Data Mining
Bagging and Random Forests

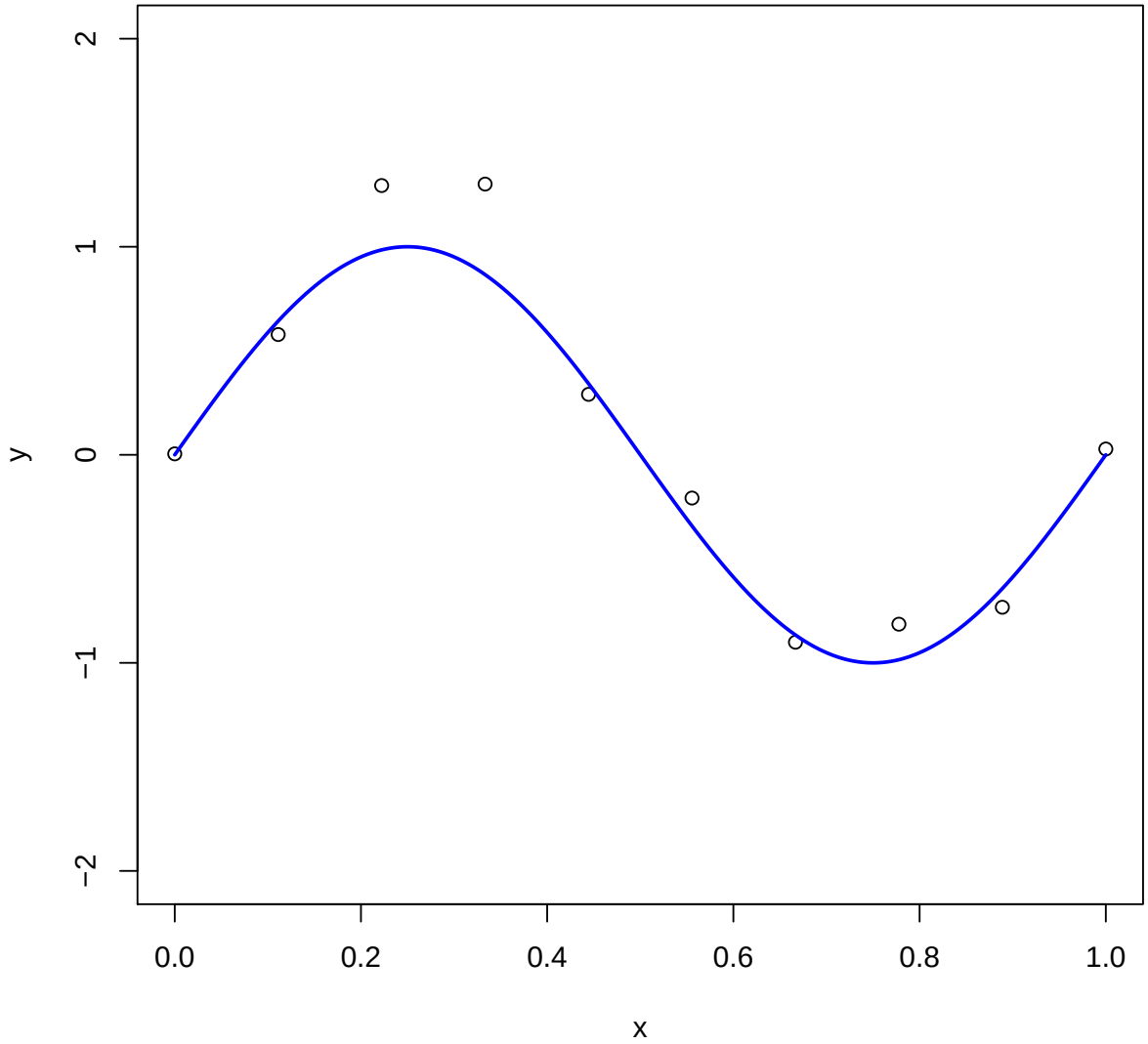
Ad Feelders

Universiteit Utrecht

Introduction

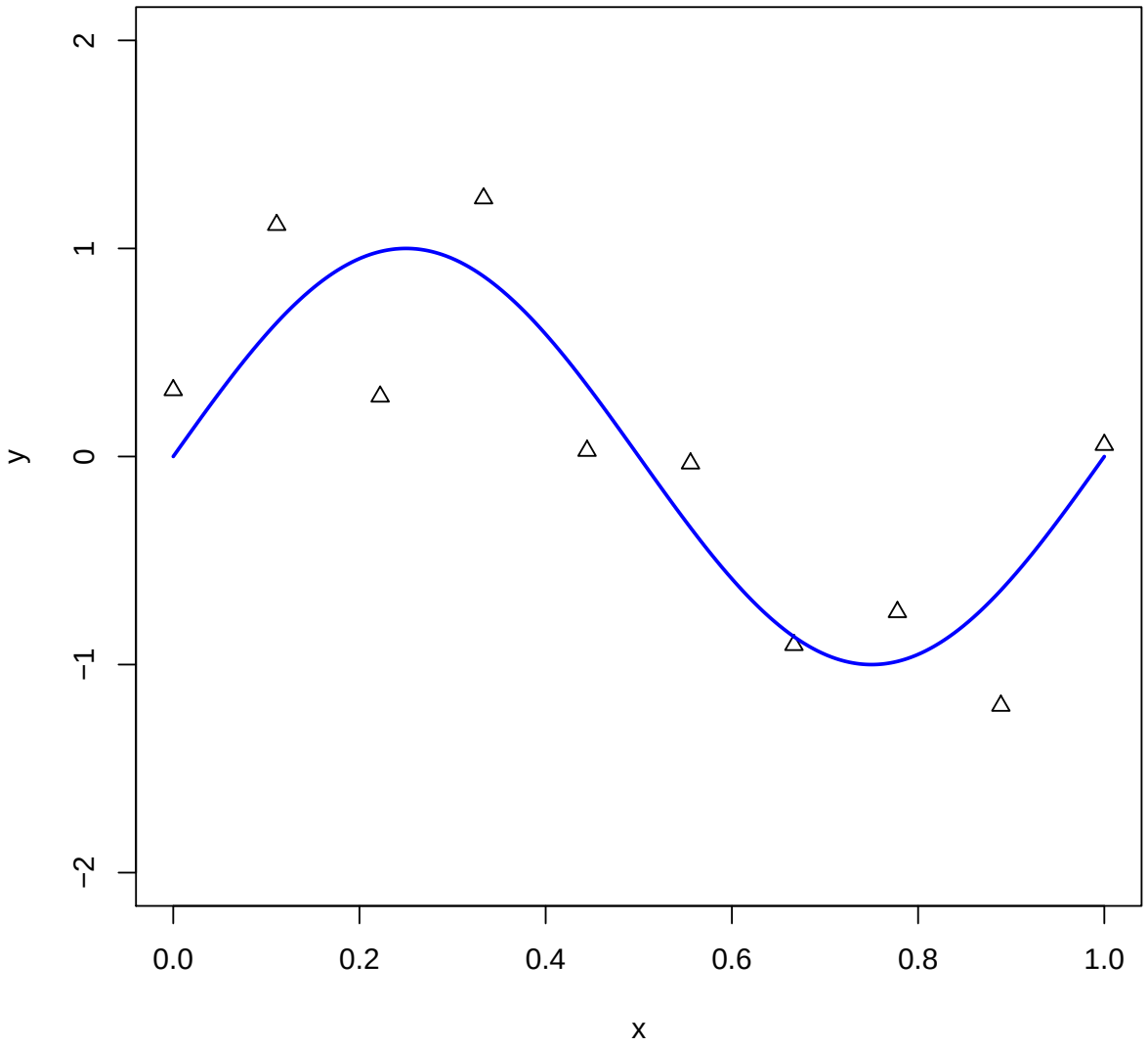
- Bad news: single trees are usually not among the top predictors.
- Good news: *ensembles* (集成模型) or *committees* (委員會（模型群體）) of trees typically perform much better.
- Why does averaging the predictions of multiple trees help to reduce error?
- To answer this question we first study the bias (偏差)-variance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

