Data Mining
Bagging and Random Forests

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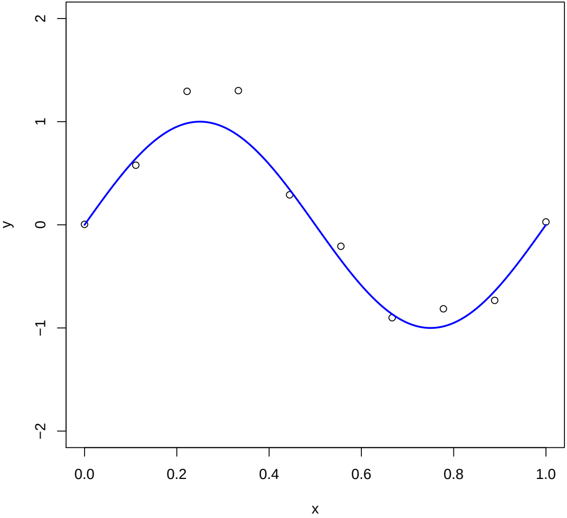
Introduction

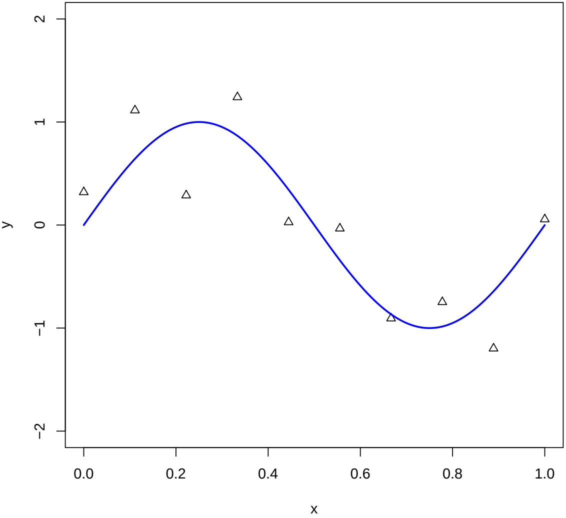
- Bad news: single trees are usually not among the top predictors.
- Good news: *ensembles* or *committees* of trees typically perform much better.
- Why does averaging the predictions of multiple trees help to reduce error?
- To answer this question we first study the bias-variance decomposition of prediction error.

Sample 1 and the True Regression Function



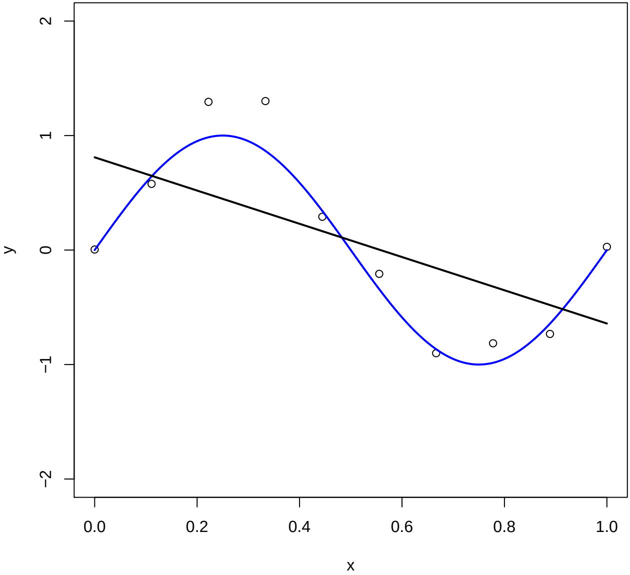
$f(x) = \sin(2\pi x)$ $\qquad$ $y_i = f(x_i) + \varepsilon_i$ with $\varepsilon_i \sim N(0, \sigma = 0.3)$

