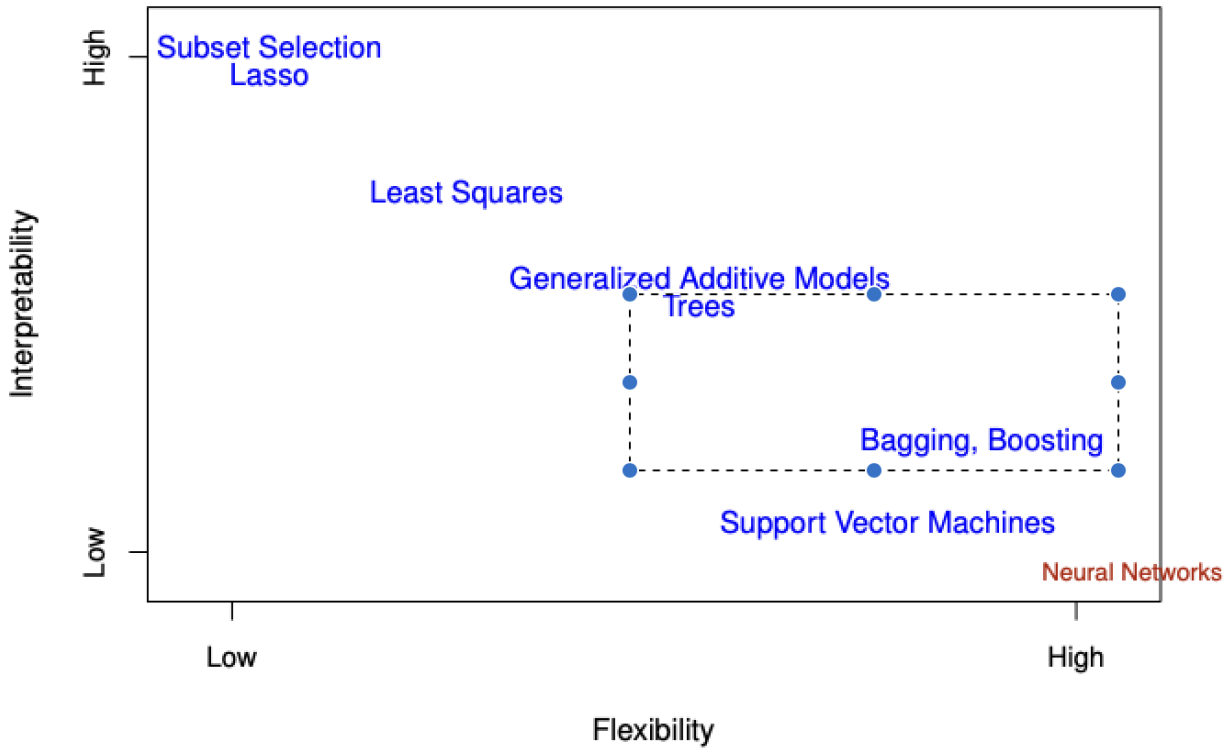
8. Appendix 2: Gradient Boosted Trees (The Workhorse)

Where Are We So Far

So far, we've focused on models with strong global structures, like linear and additive models. We now turn to a more flexible, non-parametric approach that works by partitioning the data into local regions.



Decision Trees for Regression and Classification

A simple class of methods are **tree-based**: the input space is partitioned into simple regions and a constant prediction is assigned to each region.

Definition 1: Tree-Based Model

Partition input space into M disjoint regions $R_1, \ldots, R_M$:

$$f(x) = \sum_{m=1}^{M} c_m \mathbb{I}(x \in R_m),$$

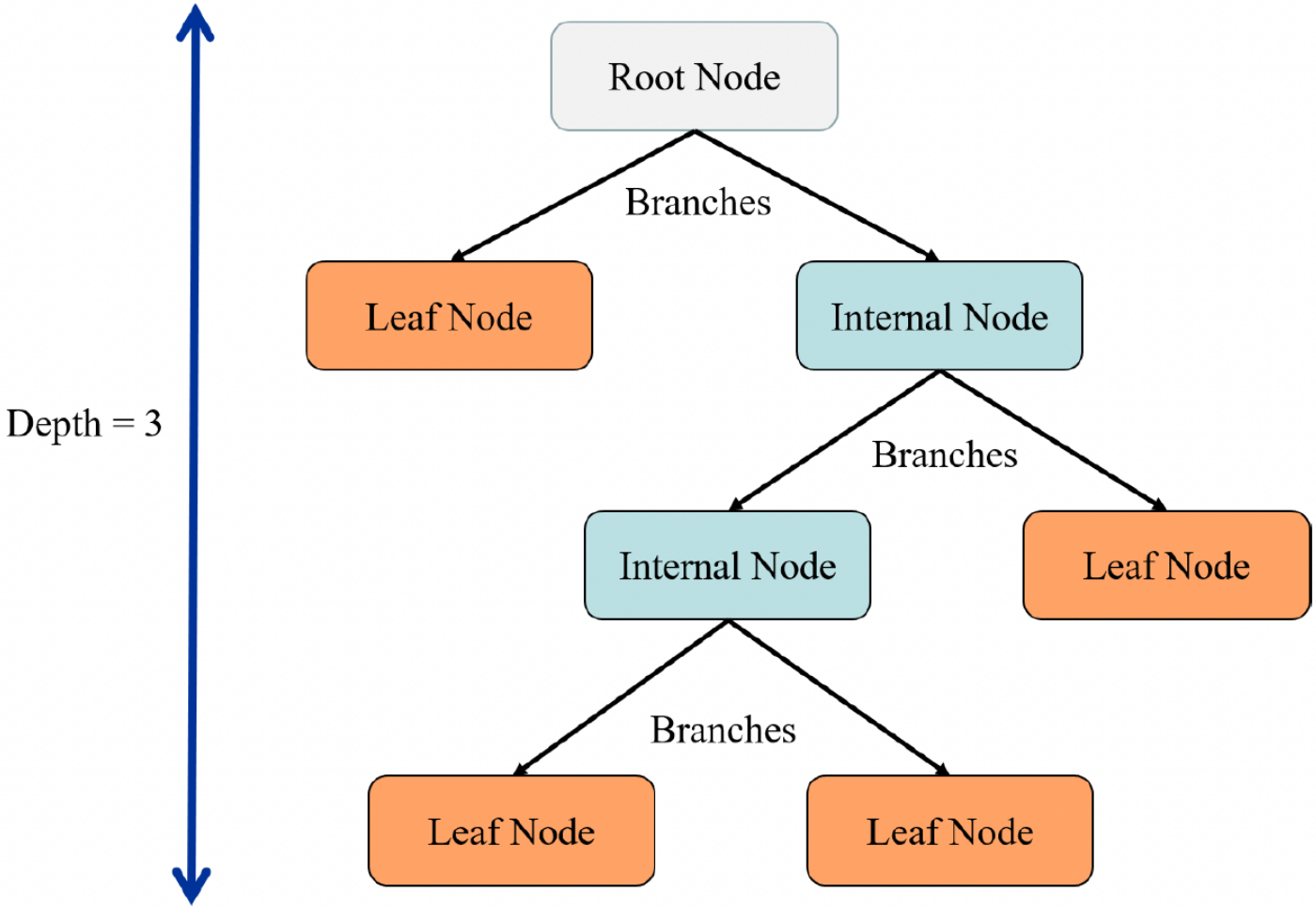
where c_m is the prediction in region R_m.

