Lecture 2: Supervised vs. unsupervised learning, bias-variance tradeoff

Reading: Chapter 2

STATS 202: Data mining and analysis

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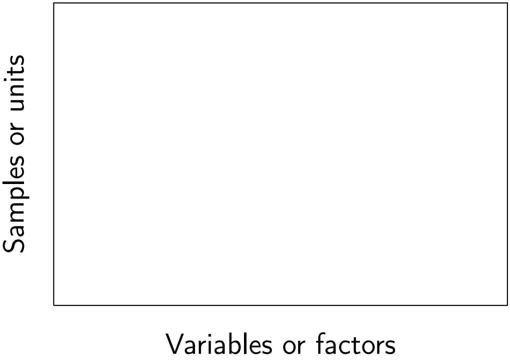
September 24, 2014

Supervised vs. unsupervised learning

In **unsupervised learning** we start with a data matrix:



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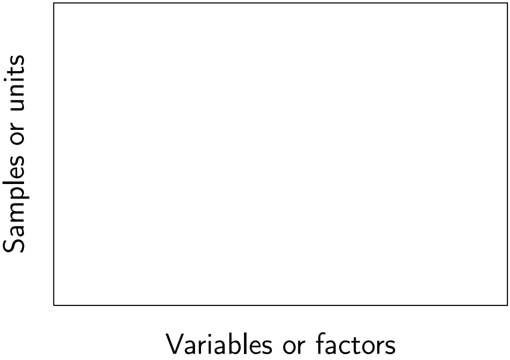

Quantitative, eg. weight, height, number of children, ...

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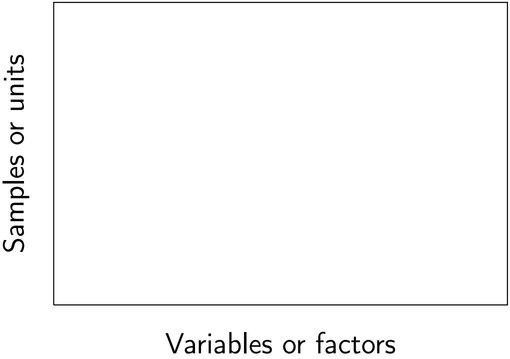


Qualitative, eg. college major, profession, gender, ...

Supervised vs. unsupervised learning

In **unsupervised learning** we start with a data matrix:

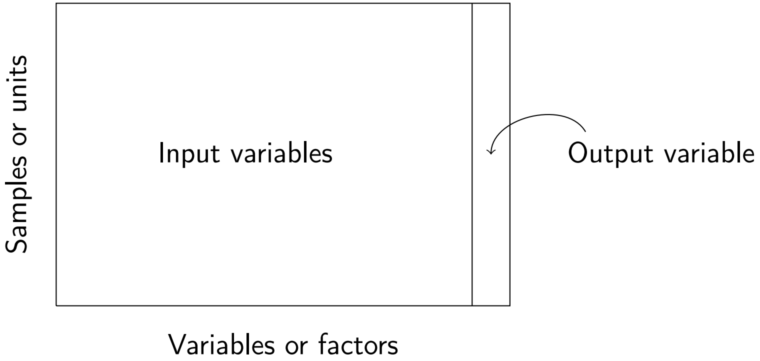
Our goal is to:

- Find meaningful relationships between the variables or units. Correlation analysis.
- Find low-dimensional representations of the data which make it easy to visualize the variables and units. PCA, ICA, isomap, locally linear embeddings, etc.
- Find meaningful groupings of the data. Clustering.

Unsupervised learning is also known in Statistics as **exploratory data analysis**.

