Part I

The basics of ensembles

Chapter 1

Ensemble methods: Hype or hallelujah?

1.1 Fit vs. complexity in individual models

Regression with support vector machines

Specifically, SVM training tries to find a model to minimize:

$$regularization + C * loss \tag{1.1}$$

The regularization term measures the flatness of the model: the more it is minimized, the more linear and less complex the learned model is. The loss term measures the fit to the training data through a *loss function* (typically, MSE): the more it is minimized, the better the fit to the training data. The *regularization* parameter C trades off between these two competing objectives:

- A small value of C means the model will focus more on regularization and simplicity, and less on training error, which causes the model to have higher training error and underfit.
- A large value of C means the model will focus more on training error and learn more complex models, which causes the model to have lower training errors and possibly overfit.

Every machine-learning algorithm, in fact, exhibits this behavior:

- Overly simple models tend to not fit the training data properly and tend to generalize poorly on future data; a model that is performing poorly on training and test data is underfitting.
- Overly complex models can achieve very low training errors but tend to generalize poorly on future data too; a model that is performing very well on training data, but poorly on test data is overfitting.
- The best models trade off between complexity and fit, sacrificing a little bit of each during training so that they can generalize most effectively when deployed.

What we've informally discussed so far as the fit versus complexity tradeoff is more formally known as the bias-variance tradeoff. The bias of a model is the error arising from the effect of modeling assumptions (such as a preference for simpler models). The variance of a model is the error arising from sensitivity to small variations in the data set.
Highly complex models (low bias) will overfit the data and be more sensitive to noise (high variance), while simpler models (high bias) will underfit the data and be less sensitive to noise (low variance). This tradeoff is inherent in every machine-learning algorithm. Ensemble methods seek to overcome this problem by combining several low-bias models to reduce their variance or combining several low-variance models to reduce their bias.

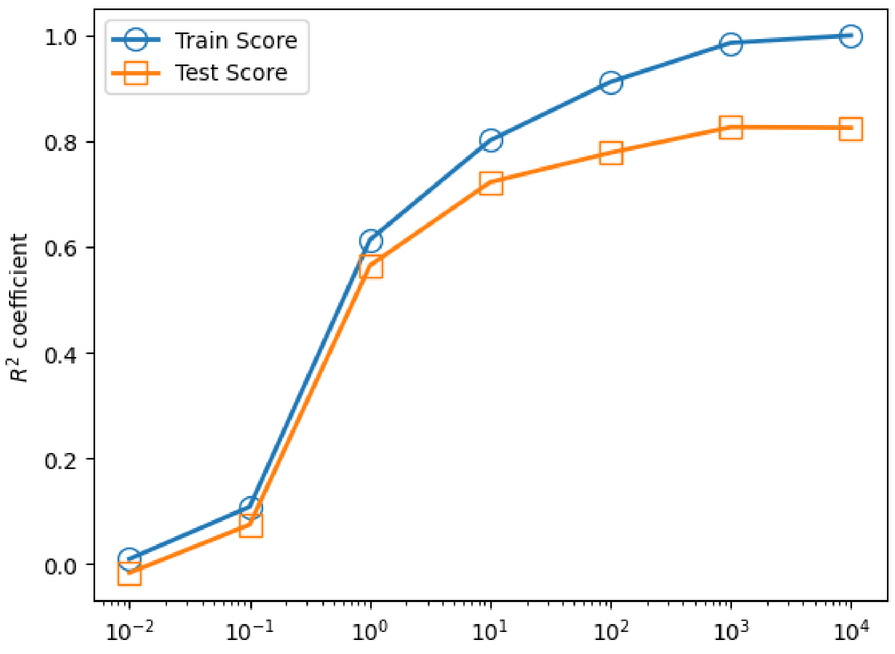


Figure 1.1: Comparing SVM regressors of different complexities on the Friedman-1 regression data set using R^2 as the evaluation metric. As with decision trees, highly complex models (corresponding to higher C values) appear to achieve fantastic fit on the training data, but they don't actually generalize as well. This means that as C increases, so does the possibility of overfitting.