The c_m is often chosen as $\arg\min_c \sum_{i:x_i \in R_m} \ell(y_i, c)$ for some loss ℓ.

- **Regression:** $\ell(y, c) = (y - c)^2 \quad \Rightarrow \quad c_m = \text{mean}(y_i : x_i \in R_m)$
- **Classification:** $\ell(y, c) = \mathbf{1}\{y \neq c\} \quad \Rightarrow \quad c_m = \text{mode}(y_i : x_i \in R_m)$

Tree-based methods are simple and useful for interpretation. See blackboard for an example (also see the baseball salary data in ISL).

The Structure of a Decision Tree



*Leaf nodes are also called terminal nodes. Picture borrowed from Qianxiao Li's NUS lecture notes (DSA5102/DSA5102X): `https://blog.nus.edu.sg/qianxiaoli/teaching/`.

General Tree-Building Process

- We divide the predictor space — that is, the set of possible values for $X_1, X_2, \ldots, X_p$ — into J distinct and non-overlapping regions, $R_1, R_2, \ldots, R_J$.
- For every observation that falls into the region R_j, we make the same prediction, which is simply the mean of the response values for the training observations in R_j.
- In theory, the regions could have any shape. However, we choose to divide the predictor space into high-dimensional rectangles (boxes), for simplicity and for ease of interpretation of the resulting predictive model.
- For regression, the goal is to find boxes $R_1, \ldots, R_J$ that minimize the RSS, given by

$$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{c}_j)^2,$$

where $\hat{c}_j$ is the mean response for the training observations within the jth box.

Top Down, Greedy Approach to Building Trees

- Unfortunately, it is computationally infeasible to consider every possible partition of the feature space into J boxes.
- For this reason, we take a top-down, greedy approach that is known as **recursive binary splitting**.
- The approach is top-down because it begins at the top of the tree and then successively splits the predictor space; each split is indicated via two new branches further down on the tree.
- It is greedy because at each step of the tree-building process, the best split is made at that particular step, rather than looking ahead and picking a split that will lead to a better tree in some future step.

 Since the set of splitting rules used to segment the predictor space can be summarized in a tree, these types of approaches are known as decision-tree methods. Trees create rectangular partitions through recursive binary splitting, making them naturally interpretable as decision rules.

Building Trees: The Recursive Binary Splitting Process

Definition 2: Binary Split

At each internal node, split data into two regions:

$$R_1(j, s) = \{X : X_j \leq s\} \tag{1}$$
$$R_2(j, s) = \{X : X_j > s\} \tag{2}$$

where j is the splitting variable and s is the split point.

Goal: Find the "best" binary split at each step: select the predictor X_j and the cutpoint s such that splitting the predictor space leads to the greatest reduction in the residual sum of squares (RSS).

Optimization Problem: For regresssion, find (j^*, s^*) that minimizes:

$$\sum_{i:x_i \in R_1(j,s)} (y_i - \hat{c}_1)^2 + \sum_{i:x_i \in R_2(j,s)} (y_i - \hat{c}_2)^2,$$

where $\hat{c}_1, \hat{c}_2$ are the within-region means.

Partitions and CART

Regression and classification models using decision trees are called CART (classification and regression trees).