Sample 1 and the True Regression Function



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

Sample 2 and the True Regression Function



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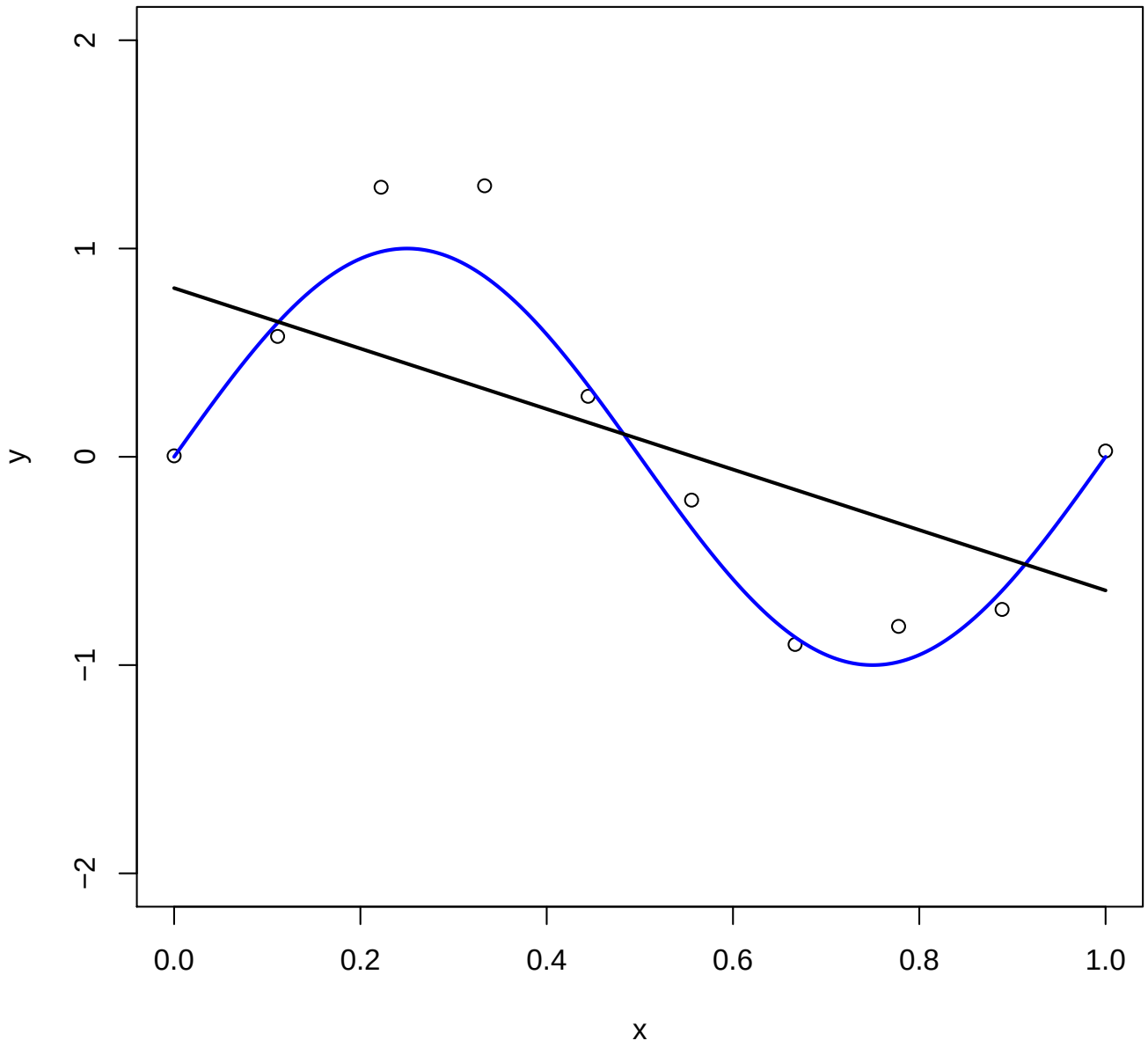
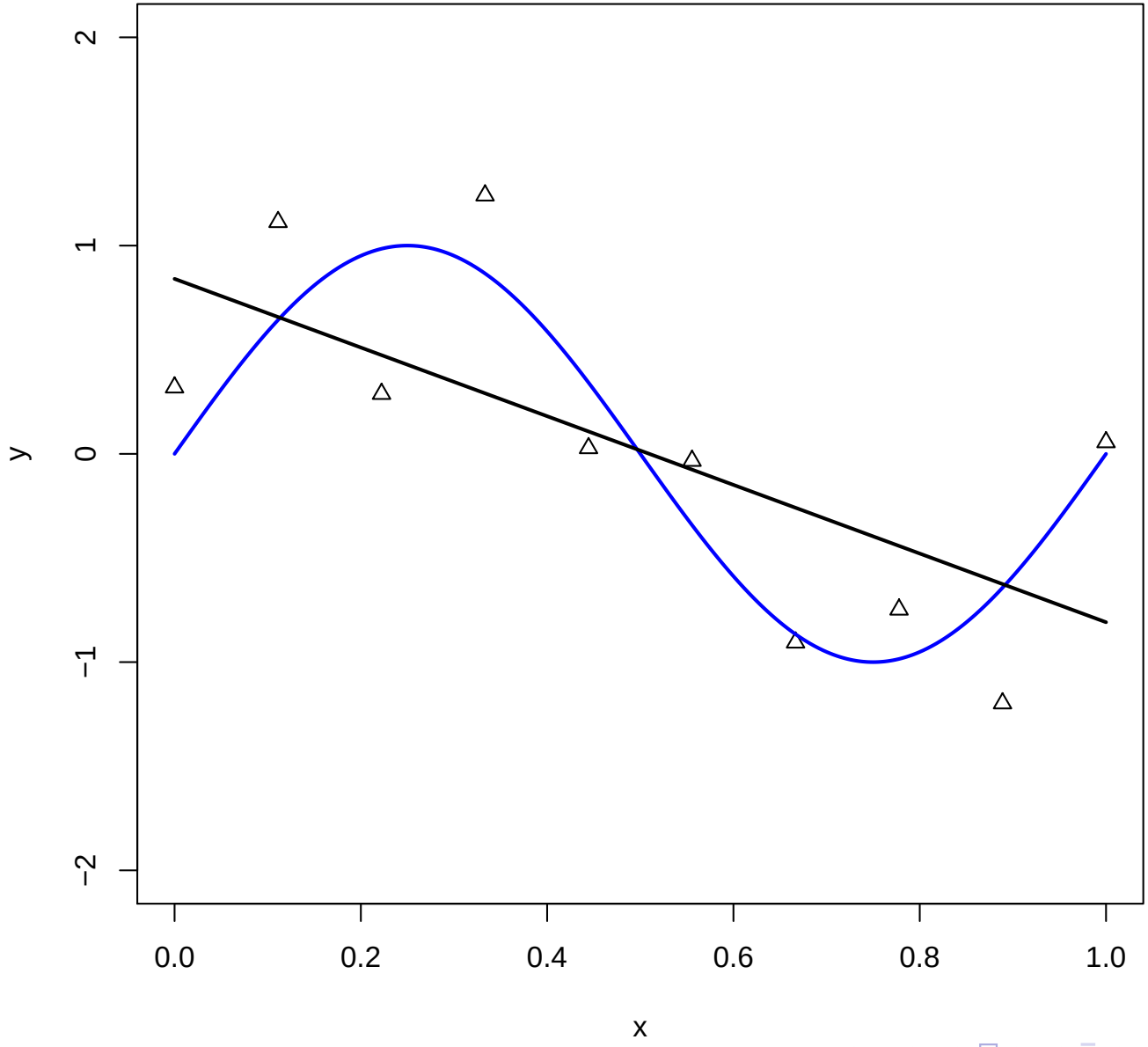
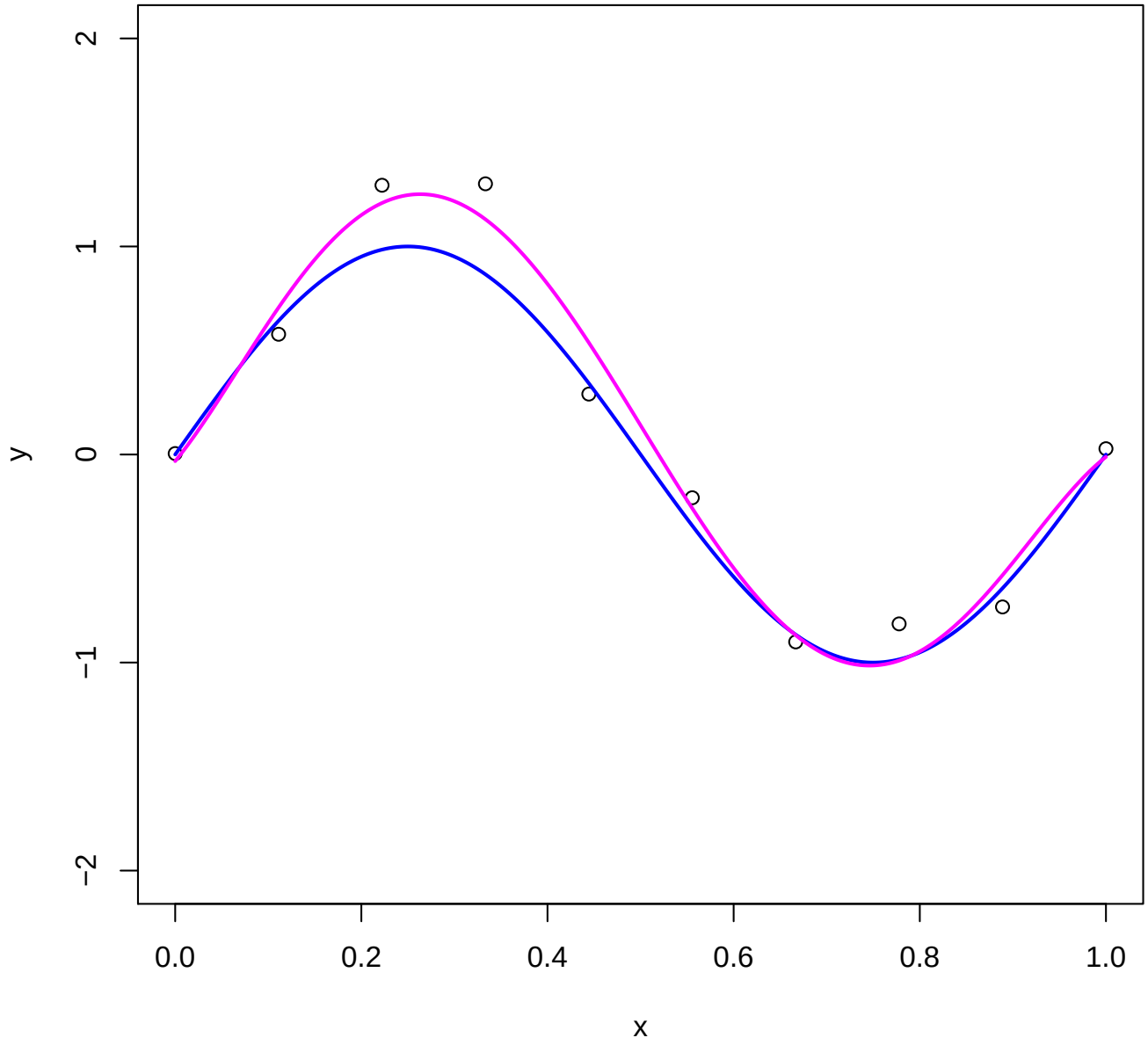
Linear Fit on Sample 1