Sample 2 and the True Regression Function

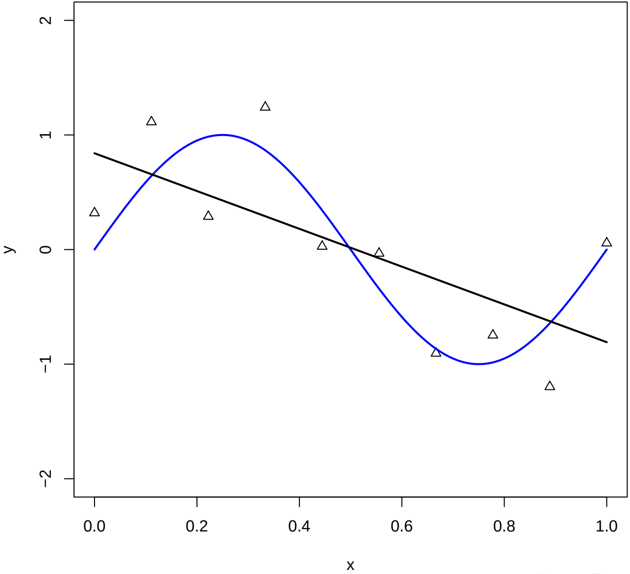


$f(x) = \sin(2\pi x)$ $\qquad$ $y_i = f(x_i) + \varepsilon_i$ with $\varepsilon_i \sim N(0, \sigma = 0.3)$