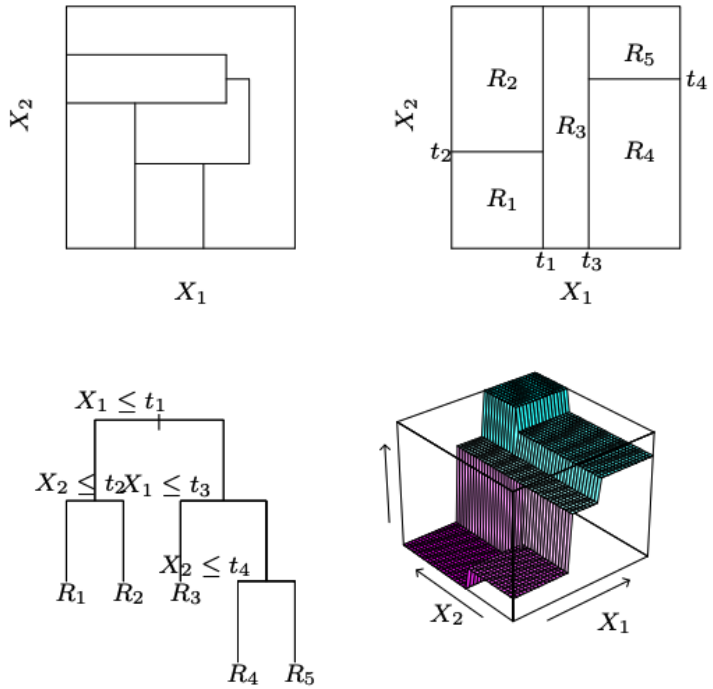


FIGURE 9.2. *Partitions and CART. Top right panel shows a partition of a two-dimensional feature space by recursive binary splitting, as used in CART, applied to some fake data. Top left panel shows a general partition that cannot be obtained from recursive binary splitting. Bottom left panel shows the tree corresponding to the partition in the top right panel, and a perspective plot of the prediction surface appears in the bottom right panel.*

Growing Regression Trees Using a Greedy Approach

CART Algorithm

Input: Training data $\{(x_i, y_i)\}_{i=1}^{N}$, stopping criteria
Initialize: Root node containing all data
for each internal node t **do**
    if stopping criterion not met **then**
        for each variable X_j and split point s **do**
            Define: $t_L = \{x \in t : x_j \leq s\}$, $t_R = \{x \in t : x_j > s\}$
            Compute improvement:

$$\Delta(s, j) = \text{RSS}(t) - \text{RSS}(t_L) - \text{RSS}(t_R)$$

        end for
        Choose: $(s^*, j^*) = \arg\max_{s,j} \Delta(s, j)$
        Split node if $\Delta(s^*, j^*) >$ threshold
    end if
end for

Here, $\text{RSS}(t) = \sum_{x_i \in t}(y_i - \bar{y}_t)^2$, and the stopping criteria could be minimum observations per region, minimum improvement, maximum depth.

The Overfitting Issue

- The process described above may produce good predictions on the training set, but is likely to **overfit** the data, leading to poor test performance (why?).
- A smaller tree with fewer splits (that is, fewer regions $R_1, \ldots, R_J$) might lead to lower variance and better interpretation, at the cost of a little bias.
- One possible alternative to the process described above is to grow the tree only so long as the decrease in the RSS due to each split exceeds some (high) threshold.
- This strategy will result in smaller trees, but is too short-sighted: a seemingly worthless split early on in the tree might be followed by a very good split — i.e., a split that leads to a large reduction in RSS later on.

Pruning a Tree: Regression Case

A better strategy is to grow a very large tree T_0, and then prune it back in order to obtain a subtree. **Cost complexity pruning** (also known as **weakest link pruning**) is used to do this.

- We consider a sequence of trees indexed by a nonnegative tuning parameter α. For each value of α there corresponds a subtree $T \subset T_0$ such that the cost

$$C_\alpha(T) := \sum_{m=1}^{|T|} \sum_{i:x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha|T|$$

  is as small as possible.
- Here $|T|$ indicates the number of terminal nodes of the tree T, R_m is the rectangle (i.e., the subset of predictor space) corresponding to the mth terminal node, and $\hat{y}_{R_m}$ is the mean of the training observations in R_m.
- The tuning parameter α controls a trade-off between the subtree's complexity and its fit to the training data.
- We select an optimal value $\hat{\alpha}$ using cross-validation, then return to the full data set and obtain the subtree corresponding to $\hat{\alpha}$.

Regression Trees: Summary of Algorithm

1. Use recursive binary splitting to grow a large tree on the training data, stopping only when each terminal node has fewer than some minimum number of observations.
2. Apply cost complexity pruning to the large tree in order to obtain a sequence of best subtrees, as a function of α.
3. Use K-fold cross-validation to choose α. For each $k = 1, \ldots, K$:
   - 3.1 Repeat Steps 1 and 2 on the $\frac{K-1}{K}$ fraction of the training data, excluding the kth fold.
   - 3.2 Evaluate the mean squared prediction error on the data in the left-out kth fold, as a function of α.

   Average the results, and pick α to minimize the average error.
4. Return the subtree from Step 2 that corresponds to the chosen value of α.


Revisit the baseball dataset example in ISL.

Classification Trees

- Very similar to a regression tree, except that it is used to predict a **qualitative response** rather than a quantitative one.
- For a classification tree, we predict that each observation belongs to the most commonly occurring class of training observations in the region to which it belongs.
- Just as in the regression setting, we use recursive binary splitting to grow a classification tree, but RSS cannot be used as a criterion for making the binary splits.
- A natural alternative to RSS is the **classification error rate**. This is simply the fraction of the training observations in that region that do not belong to the most common class:

$$E_m = 1 - \max_k(\hat{p}_{mk}),$$

  where $\hat{p}_{mk}$ represents the proportion of training observations in the mth region that are from the kth class.
- However, classification error is not sufficiently sensitive for tree-growing, and in practice two other measures are preferable.

Node Impurity Measures

Node impurity tells us how "mixed up" a node m is in terms of class labels:

1. **Gini Index:** $G_m = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk}) = 1 - \sum_{k=1}^{K} \hat{p}_{mk}^2$
2. **Cross-Entropy (Deviance):** $CE_m = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$

Properties:

- E_m, G_m, CE_m are zero when node is pure (all same class), and are maximum when classes are equally represented: $\hat{p}_{mk} = 1/K$.
- G_m is a measure of total variance across the K classes, and takes on a small value if all of the $\hat{p}_{mk}$'s are close to zero or one.
- That's why the Gini index is also a measure of **node impurity,** with small values indicating high purity (most observations in a single class).
- G_m[1] and CE_m are more sensitive to probability changes than misclassification. They are differentiable (better for optimization) and lead to better intermediate splits during construction.
- Use Gini or entropy for growing; classification error for pruning.