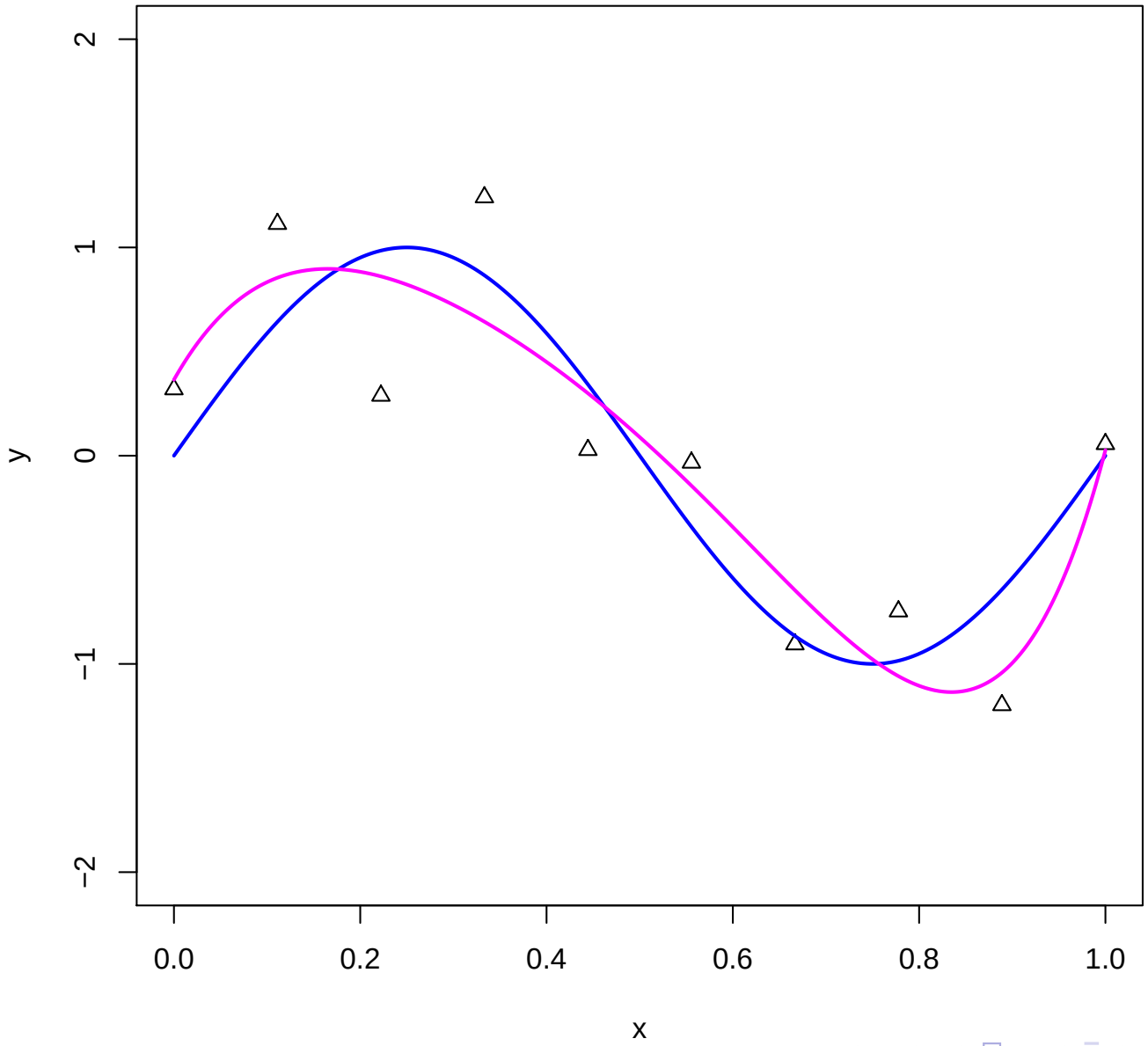
Linear Fit on Sample 2



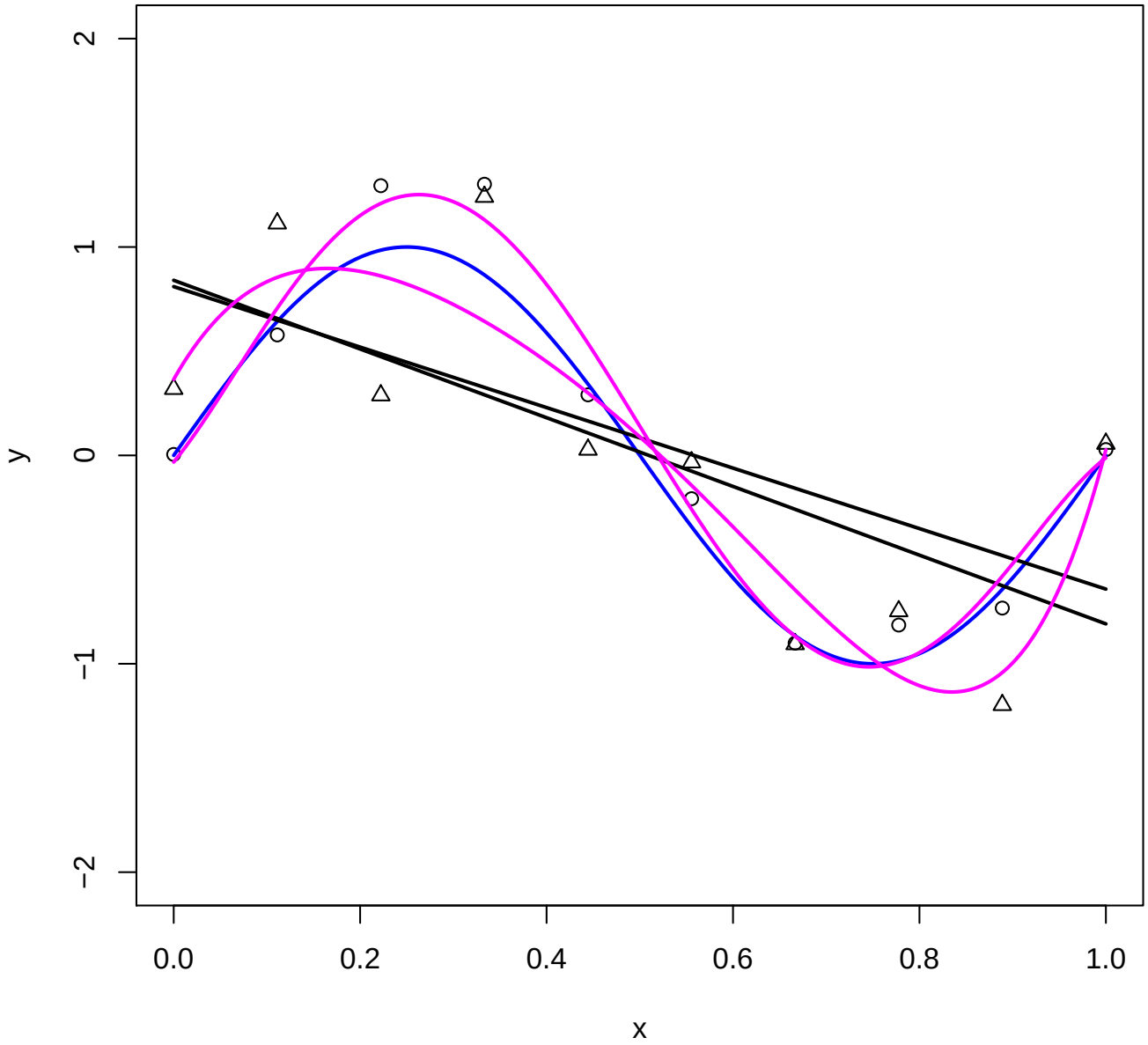
Polynomial of Degree 5 on Sample 1



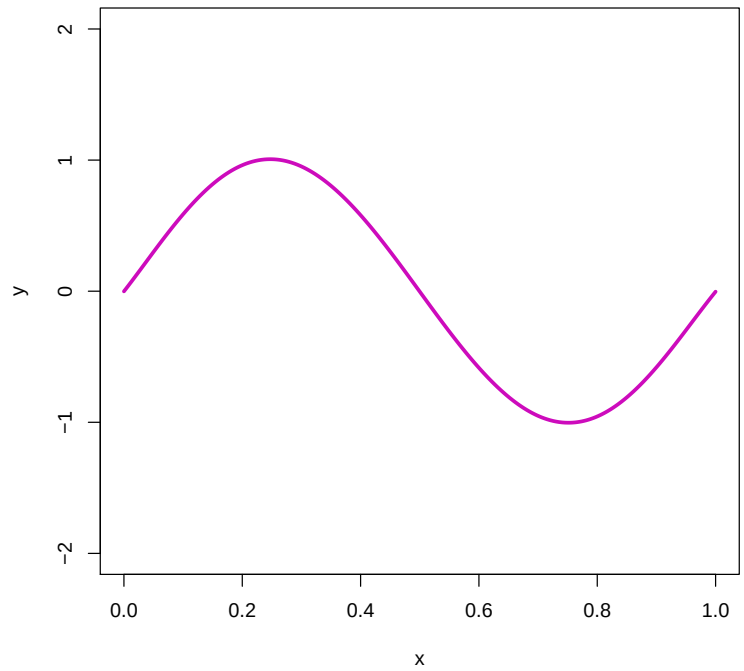