1.2 Our first ensemble

We train a set of *base estimators* (also known as *base learners*) using diverse base-learning algorithms on the same data set. That is, **we count on the significant variations in each learning algorithm to produce a diverse set of base estimators.**

1.3 Terminology and taxonomy for ensemble methods

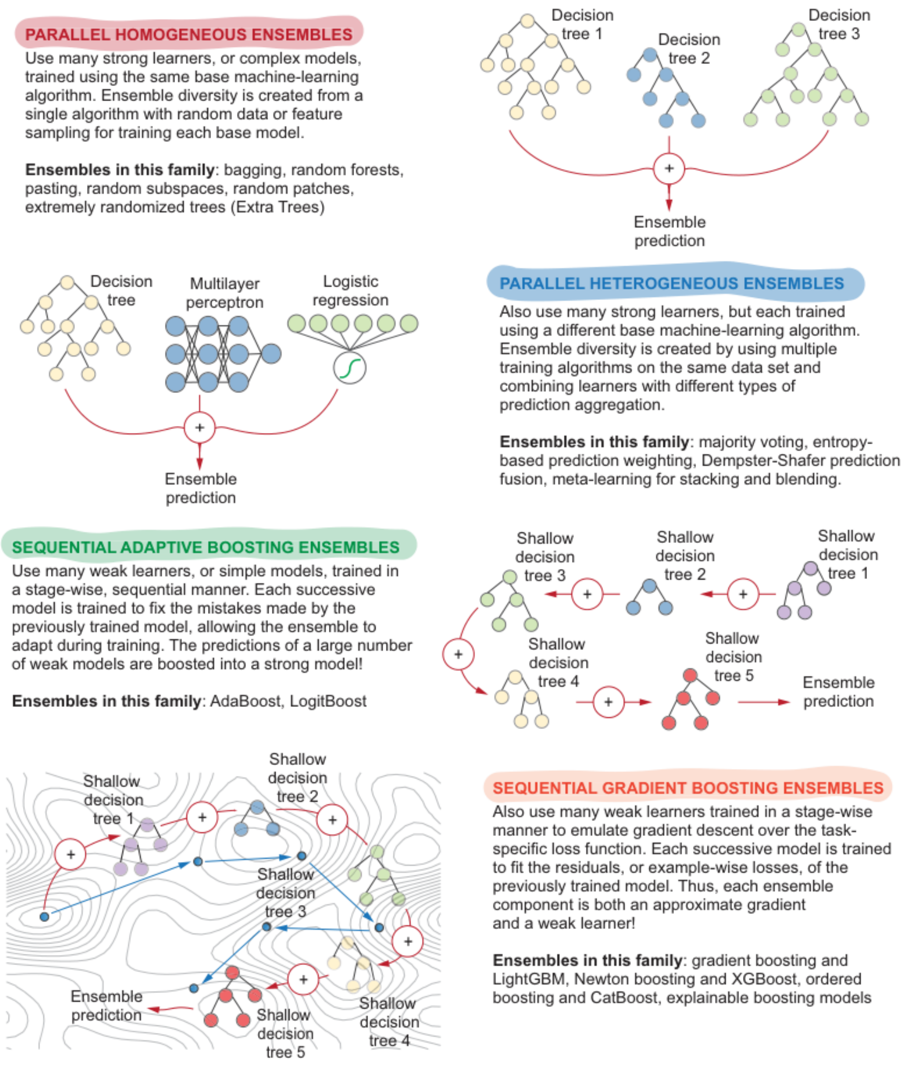
All ensembles are composed of individual machine-learning models called base models, base learners, or base estimators (these terms are used interchangeably throughout the book) and are trained using base machine-learning algorithms. Base models are often described in terms of their complexity. Base models that are sufficiently complex (e.g., a deep decision tree) and have "good" prediction performance (e.g., accuracy over 80% for a binary classification task) are typically known as strong learners or strong models.

In contrast, base models that are pretty simple (e.g., a shallow decision tree) and achieve barely acceptable performance (e.g., accuracy around 51% for a binary classi- fication task) are known as weak learners or weak models. More formally, a weak learner only has to do slightly better than random chance, or 50% for a binary classification task.