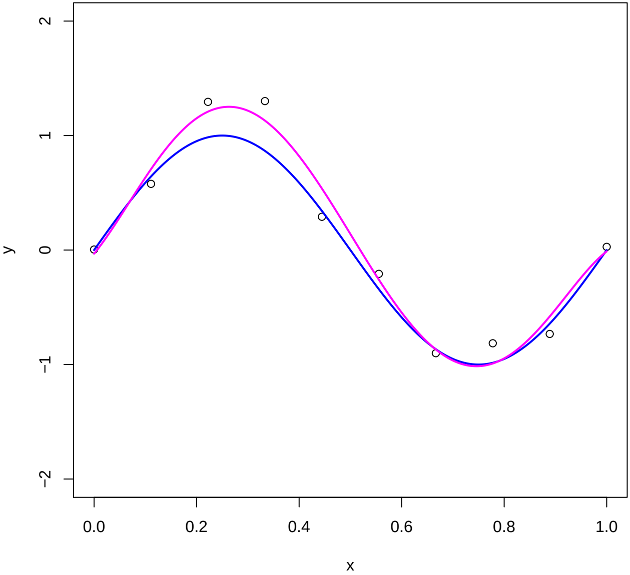
Linear Fit on Sample 1



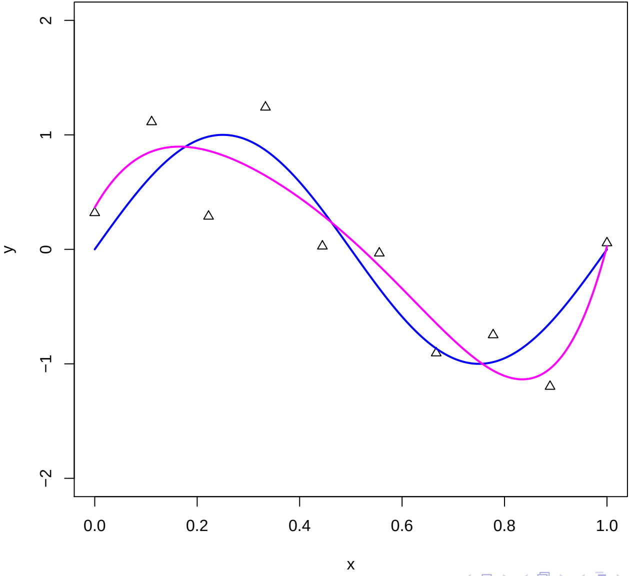
Linear Fit on Sample 2



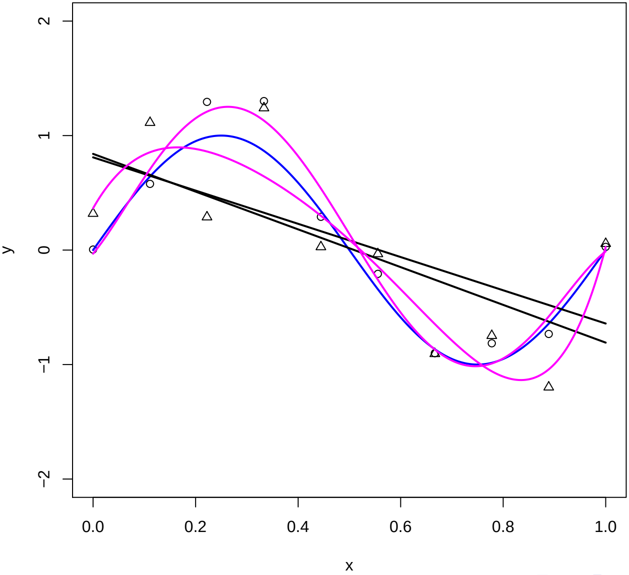
Polynomial of Degree 5 on Sample 1



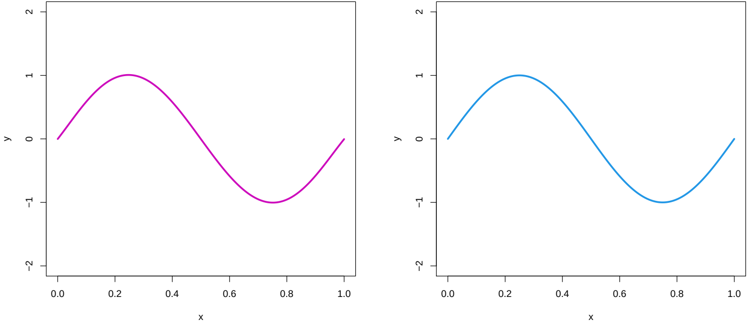
Polynomial of Degree 5 on Sample 2



All Together Now

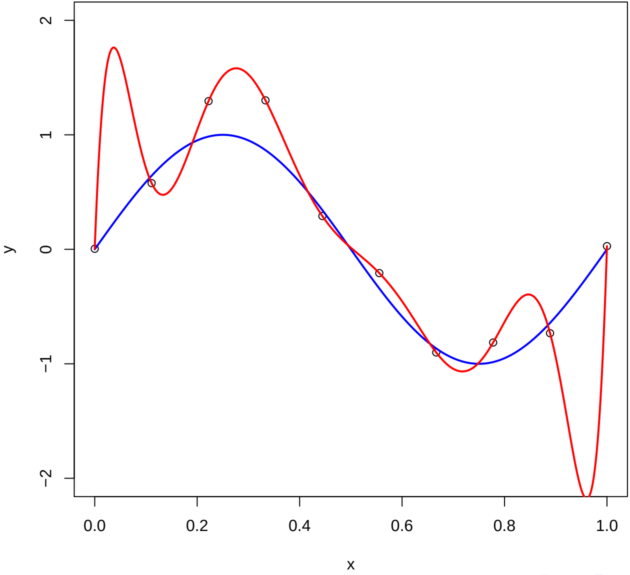


Average of degree 5 polynomials

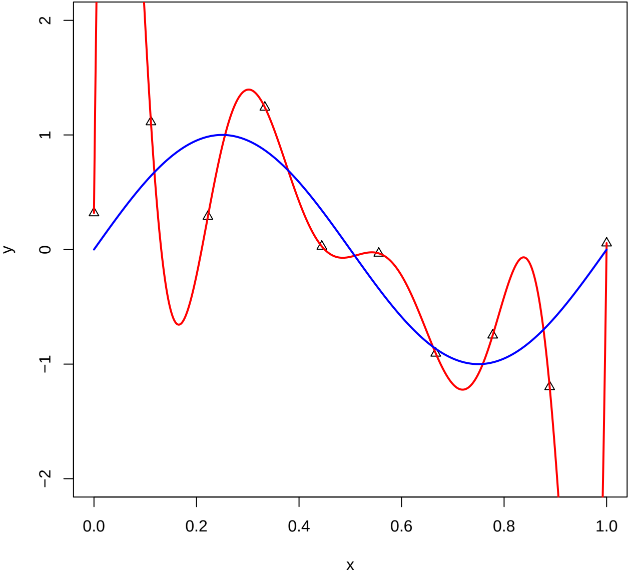


Average predictions of degree 5 polynomials estimated on 10,000 samples of size 10 (on the left), and $\sin(2\pi x)$ (on the right).
Can you see the difference?