Polynomial of Degree 5 on Sample 2

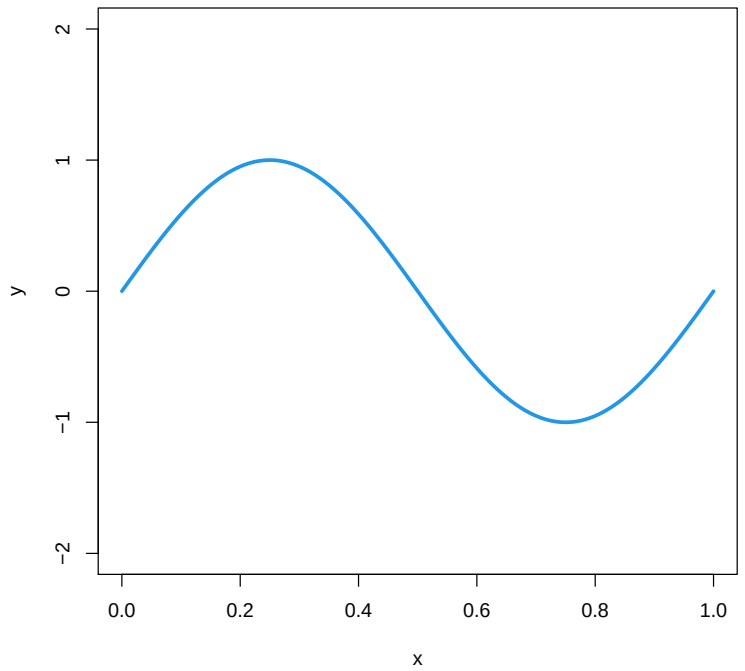


All Together Now



Average of degree 5 polynomials



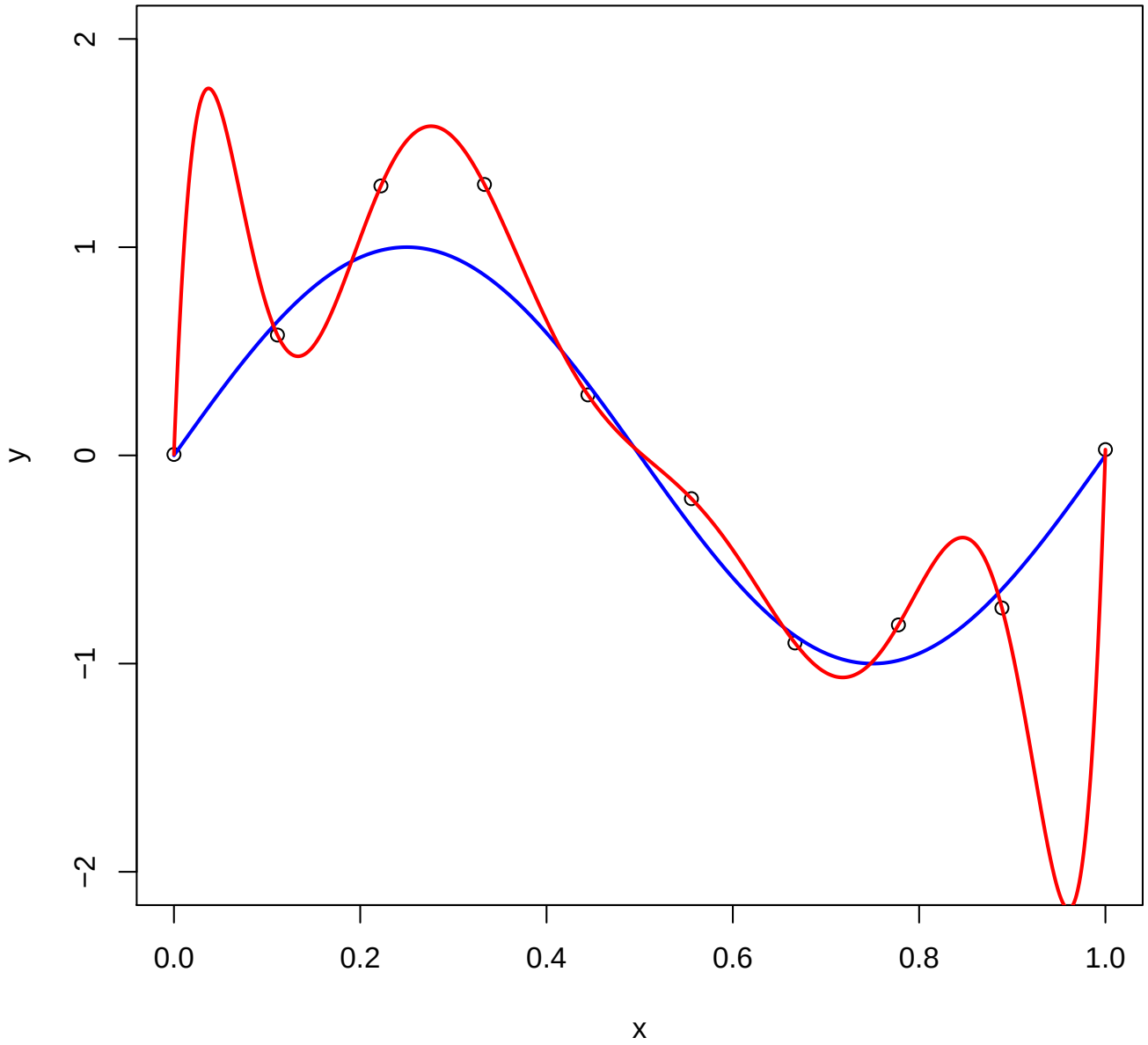