[1] Both G_m and CE_m are surrogates for E_m. In fact, G_m can be interpreted as the expected misclassification error under random assignment according to node proportions (show this).

Tree Pruning: Cost-Complexity Pruning

⚠ Large trees overfit; simple stopping rules are suboptimal.

💡 To overcome this, we usually devise a pruning procedure that involves minimizing a loss function plus a term that penalizes the complexity of a tree.

For subtree $T \subseteq T_0$ (full tree), minimize: $C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha|T|$, where $|T|$ = number of terminal nodes (leaves), N_m = number of observations in node m, $Q_m(T)$ = node impurity, α = complexity parameter.

💡 For any α, there exists a unique smallest subtree T_α minimizing $C_\alpha(T)$.
This means instead of searching over all subtrees, we only need to work with a sequence of nested candidates.

Minimal Cost-Complexity Pruning

1: Grow large tree T_0 using stopping rule (e.g., min 5 obs per node)
2: Compute sequence $T_0 \supset T_1 \supset \ldots \supset \{t_1\}$ by iteratively pruning weakest link
3: For each subtree, estimate generalization error via cross-validation
4: Choose subtree with minimum CV error (or within 1 SE rule)

Understanding Tree Instability

High Variance Problem: Small changes in training data can lead to very different tree structures and predictions.

Sources of instability:

- **Hierarchical Effect:** Errors in early splits propagate throughout tree
- **Greedy Selection:** Locally optimal splits may be globally suboptimal
- **Discrete Splits:** Small data changes can move split points dramatically
- **Hard Boundaries:** Abrupt transitions between regions (see ESL Ch. 9.5 for an alternative method based on probabilistic splits)

Bias-Variance Tradeoff for Trees

- **Low Bias:** Can approximate complex decision boundaries
- **High Variance:** Very sensitive to training data

 Poor generalization despite good training fit! If x is near split point s, small training changes can move x to different sides, causing completely different predictions. MARS is a more stable alternative (see ESL Ch. 9.4).

Overview: From Single Trees to Powerful Ensembles

Decision Trees: The Building Blocks

- Decision trees work by sequentially splitting variables to create rectangular regions in the feature space. Predictions are then made locally within each of these regions.
- They are intuitive, robust to data types, and can be highly interpretable.
- However, in addition to high variance, they generally have lower prediction accuracy on their own and are considered **weak learners**.

Ensembling Methods: The Solution

- This leads to the famous "Boosting Problem" posed by Kearns & Valiant: *Can a set of weak learners*[2] *be combined to create a single strong learner?*
- **Bagging**, **random forests** and **boosting** are methods that achieve this by making predictions based on an ensemble of many trees.
- Bagging and boosting are **general methodologies** and are not limited to just trees, even though that is our focus.

[2] Weak learners perform just slightly better than random chance. In practice, people still prefer to use strong base learners.

Ensembling Methods

Instead of finding one "perfect" model, we combine many "good" models to achieve better performance than any individual model. In fact, we often need both accurate and diverse learners to increase the generalization ability of the ensemble (see Exercise 9.1).

Why ensembles work:

- **Variance Reduction:** Averaging reduces variance without increasing bias.
- **Bias Reduction:** Sequential methods can systematically reduce bias.
- **Improved Stability:** Less sensitive to outliers and data peculiarities.
- **Better Generalization:** Combine different "views" of the data.

Two main approaches:

1. **Parallel:** Create individual learners independently and parallelize the generation process, then combine (bagging, random forest).
2. **Sequential:** Create individual learners with strong correlations and generate the learners sequentially, each learning from the previous one's mistakes (boosting).

Bagging: Bootstrap Aggregating

Bagging is a general-purpose procedure for reducing the variance of a method.

The Bagging Algorithm

1. For $b = 1, \ldots, B$:
   - 1.1 Draw a bootstrap sample $\mathcal{Z}^{*b}$ of size N from the original data (i.e., sampling with replacement).
   - 1.2 Train a model $\hat{f}_b$ on the bootstrap sample $\mathcal{Z}^{*b}$.
2. **Final prediction:** Aggregate the results.
   - Regression: $\hat{f}_{\text{bag}}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}_b(x)$
   - Classification: Take the majority vote

Bagging is most effective for high-variance, low-bias models like fully grown decision trees. Intuitively, bagging is useful because it can be viewed as a smoothing operator (see `https://www.stat.cmu.edu/~larry/=sml/forests.pdf`).

Out-of-Bag (OOB) Error Estimation

- There is a straightforward way to estimate the test error of a bagged model.
- Recall: the key to bagging is that trees are repeatedly fit to bootstrapped subsets of the observations. On average, each bagged tree makes use of about two-thirds of the observations (see Lecture 8).
- Consequently, each bootstrap sample omits about 36.8% of the data. These **out-of-bag (OOB)** samples can be used as a built-in validation set to estimate test error, removing the need for separate cross-validation.
- We can predict the response for the ith observation using each of the trees in which that observation was OOB. This yields around $B/3$ predictions for the ith observation, which we then average.
- This estimate is essentially the leave-one-out (LOO) cross-validation error for bagging, provided B is large.