Supervised vs. unsupervised learning

In **supervised learning**, there are *input* variables, and *output* variables:



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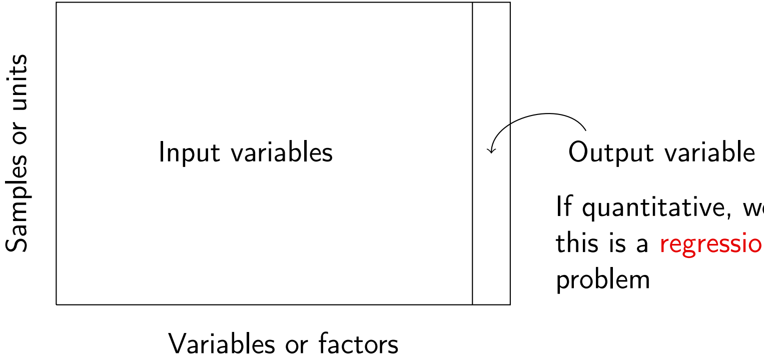

If quantitative, we say this is a regression problem

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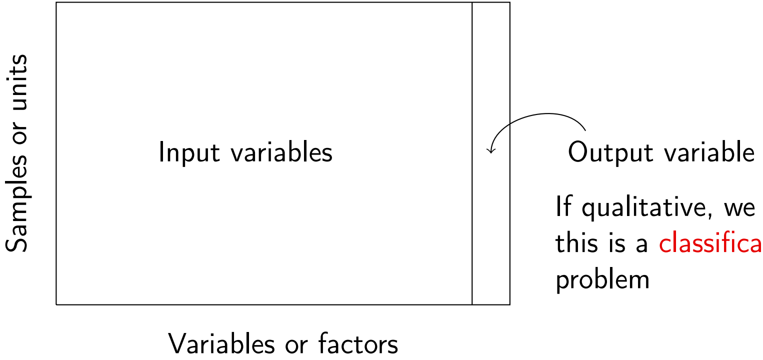


If qualitative, we say this is a classification problem

Supervised vs. unsupervised learning

In **supervised learning**, there are *input* variables, and *output* variables:

If X is the vector of inputs for a particular sample. The output variable is modeled by:

$$Y = f(X) + \underbrace{\varepsilon}_{\text{Random error}}$$

Our goal is to learn the function f, using a set of training samples.

Supervised vs. unsupervised learning

$$Y = f(X) + \underbrace{\varepsilon}_{\text{Random error}}$$

Motivations:

- **Prediction:** Useful when the input variable is readily available, but the output variable is not.

  Example: Predict stock prices next month using data from last year.

- **Inference:** A model for f can help us understand the structure of the data — which variables influence the output, and which don't? What is the relationship between each variable and the output, e.g. linear, non-linear?

  Example: What is the influence of genetic variations on the incidence of heart disease.

Parametric and nonparametric methods:

There are two kinds of supervised learning method:

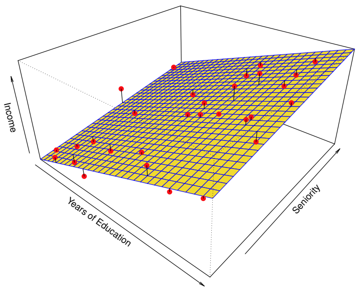
- **Parametric methods:** We assume that f takes a specific form. For example, a linear form:

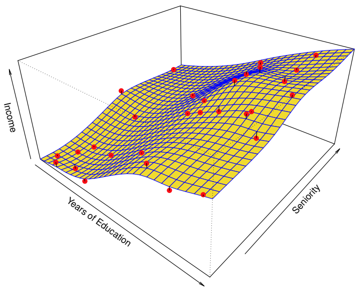
  $$f(X) = X_1\beta_1 + \cdots + X_p\beta_p$$

  with parameters $\beta_1, \ldots, \beta_p$. Using the training data, we try to *fit* the parameters.

- **Non-parametric methods:** We don't make any assumptions on the form of f, but we restrict how "wiggly" or "rough" the function can be.

Parametric vs. nonparametric prediction





Figures 2.4 and 2.5

Parametric methods have a limit of fit quality. Non-parametric methods keep improving as we add more data to fit.

Parametric methods are often simpler to interpret.

Prediction error

Training data: $(x_1, y_1), (x_2, y_2) \dots (x_n, y_n)$
Predicted function: $\hat{f}$.