Average predictions of degree 5 polynomials estimated on 10,000 samples of size 10 (on the left), and $\sin(2\pi x)$ (on the right).

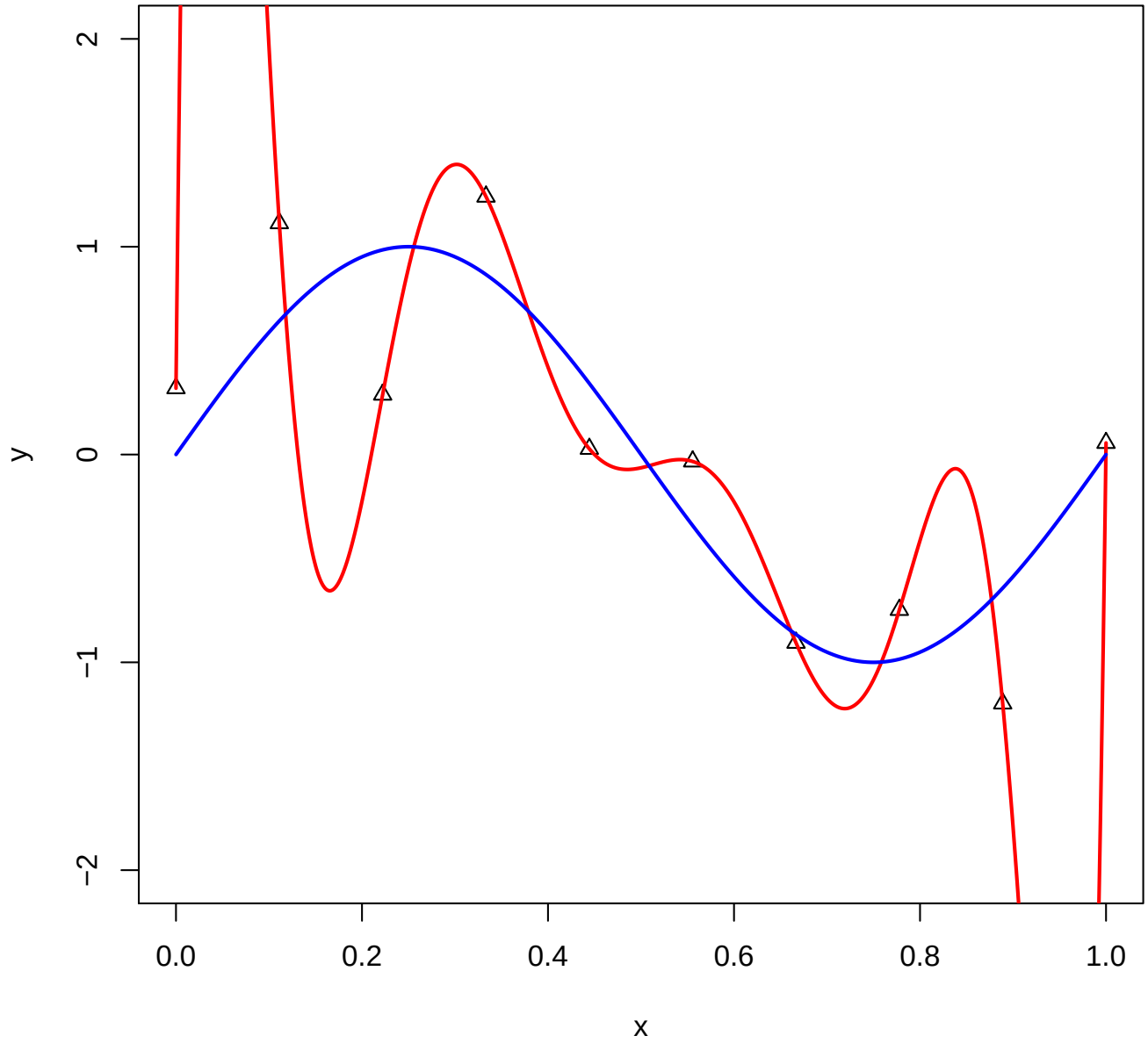
10000次樣本大小是10的抽樣

Can you see the difference?