Why Bagging Works: Variance Reduction

Assume each trained model $\hat{f}_b$ is the approximation of the true function $f^* : \mathbb{R}^d \to \mathbb{R}$:

$$\hat{f}_b(x) = f^*(x) + \epsilon_b(x)$$

where ϵ_b is a random error function with mean 0 and variance $\sigma^2(x)$. The aggregated prediction is $\hat{f}(x) = \frac{1}{B}\sum_{b=1}^{B} \hat{f}_b(x)$.

Averaging reduces variance! If the errors ϵ_b were uncorrelated, the variance of the final prediction would be reduced by a factor of B (see below).

- **Mean Squared Error (MSE) of a single model $\hat{f}_b$:**

$$\mathbb{E}[(f^*(x) - \hat{f}_b(x))^2] = \mathbb{E}[\epsilon_b(x)^2] = \sigma^2(x).$$

- **MSE of the aggregated model $\hat{f}$ (uncorrelated case):**

$$\mathbb{E}[(f^*(x) - \hat{f}(x))^2] = \mathbb{E}\left[\left(\frac{1}{B}\sum_{b=1}^{B}\epsilon_b(x)\right)^2\right] = \frac{1}{B^2}\sum_{b=1}^{B}\mathbb{E}[\epsilon_b(x)^2] = \frac{\sigma^2(x)}{B}.$$

What if $\mathbb{E}[\epsilon_b] \neq 0$? How will this change the bias and variance of MSE?

Why Bagging Isn't Enough: The Correlation Problem

If we average B identically distributed variables Y_b, each with variance σ^2 and positive pairwise correlation ρ, the variance of the average is (Exercise 9.2 (a)):

$$\text{Var}\left(\frac{1}{B}\sum_{b=1}^{B} Y_b\right) = \rho\sigma^2 + \frac{1-\rho}{B}\sigma^2.$$

As B grows, the second term vanishes, but the first term, $\rho\sigma^2$, remains. This correlation limits the variance reduction we can achieve with bagging.

- Bootstrap samples are correlated (all drawn from the same dataset), so the variance reduction is **less than the ideal** $1/B$.
- Bagging **does not reduce bias** — it only reduces variance.
- If the base learner is already stable, bagging provides little benefit (see Exercise 9.2 (b)). Most effective with high-variance, low-bias learners.

To improve on bagging, we need to reduce the correlation ρ between the trees. This is the core idea behind **Random Forests**, which give a small tweak that decorrelates the trees to reduce the variance when we average the trees.

Random Forests: Improving on Bagging

⚠ If the dataset has a very strong predictor, most bagged trees will use it as the top split. This makes the trees look similar and become correlated, which limits the variance reduction from averaging.

Definition 3: The Random Forest Algorithm

The Random Forest algorithm is identical to bagging, with one crucial modification during the training of each tree $\hat{f}_b$:

- **At each candidate split in the tree, randomly select a small subset of $m \ll p$ predictors from the full set of p predictors. Only these m predictors are considered for finding the best split.**

💡 This simple tweak decorrelates the trees without increasing the variance too much. It prevents strong predictors from dominating every tree, forcing the ensemble to explore a more diverse set of predictive rules.

*The Random Forest is one of the best, most popular and easiest to use out-of-the-box classifier. However, it's difficult to develop precise theory since the splitting is done using greedy methods. It is still a mystery why they work so well; see `https://www.stat.cmu.edu/~larry/=sml/forests.pdf`.

Random Forests: The Algorithm

Random Forest (Breiman 2001)

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

Prediction at new point x:

- Regression: $\hat{f}_{rf}^{B}(x) = \frac{1}{B}\sum_{b=1}^{B} T_b(x)$
- Classification: $\hat{C}_{rf}^{B}(x) = \text{majority vote } \{\hat{C}_b(x)\}_{b=1}^{B}$

Key parameters:

- B: Number of trees (larger is usually better, until performance plateaus).
- m: Number of predictors per split (typically, $m \approx \sqrt{p}$ for classification, $m \approx p/3$ for regression).

Random Forest: Variable Importance

Two common methods for measuring a predictor's/feature's importance:

1. Mean Decrease in Impurity (Gini Importance)

- For each predictor/feature j, sum the impurity decrease over all splits in a tree where j was used.
- Average this sum across all trees in the forest.
- **Pros:** Fast to compute.
- **Cons:** Can be biased towards features with high cardinality.

2. Permutation Importance (Preferred Method)

- First, record the baseline OOB error of the trained forest.
- For each feature j: randomly permute (shuffle) the values of feature j in the OOB samples and recompute the OOB error.
- The importance of feature j is the increase in error caused by permuting it.
- **Pros:** More reliable, model-agnostic, and unbiased.

Boosting

- Boosting works similarly to bagging, except that the trees are grown **sequentially** instead of in parallel: each tree is grown using information from previously grown trees.
- Boosting does not involve bootstrap sampling; instead each tree is fit on a modified version of the original dataset.
- Like bagging, boosting is a general approach that can be applied to many statistical learning methods for regression or classification.

The Boosting Strategy In General:

1. Start with equal weights on all training observations.
2. Fit a weak learner to the weighted data.
3. **Increase the weights** on observations that were misclassified.
4. Repeat: each new learner is forced to focus on the "hard" cases.
5. Combine all learners via a weighted vote, **giving more accurate learners weights**.

Boosting Algorithm for Regression Trees

We first discuss boosting for decision trees[3].

Boosting Algorithm for Regression Trees

1. Initialize: set $\hat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set.
2. For $b = 1, 2, \ldots, B$, repeat:
   - 2.1 Fit a regression tree $\hat{f}_b$ with d splits ($d + 1$ terminal nodes) to the training data (X, r).
   - 2.2 Update the current model by adding a shrunken tree:
   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}_b(x).$$
   - 2.3 Update the residuals:
   $$r_i \leftarrow r_i - \lambda \hat{f}_b(x_i).$$
3. Output the boosted model:
$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}_b(x).$$

[3] For a Bayesian approach (BART) to fitting an ensemble of trees, see Ch. 8.2.4 in ISL.