Our goal in supervised learning is to minimize the prediction error. For regression models, this is typically the *Mean Squared Error*:

$$MSE(\hat{f}) = E(y_0 - \hat{f}(x_0))^2.$$

Unfortunately, this quantity cannot be computed, because we don't know the joint distribution of (X, Y). We can compute a sample average using the training data; this is known as the training MSE:

$$MSE_{\text{training}}(\hat{f}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2.$$

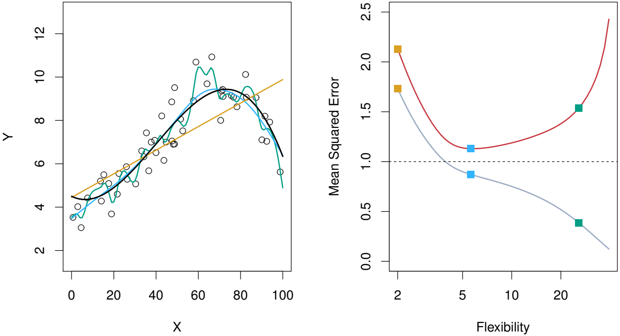
Prediction error

The main challenge of statistical learning is that *a low training MSE does not imply a low MSE.*

If we have test data $\{(x_i', y_i'); i = 1, \ldots, m\}$ which were not used to fit the model, a better measure of quality for $\hat{f}$ is the test MSE:

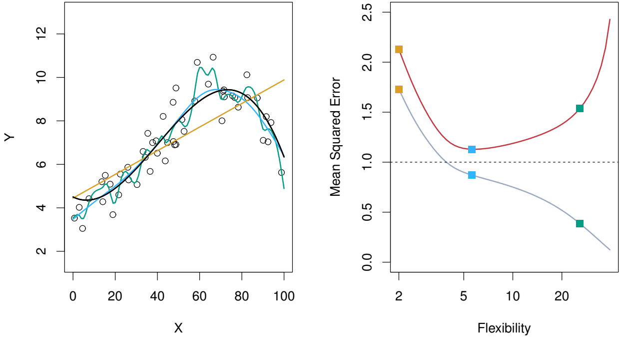
$$MSE_{\text{test}}(\hat{f}) = \frac{1}{m} \sum_{i=1}^{m} (y_i' - \hat{f}(x_i'))^2.$$

Figure 2.9.



The circles are simulated data from the black curve. In this artificial example, we *know* what f is.

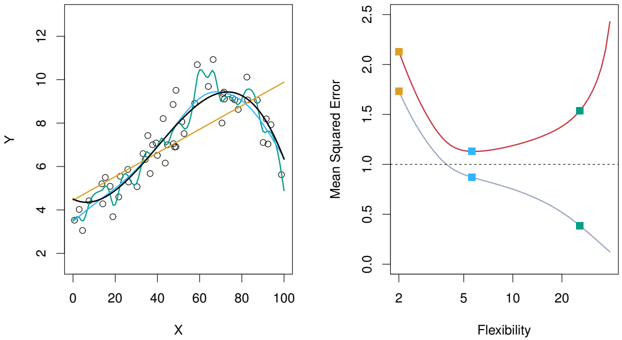
Figure 2.9.



Three estimates $\hat{f}$ are shown:

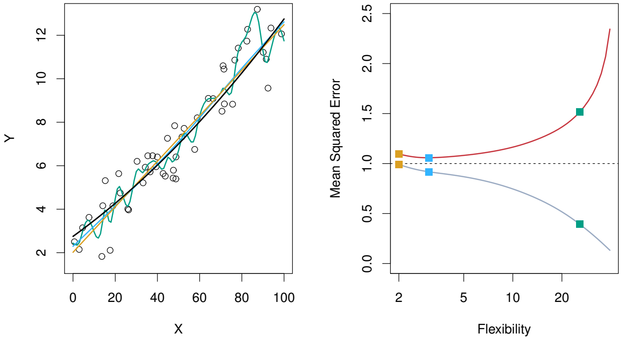
1. Linear regression.
2. Splines (very smooth).
3. Splines (quite rough).

Figure 2.9.