More broadly, ensemble methods can be classified into two types depending on how they are trained: **parallel** and **sequential ensembles**.

Parallel ensemble methods, as the name suggests, train each component base model *independently* of the others, which means that they can be trained in parallel. Parallel ensembles are often constructed out of strong learners and can further be categorized into the following:

- **Homogeneous parallel ensembles**—All the base learners are of the same type (e.g., all decision trees) and trained using the same base-learning algorithm. Several well-known ensemble methods, such as bagging, random forests, and extremely randomized trees (Extra Trees), are parallel ensemble methods.



PARALLEL HOMOGENEOUS ENSEMBLES

Use many strong learners, or complex models, trained using the same base machine-learning algorithm. Ensemble diversity is created from a single algorithm with random data or feature sampling for training each base model.

Ensembles in this family: bagging, random forests, pasting, random subspaces, random patches, extremely randomized trees (Extra Trees)

PARALLEL HETEROGENEOUS ENSEMBLES

Also use many strong learners, but each trained using a different base machine-learning algorithm. Ensemble diversity is created by using multiple training algorithms on the same data set and combining learners with different types of prediction aggregation.

Ensembles in this family: majority voting, entropy-based prediction weighting, Dempster-Shafer prediction fusion, meta-learning for stacking and blending.

SEQUENTIAL ADAPTIVE BOOSTING ENSEMBLES

Use many weak learners, or simple models, trained in a stage-wise, sequential manner. Each successive model is trained to fix the mistakes made by the previously trained model, allowing the ensemble to adapt during training. The predictions of a large number of weak models are boosted into a strong model!

Ensembles in this family: AdaBoost, LogitBoost

SEQUENTIAL GRADIENT BOOSTING ENSEMBLES

Also use many weak learners trained in a stage-wise manner to emulate gradient descent over the task-specific loss function. Each successive model is trained to fit the residuals, or example-wise losses, of the previously trained model. Thus, each ensemble component is both an approximate gradient and a weak learner!

Ensembles in this family: gradient boosting and LightGBM, Newton boosting and XGBoost, ordered boosting and CatBoost, explainable boosting models

Figure 1.2: A taxonomy of ensemble methods

- **Heterogeneous parallel ensembles**—The base learners are trained using different base-learning algorithms. Meta-learning by stacking is a well-known exemplar of this type of ensembling technique.

Sequential ensemble methods, unlike parallel ensemble methods, exploit the dependence of base learners. More specifically, during training, sequential ensembles train a new base learner in such **a manner that it minimizes mistakes made by the base learner trained in the previous step.** These methods construct ensembles sequentially in stages and often use weak learners as base models. They can also be further categorized into the following:

- **Adaptive boosting ensembles**—Also called vanilla boosting, these ensembles train successive base learners by reweighting examples adaptively to fix mistakes in previous iterations. AdaBoost, the granddaddy of all the boosting methods, is an example of this type of ensemble method.
- **Gradient-boosting ensembles**—These ensembles extend and generalize the idea of adaptive boosting and aim to mimic gradient descent, which is often used under the hood to actually train machine-learning models. Some of the most powerful modern ensemble learning packages implement some form of gradient boosting (LightGBM), Newton boosting (XGBoost), or ordered boosting (CatBoost).

1.4 Summary

- Ensemble learning aims to improve predictive performance by training multi- ple models and combining them into a meta-estimator. The component models of an ensemble are called base estimators or base learners.
- Ensemble methods use the power of "the wisdom of crowds," which relies on the principle that the collective opinion of a group is more effective than any single individual in the group.
- Ensemble methods are widely used in several application areas, including finan- cial and business analytics, medicine and health care, cybersecurity, education, manufacturing, recommendation systems, entertainment, and many more.
- Most machine-learning algorithms contend with a fit versus complexity (also called bias-variance) tradeoff, which affects their ability to generalize well to future data. Ensemble methods use multiple component models to overcome this tradeoff.
- An effective ensemble requires two key ingredients: (1) ensemble diversity and (2) model aggregation for the final predictions.