What is the Idea Behind This Procedure?

- Unlike fitting a single large decision tree to the data, which amounts to fitting the data hard and potentially overfitting, the boosting approach instead **learns slowly**.
- Given the current model, we fit a decision tree to the residuals from the model. We then add this new decision tree into the fitted function in order to update the residuals.
- Each of these trees can be rather small, with just a few terminal nodes, determined by the parameter d in the algorithm.
- By fitting small trees to the residuals, we slowly improve $\hat{f}$ in areas where it does not perform well.
- The shrinkage parameter λ slows the process down even further, allowing more and different shaped trees to attack the residuals.

Boosting: Tuning Parameters

- **Number of trees** B: Unlike bagging and random forests, boosting can overfit if B is too large, although this overfitting tends to occur slowly if at all. We use cross-validation to select B.
- **Shrinkage parameter** λ: A small positive number controlling the learning rate. Typical values are 0.01 or 0.001, and the right choice can depend on the problem. Very small λ may require using a very large B to achieve good performance.
- **Number of splits** d **in each tree**: Controls the complexity of the boosted ensemble. Often $d = 1$ works well, in which case each tree is a **stump** (a single split). More generally, d is the *interaction depth*, controlling the maximum interaction order of the boosted model (up to d variables).

 The boosted stump ensemble fits an additive model (more interpretable), since each term involves only a single variable (see Exercise 9.3).

Boosting for Classification: AdaBoost

Boosting for classification is similar in spirit to boosting for regression, but is a bit more complex. Let's consider binary classification with $Y \in \{-1, +1\}$ and weak learners $G_m(x) \in \{-1, +1\}$.

AdaBoost.M1 (Freund-Schapire 1996)

1: **Initialize:** observation weights $w_i^{(1)} = 1/N$ for $i = 1, \ldots, N$.
2: **for** $m = 1$ to M **do**
3: **Fit a weak classifier** $G_m(x)$ to the training data using weights $w_i^{(m)}$.
4: **Compute the weighted error:** $\text{err}_m = \dfrac{\sum_{i=1}^N w_i^{(m)} \mathbb{I}(y_i \neq G_m(x_i))}{\sum_{i=1}^N w_i^{(m)}}$.
5: **Compute the classifier's weight:** $\alpha_m = \log\left(\dfrac{1-\text{err}_m}{\text{err}_m}\right)$.
6: **Update observation weights:**

$$w_i^{(m+1)} = w_i^{(m)} \exp[\alpha_m \mathbb{I}(y_i \neq G_m(x_i))].$$

7: **end for**
8: **Output Final Model:** $G(x) = \text{sign}\left[\sum_{m=1}^M \alpha_m G_m(x)\right]$.

AdaBoost: A Visual Intuition

Much of success of AdaBoost centered around using classification trees as the base learner, where improvements are often most dramatic[4] .

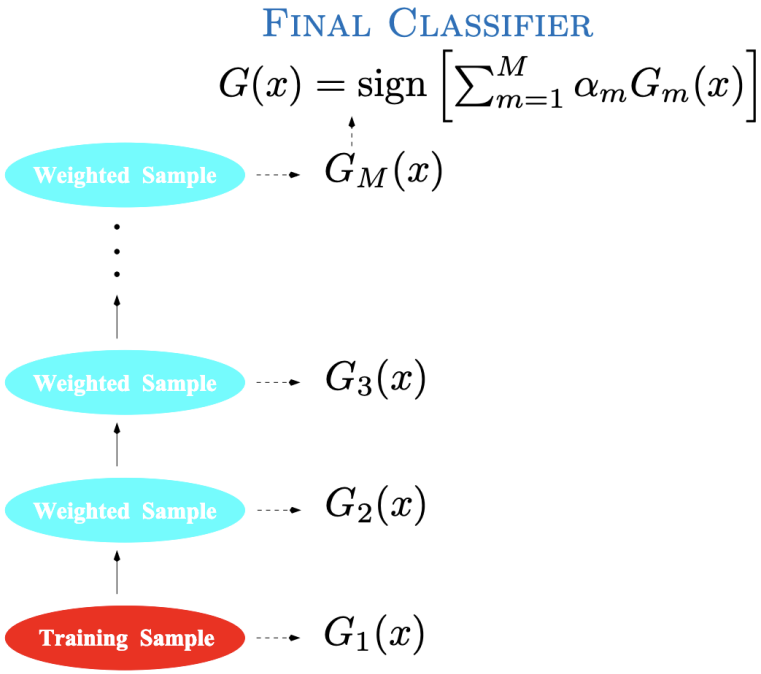


FIGURE 10.1. *Schematic of AdaBoost. Classifiers are trained on weighted versions of the dataset, and then combined to produce a final prediction.*

[4] Breiman called it the best off-the-shelf classifier in the world (in 1996). The training error can be shown to decrease exponentially fast as long as each weak learner is slightly better than random (see `https://www.stat.cmu.edu/~larry/=sml/Boosting.pdf`).

AdaBoost: The Statistical View

AdaBoost is not just a clever algorithm; it is a procedure for minimizing the **exponential loss function** in a stagewise fashion.

- Why minimizing the exponential loss? See Exercise 9.4 for a statistical view.

Exponential Loss

For a binary outcome $y \in \{-1, 1\}$, the exponential loss for a prediction score $f(x)$ is

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

The goal is to find an additive model

$$f(x) = \sum_{m=1}^{M} \alpha_m G_m(x)$$

that minimizes $\sum_{i=1}^{N} \exp(-y_i f(x_i))$.