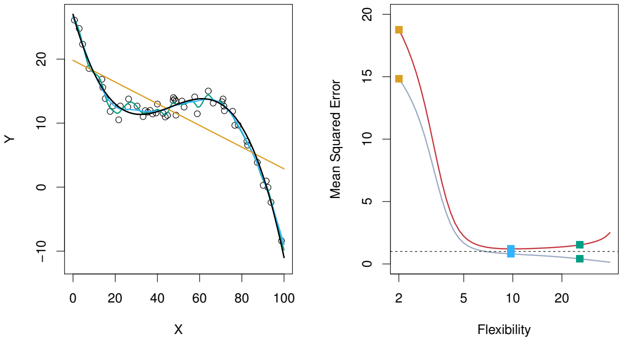
Red line: Test MSE.
Gray line: Training MSE.

Figure 2.10



The function f is now almost linear.

Figure 2.11



When the noise ε has small variance, the third method does well.

The bias variance decomposition

Let x_0 be a fixed test point, $y_0 = f(x_0) + \varepsilon_0$, and $\hat{f}$ be estimated from n training samples $(x_1, y_1) \ldots (x_n, y_n)$.

Let E denote the expectation over y_0 and the training outputs $(y_1, \ldots, y_n)$. Then, the Mean Squared Error at x_0 can be decomposed:

$$MSE(x_0) = E(y_0 - \hat{f}(x_0))^2 = \text{Var}(\hat{f}(x_0)) + [\text{Bias}(\hat{f}(x_0))]^2 + \text{Var}(\varepsilon_0).$$

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Irreducible error

The bias variance decomposition

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The variance of the estimate of Y: $E[\hat{f}(x_0) - E(\hat{f}(x_0))]^2$

This measures how much the estimate of $\hat{f}$ at x_0 changes when we sample new training data.

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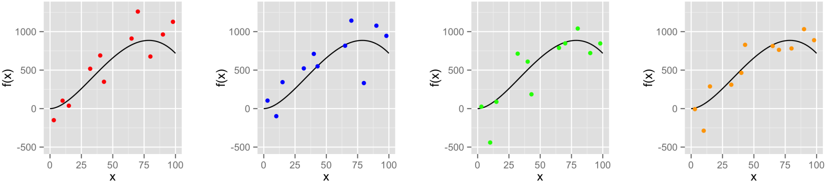
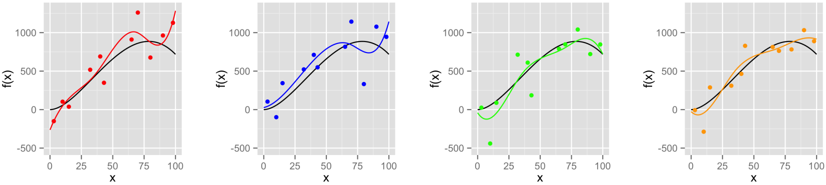
The squared bias of the estimate of Y: $[E(\hat{f}(x_0)) - f(x_0)]^2$

This measures the deviation of the average prediction $\hat{f}(x_0)$ from the truth $f(x_0)$.



1000
500
0
-500
f(x)
0
25
50
75
100
x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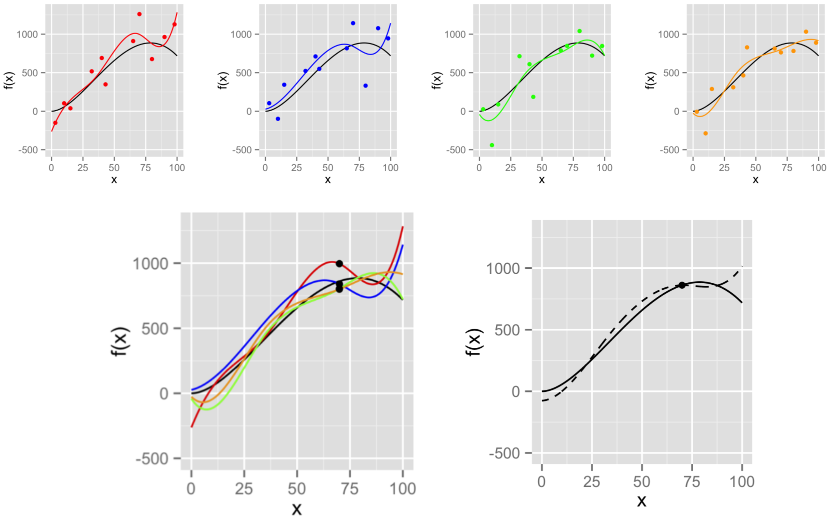