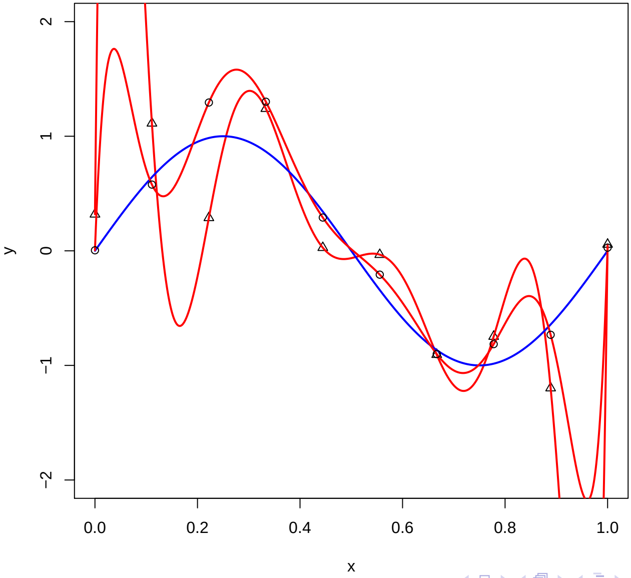
Polynomial of Degree 9 on Sample 1



Polynomial of Degree 9 on Sample 2



A High Variance Predictor!



Reducible and Irreducible Error

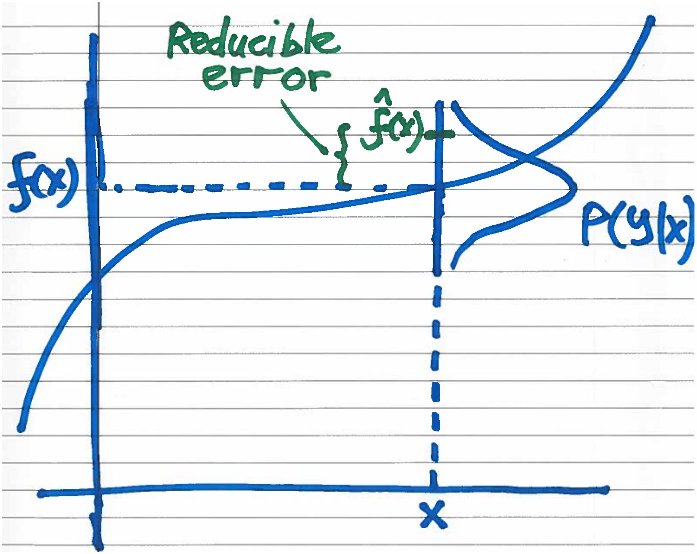
Consider a model created by an algorithm on a single data set, sampled from some population. What is the mean squared prediction error of this model on the population? For simplicity, we restrict our analysis to some fixed point x.

$$\begin{aligned}\mathbb{E}_{P(Y\mid x)}\left[(Y-\hat{f}(x))^2\right] &= (f(x)-\hat{f}(x))^2 && \text{(Reducible Error)}\\ &+\mathbb{E}_{P(Y\mid x)}\left[(Y-f(x))^2\right], && \text{(Irreducible Error)}\end{aligned}$$

where $f(x) \equiv \mathbb{E}[Y \mid x]$ is the true (population) regression function, and the expectation is taken with respect to $P(Y \mid x)$. $\hat{f}(x)$ is the model prediction at x.

The irreducible error is the error of the best possible prediction (which is $f(x) \equiv \mathbb{E}[Y \mid x]$), and is equal to the variance of Y around the regression line at the point x.

Reducible and Irreducible Error



Bias-Variance Decomposition of Estimation Error

Now let's focus on reducible error.

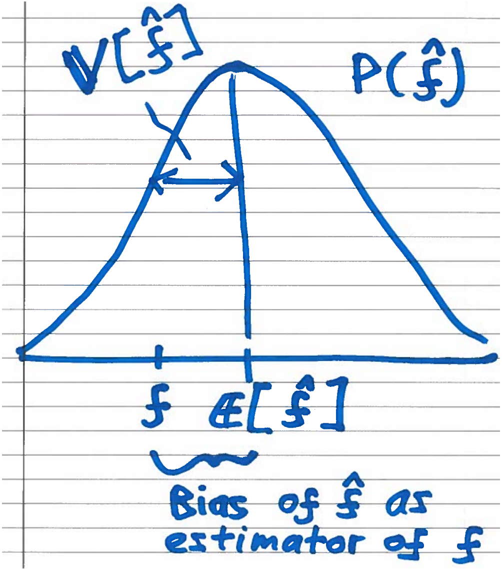
Consider the collection of models created by an algorithm on different data sets, sampled from the same population. We use each sample to estimate $f(x)$. What is the mean squared estimation error of these models?