Stagewise Additive Fitting in AdaBoost

Adaboost can be viewed as sequential minimization of the exponential loss and can be shown to be equivalent to the FSAM below (see blackboard).

Forward Stagewise Additive Modeling (FSAM)

1: **Initialize:** $f_0(x) = 0$.
2: **for** $m = 1$ to M **do**
3: Compute

$$(\beta_m, \gamma_m) = \arg\min_{\beta,\gamma} \sum_{i=1}^{N} L\big(y_i,\ f_{m-1}(x_i) + \beta\, b(x_i;\gamma)\big).$$

4: Update: $f_m(x) = f_{m-1}(x) + \beta_m\, b(x;\gamma_m)$.
5: **end for**

- The AdaBoost steps for finding the best G_m (via minimizing weighted error) and α_m are the solution to this minimization problem.
- **Limitation:** The exponential loss is very sensitive to outliers and mislabeled data points (see loss functions and their robustness in ESL Ch. 10.6).

We have focused on the binary case so far. But how about AdaBoost for multi-class case? See Exercise 9.5.

Boosting Trees: Why Use Trees as Weak Learners

Decision trees are ideal weak learners for boosting because they:

- Handle mixed data types naturally (numerical + categorical).
- Capture complex non-linear interactions automatically.
- Require little data preprocessing: they naturally handle features on different scales and units, which is especially useful in heterogeneous data (e.g., medical records combining blood pressure, age, gender, etc.).
- Are computationally efficient to train.
- Have a tunable complexity (e.g., depth) that provides a good bias-variance trade-off when kept shallow.

 See various details on how we can boost trees in ESL Ch. 10.9-10.12.

 Moreover, decision trees are higly interpretable; see ESL Ch. 10.13-10.14 for some useful interpretability tools and examples.

Ensembling Method Comparison

Combining many weak learners can be more powerful than creating a single, highly complex strong learner.

Aspect	**Boosting**	**Bagging**	**Random Forest**
Construction	Sequential	Parallel	Parallel
Primary Goal	Bias reduction	Variance reduction	Variance reduction & decorrelation
Base Learners	Weak (simple)	Strong (complex)	Strong (complex)
Overfitting Risk	Moderate to High	Low	Very low
Noise Sensitivity	High	Low	Low
Parallelization	Limited	Full	Full
Parameter Tuning	More Complex	Simple	Simple
Performance	Excellent (tabular data)	Good	Very good

 In practice, random forest is a robust and easy-to-use baseline. For maximum performance on structured/tabular data, a well-tuned gradient boosting[5] model often shines. We won't have time to cover gradient boosting (see Appendix for an intro).

[5] Gradient boosting also powers the ranking engines behind Google, Bing, and major e-commerce sites. In ranking, instead of predicting values, boosting optimizes order — e.g., ranking documents for a query. LambdaMART is a natural extension of boosting ideas to ranking problems.

Exercises

Exercise 9

1. **The Accuracy-Diversity Tradeoff in Ensemble Learning.**

   Consider an ensemble of n binary classifiers for a classification problem. Let $E_i \in \{0, 1\}$ be the error indicator for the ith classifier, where $E_i = 1$ if classifier i makes an error ($E_i = 0$ otherwise). Each classifier has individual error rate $\varepsilon := P(E_i = 1) < 1/2$. The ensemble uses majority voting and predicts the class chosen by more than half the classifiers. Denote $S_n = \sum_{i=1}^{n} E_i$ and $\bar{E}_n = S_n/n$.

   (a) Independent Classifiers: Assume E_i independent, so $S_n \sim \text{Binomial}(n, \varepsilon)$. Show that $\mathbb{P}(\bar{E}_n \geq 1/2) = \sum_{k=\lceil n/2 \rceil}^{n} \binom{n}{k} \varepsilon^k (1-\varepsilon)^{n-k}$, and use Hoeffding's inequality (Prop. 1.2 in Bach) to show: $\mathbb{P}(\bar{E}_n \geq 1/2) \leq \exp(-2n(1/2-\varepsilon)^2)$.

   (b) Correlated Classifiers: Assume $\text{Corr}(E_i, E_j) = \rho$ for $i \neq j$.

   Derive $\text{Var}(\bar{E}_n) = \frac{\varepsilon(1-\varepsilon)}{n}[1 + (n-1)\rho]$, and use Chebyshev's inequality (see page 8 in Bach) to bound the majority vote error probability. What happen as $n \to \infty$ when $\rho > 0$?

   (c) Use the above results to explain why effective ensembles require both *individual accuracy* ($\varepsilon < 1/2$) and *diversity* (low ρ).

Exercises

Exercise 9

2. **Understanding Bagging: Error Estimation and Estimator Correlation.**
   (a) Solve Exercise 15.1 in ESL.
   (b) Solve Exercise 15.4 in ESL.
3. **Boosting Using Depth-One Trees.** Solve Exercise 8.4.2 in ISL.
4. **Population Minimizer for the Exponential Loss.** For binary classification with $y \in \{-1, 1\}$, show that the population minimizer for the exponential loss $L(y, f) = \exp(-yf)$ is $f(x) = \frac{1}{2} \log \frac{P(Y=1|x)}{P(Y=-1|x)}$ and deduce the Bayes classifier.
5. **Multiclass Exponential Loss.** Solve Exercise 10.5 in ESL.
6. **[Experimental]**
   (a) **Random Forest Classifiers.** Solve Exercise 15.6 in ESL.
   (b) **AdaBoost with Trees.** Solve Exercise 10.4 in ESL.

Appendix: From AdaBoost to Gradient Boosting

Boosting can be viewed as **gradient descent**[6] **in function space**. Instead of updating parameters, we update our predictor by *adding a new function* (weak learner).