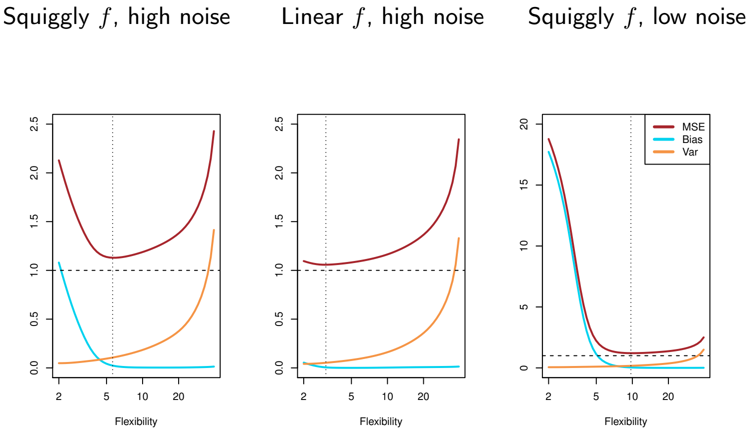
1000
500
0
-500
f(x)
0
25
50
75
100
x

Implications of bias variance decomposition

$$MSE(x_0) = E(y_0 - \hat{f}(x_0))^2 = \mathsf{Var}(\hat{f}(x_0)) + [\mathsf{Bias}(\hat{f}(x_0))]^2 + \mathsf{Var}(\varepsilon).$$

- The MSE is always positive.
- Each element on the right hand side is always positive.
- Therefore, typically when we decrease the bias beyond some point, we increase the variance, and vice-versa.

More flexibility $\iff$ Higher variance $\iff$ Lower bias.



Squiggly f, high noise
Linear f, high noise
Squiggly f, low noise
MSE
Bias
Var
0.0
0.5
1.0
1.5
2.0
2.5
0
5
10
15
20
2
5
10
20
Flexibility

Figure 2.12

Classification problems

In a classification setting, the output takes values in a discrete set.

For example, if we are predicting the brand of a car based on a number of variables, the function f takes values in the set $\{$Ford, Toyota, Mercedes-Benz, $\ldots\}$.

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becomes insufficient, as X is not necessarily real-valued.

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We will use slightly different notation:

$$\begin{aligned} P(X,Y) &: \text{joint distribution of } (X,Y), \\ P(Y \mid X) &: \text{conditional distribution of } X \text{ given } Y, \\ \hat{y}_i &: \text{prediction for } x_i. \end{aligned}$$

Loss function for classification

There are many ways to measure the error of a classification prediction. One of the most common is the 0-1 loss:

$$E(\mathbf{1}(y_0 \neq \hat{y}_0))$$

Like the MSE, this quantity can be estimated from training and test data by taking a sample average:

$$\frac{1}{n}\sum_{i=1}^{n} \mathbf{1}(y_i \neq \hat{y}_i)$$

Bayes classifier

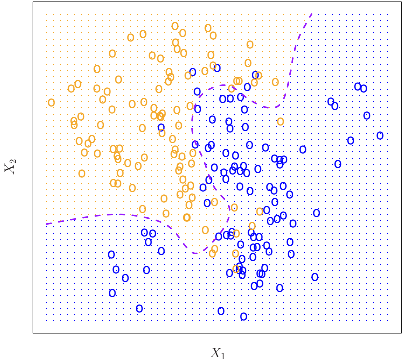

Figure 2.13

In practice, we never know the joint probability P. However, we can assume that it exists.

The Bayes classifier assigns:

$$\hat{y}_i = \text{argmax}_j \;\; P(Y = j \mid X = x_i)$$

It can be shown that this is the best classifier under the 0-1 loss.