$$\begin{aligned} \mathbb{E}_D\left[(f(x)-\hat{f}(x))^2\right] &= (f(x)-\mathbb{E}_D[\hat{f}(x)])^2 && \text{(Squared Bias)} \\ &+ \mathbb{E}_D\left[(\hat{f}(x)-\mathbb{E}_D[\hat{f}(x)])^2\right] && \text{(Variance)} \end{aligned}$$

where expectation is taken with respect to repeated sampling from the same population.

$$\boxed{\text{Mean Squared Error} = \text{Squared Bias} + \text{Variance}}$$

Bias and Variance of $\hat{f}$ as estimator of f



Bias-Variance Decomposition

Some observations:

- Simple (inflexible) models tend to have high bias and low variance.
- Complex (flexible) models tend to have low bias and high variance.
- As sample size increases, variance goes down, but bias doesn't.
- Hence, we can afford to fit more complex models if the data set is large.
- In practice, we have to find the right trade-off between bias and variance in order to get small prediction error.

Reducing Variance by Bagging

- Classification trees are high variance classifiers.
- Variance can be reduced by averaging.
- Average how?
- Bootstrapping!

Reducing Variance by Bagging

Bagging is short for Bootstrap Aggregating.

Training:

1. Draw a sample *with replacement* from the training set.
   The sample should be of the same size as the training set.
2. Grow a tree on this bootstrap sample (pruning not necessary).
3. Repeat these steps M times to create M different trees.

Prediction:

1. Predict on a test sample using each of the M trees in turn.
2. Take the majority vote of the M predictions as the final prediction.

Reducing Variance by Bagging

For regression problems, generate M bootstrap samples, and combine the predictions by averaging:

$$\hat{f}_{\mathrm{BAG}}(x) = \frac{1}{M} \sum_{m=1}^{M} \hat{f}_m(x),$$

where $\hat{f}_m(x)$ is the prediction of the model trained on the $m - th$ bootstrap sample.

Notice that we never actually average *models*, we average their *predictions*.

Reducing Variance by Bagging

The true regression function is $f(x)$, so the output of each model can be written as the true value plus an error term in the form:

$$\hat{f}_m(x) = f(x) + e_m(x)$$
$$e_m(x) = \hat{f}_m(x) - f(x)$$

The expected squared error of the $m-th$ model then becomes

$$\mathbb{E}_{P(x)}\left[(\hat{f}_m(x) - f(x))^2\right] = \mathbb{E}_{P(x)}\left[e_m(x)^2\right],$$

where the expectation is taken with respect to the distribution of x.

Note: the models $\hat{f}_m$ are fixed now!

Reducing Variance by Bagging

The average error made by the models acting individually is therefore:

$$E_{\mathrm{AV}} = \frac{1}{M} \sum_{m=1}^{M} \mathbb{E}_{P(x)} \left[e_m(x)^2 \right]$$

Similarly, the expected error of the committee is given by

$$\begin{aligned} E_{\mathrm{BAG}} &= \mathbb{E}_{P(x)} \left[\left(\frac{1}{M} \sum_{m=1}^{M} \hat{f}_m(x) - f(x) \right)^2 \right] \\ &= \mathbb{E}_{P(x)} \left[\left(\frac{1}{M} \sum_{m=1}^{M} e_m(x) \right)^2 \right] = \frac{1}{M^2} \mathbb{E}_{P(x)} \left[\left(\sum_{m=1}^{M} e_m(x) \right)^2 \right] \end{aligned}$$

Reducing Variance by Bagging

If we assume that the errors have zero mean and are uncorrelated, so that:

$$\mathbb{E}_{P(x)}\left[e_m(x)e_n(x)\right] = 0, \text{ for all } m \neq n,$$

then we obtain

$$E_{\mathrm{BAG}} = \frac{1}{M^2}\sum_{m=1}^{M}\mathbb{E}_{P(x)}\left[e_m(x)^2\right] = \frac{1}{M}E_{\mathrm{AV}}$$

This is a sensational reduction!

In practice, the errors of individual models tend to be positively correlated, and the reduction in overall error tends to be much smaller than suggested by this formula.

Random Forests

- Random forests can be regarded as an attempt to “de-correlate” the predictions of the individual trees, so

  $$\mathbb{E}_{P(x)}\left[e_m(x)e_n(x)\right]$$

  is closer to zero.
- Each time we have to determine the best split in a node, we first randomly select a subset of the features.
- The size of this subset is a hyper-parameter of the random forest algorithm.
- We then determine the best split on this random subset of features, and perform that split.
- Otherwise, the procedure is identical to that described for bagging.