The Gradient Boosting Idea (Friedman, 2001): We want to improve our model f_{m-1} by adding a small function αh. Using a first-order Taylor expansion:

$$L(f_{m-1} + \alpha h) \approx L(f_{m-1}) + \alpha \langle \nabla L(f_{m-1}), h \rangle,$$

with inner product $\langle g, h \rangle := \sum_{i=1}^{N} g(x_i)h(x_i)$. To reduce the loss, we choose h aligned with the **negative gradient**.

This gives the **pseudo-residuals**:

$$r_{im} = - \left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)} \right]_{f=f_{m-1}}.$$

We then fit a weak learner h_m to $\{(x_i, r_{im})\}$, the functional analogue of taking a gradient step. That's why the method is called gradient descent in function space.

[6] We will see gradient descent in the next lecture on neural networks.

Common Loss Functions and The Generic Algorithm

This idea generalizes boosting to **any differentiable loss function**. We have already seen that AdaBoost corresponds to gradient descent on exponetial loss.

- **Squared Loss:** $L(y, f) = \frac{1}{2}(y - f)^2 \implies r_i = y_i - f(x_i)$ (ordinary residuals!)
- **Absolute Loss:** $L(y, f) = |y - f| \implies r_i = \text{sign}(y_i - f(x_i))$
- **Huber Loss:** Robust combination of squared and absolute loss.
- **Logistic/Bernoulli (labels $y \in \{0, 1\}$, $f = \text{logit}(p)$):** $L(y, f) = \log(1 + \exp(-f))$ if $y = 1$ and $\log(1 + \exp(f))$ if $y = 0$, with $p = \sigma(f)$. Then $r_i = y_i - p_i$.

Generic Gradient Boosting (Friedman 2001)

1: **Initialize:** $f_0(x) = \arg\min_\gamma \sum_{i=1}^N L(y_i, \gamma)$
2: **for** $m = 1$ to M **do**
3: **Compute pseudo-residuals:** $r_{im} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f=f_{m-1}}$
4: **Fit weak learner:** Fit $h_m(x)$ to $\{(x_i, r_{im})\}_{i=1}^N$.
5: **Line search (step size):** $\rho_m = \arg\min_\rho \sum_{i=1}^N L(y_i, f_{m-1}(x_i) + \rho\, h_m(x_i))$
6: **Update:** $f_m(x) = f_{m-1}(x) + \nu\, \rho_m\, h_m(x)$
7: **end for**

Schapire & Singer (1999) introduced **AnyBoost**, a general framework showing that AdaBoost, Gradient Boosting, and many other variants are all special cases of functional gradient descent.

Gradient Tree Boosting: The Algorithm

Gradient boosting with regression trees as weak learners is often called Gradient Boosted Regression Trees (GBRT).

Gradient Tree Boosting

1: **Initialize:** $f_0(x) = \arg\min_\gamma \sum_{i=1}^N L(y_i, \gamma)$
2: **for** $m = 1$ to M **do**
3: **Compute pseudo-residuals:** $r_{im} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f=f_{m-1}}$
4: **Fit a regression tree** T_m to the pseudo-residuals $\{(x_i, r_{im})\}_{i=1}^N$.
5: The tree produces terminal regions (leaves) $R_{jm}, j = 1, \ldots, J_m$.
6: **for** $j = 1$ to J_m **do**
7: **Optimize leaf values:**
Find the optimal constant update γ_{jm} for each leaf by solving a simple 1D optimization problem: $\gamma_{jm} = \arg\min_\gamma \sum_{x_i \in R_{jm}} L(y_i, f_{m-1}(x_i) + \gamma)$
8: **end for**
9: **Update model:** $f_m(x) = f_{m-1}(x) + \nu \sum_{j=1}^{J_m} \gamma_{jm} \mathbb{I}(x \in R_{jm})$
10: **end for**
11: **Output:** $\hat{f}(x) = f_M(x)$

The learning rate ν (shrinkage) is a crucial regularization parameter.

Tuning and Regularization

1. Key Hyperparameters

- **Number of Trees (M):** Controls model complexity. Best set via **early stopping** on a validation set.
- **Learning Rate / Shrinkage (ν):** Scales the contribution of each tree. Smaller ν (e.g., 0.01-0.1) requires larger M but often leads to better generalization.
- **Tree Depth (J):** Controls the maximum level of feature interactions. Depths of 4-8 are common.

2. Advanced Regularization Techniques

- **Stochastic Gradient Boosting (Subsampling):** At each iteration, train the tree on a random subsample (e.g., 50-80%) of the data. This reduces overfitting and speeds up computation.
- **Feature Subsampling:** At each tree or each split, consider only a random subset of features to further reduce variance.

Key Takeaways

Combining many weak learners can be more powerful than creating a single, highly complex strong learner.

- **Bagging & Random Forest:** A parallel combination of models that reduces variance by averaging.
- **Boosting (AdaBoost & Gradient Bossting):** A sequential combination of models that reduces bias by focusing on errors.

 We only have time to introduce how these methods work. To understand them deeper, see Ch. 10 in Bach.

Practical Guidance:

- Use **Random Forest** for robustness, ease of use, and a strong baseline.
- Use **Gradient Boosting** for maximum predictive accuracy, especially on tabular data, but be prepared to tune hyperparameters carefully. Always use a validation set and early stopping when training boosting models.
- **Gradient Boosted Trees are among the strongest supervised learners.** Modern implementations like *XGBoost*[7] and *LightGBM*[8] make them fast, regularized, and scalable.

[7] `https://xgboost.readthedocs.io/en/stable/`.
[8] `https://lightgbm.readthedocs.io/en/stable/`