Polynomial of Degree 9 on Sample 1

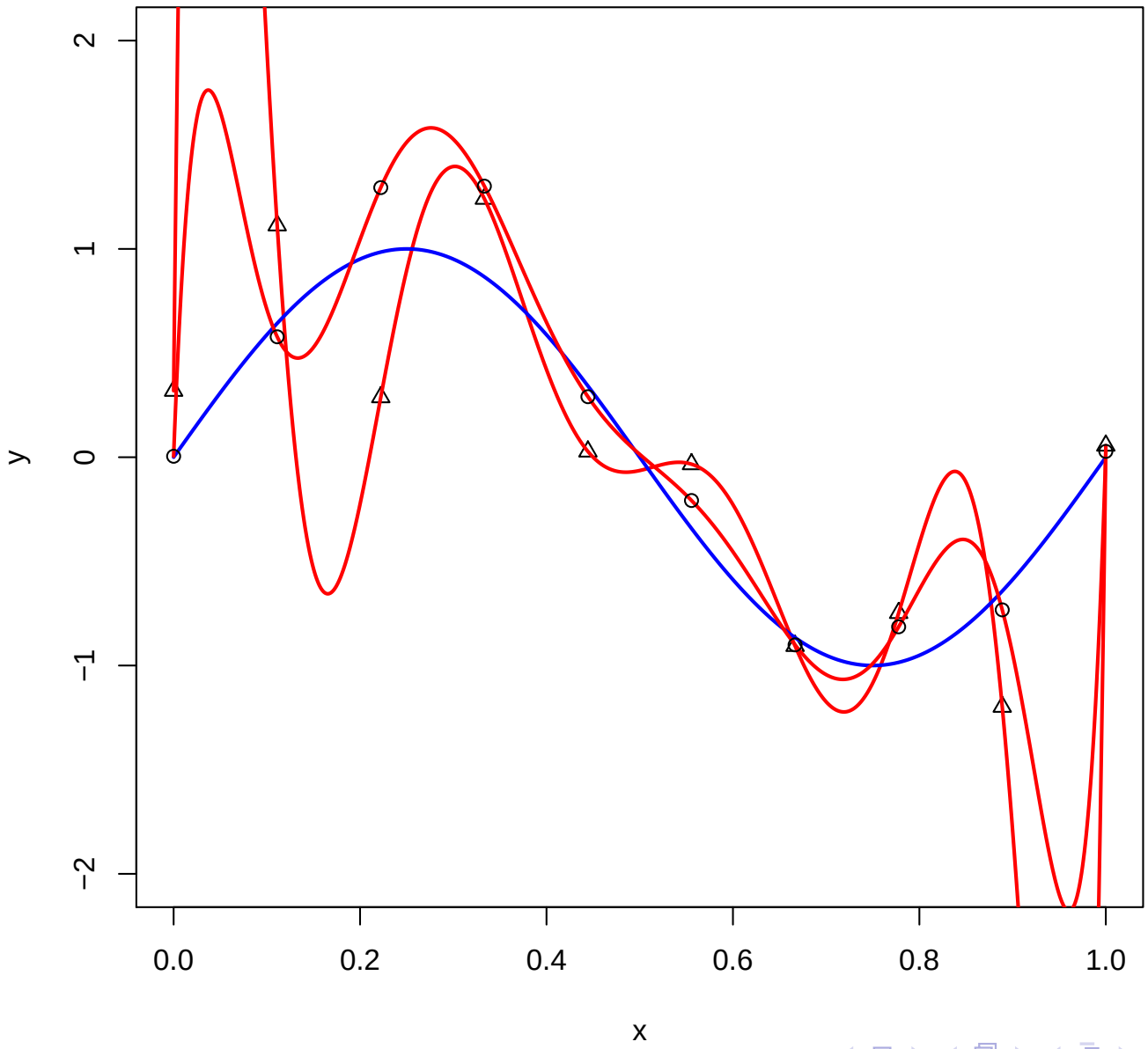


Polynomial of Degree 9 on Sample 2



A High Variance Predictor!

Bias（偏差） 很低 → 平均起來接近真實函數。
Variance（變異） 很高 → 單個模型不穩定，差異大。



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 母體
population? For simplicity, we restrict our analysis to some fixed point x.

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

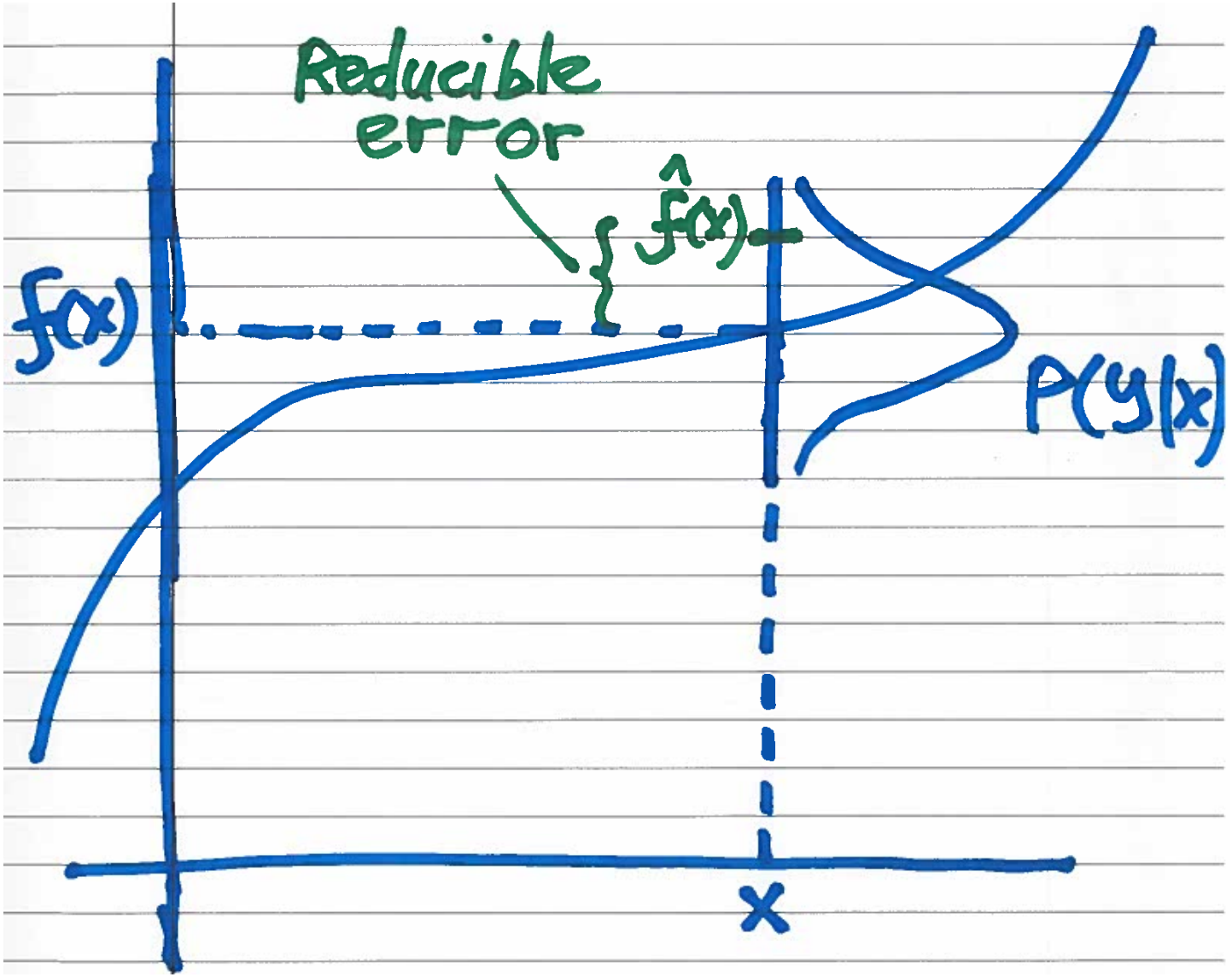
where $f(x) \equiv \mathbb{E}[Y \mid x]$ is the true (population) regression function, and the expectation is taken with respect to $P(Y \mid x)$. $\hat{f}(x)$ is the model prediction at x.

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.

Y : 真實的輸出值（帶有隨機噪音的觀測）
f^(x) : 模型在輸入 x 時的預測值。它是固定的（因為你已經有一個模型）。
(Y– f^ (x)) 2 : 這是「在輸入 x 時，模型預測和真實輸出之間的平方誤差」。但注意：因為 Y 是隨機的（有雜訊），這個值本身也是隨機的。
P(Y|x) = 在輸入 x 時，隨機變數 Y 的條件分布
EP(Y|x)[·] :「對條件分布 P(Y|x) 取期望值」。意思是：我們把所有可能出現的 Y 值代進去計算，然後加權平均（根據 P(Y|x) 的機率）。

E P(Y|x) [(Y– f^ (x)) 2] : = 「在固定輸入 x 的情況下，模型預測與真實輸出之間的平均平方誤差」
= MSE at a fixed x

Reducible and Irreducible Error



Bias-Variance Decomposition of Estimation Error

Now let's focus on reducible error.

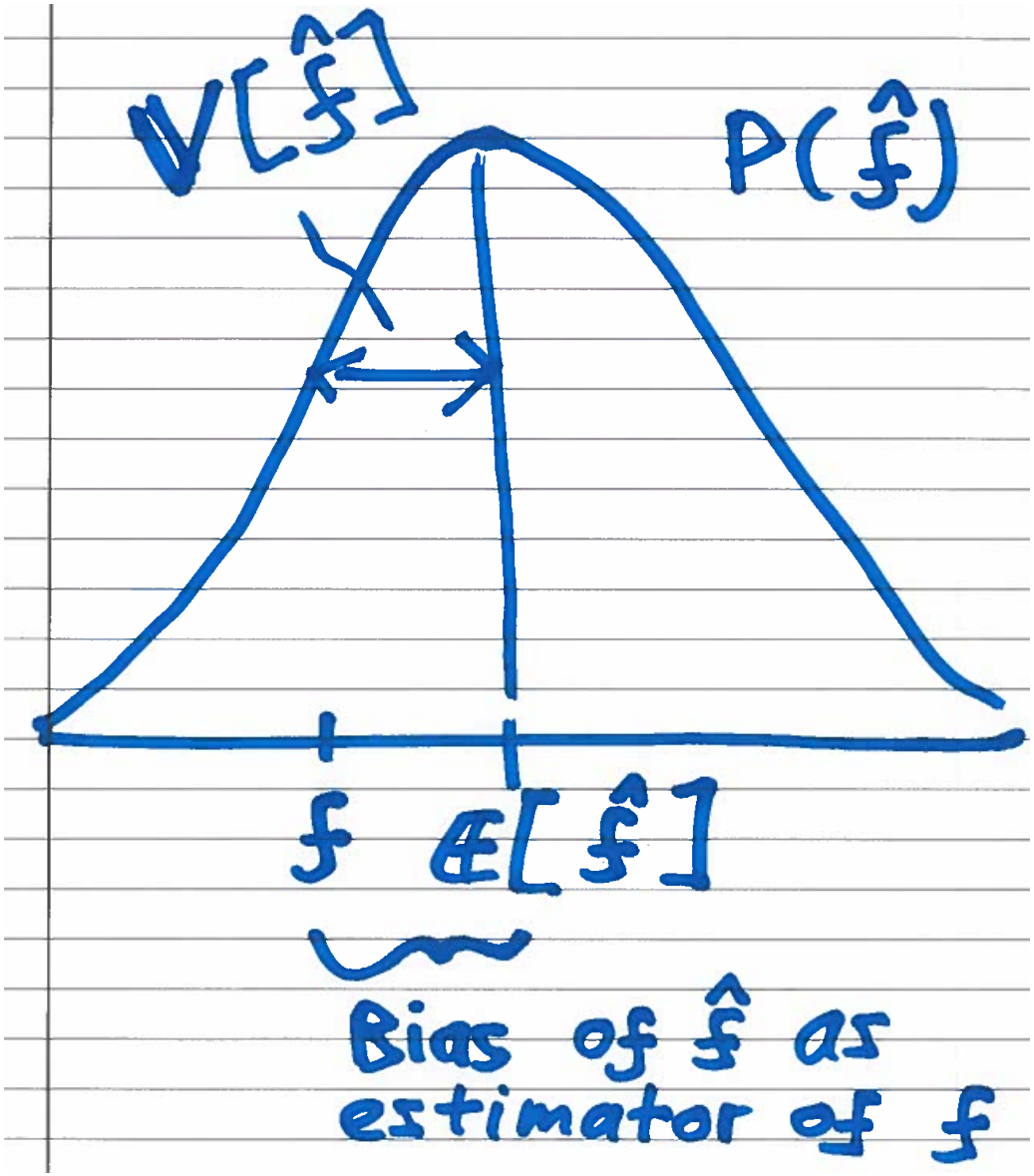
Consider the collection of models created by an algorithm on different data sets, sampled from the same population. We use each sample to estimate $f(x)$. What is the mean squared estimation error of these models?

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

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

Mean Squared Error = Squared Bias + 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!

自助抽樣：
從原始資料隨機抽取樣本（有放回）形成不同的訓練集
每個訓練集訓練一棵樹

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

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

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

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.