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

Reading: Chapter 2

STATS 202: Data mining and analysis

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In unsupervised learning we start with a data matrix:

Variables or factors

Samples or units
Supervised vs. unsupervised learning

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

- **Variables or factors**: Quantitative, eg. weight, height, number of children, ...
- **Samples or units**
In **unsupervised learning** we start with a data matrix:

```
+----------------+----------------+
| Samples or units | Variables or factors |
+----------------+----------------+
| Qualitative, eg. college major, profession, gender, ... |
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Supervised vs. unsupervised learning

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Our goal is to:

- Find meaningful relationships between the variables or units.
  - Correlation analysis.
  - PCA, ICA, isomap, locally linear embeddings, etc.
  - Clustering.

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

![Diagram showing supervised learning with input variables and output variable]
Supervised vs. unsupervised learning

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- **Input variables**
- **Output variable**

If quantitative, we say this is a *regression* problem.
In **supervised learning**, there are *input* variables, and *output* variables:

If qualitative, we say this is a **classification** problem.
Supervised vs. unsupervised learning

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

$$ Y = f(X) + \varepsilon $$

Random error
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:

$$Y = f(X) + \varepsilon$$

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

Typically we assume $\varepsilon$ independent of $X$ given $f(X)$, i.e.

$Y|X \sim N(f(X), \sigma^2)$ though this is not necessary.
Supervised vs. unsupervised learning

\[ Y = f(X) + \varepsilon \]

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.
Supervised vs. unsupervised learning

\[ Y = f(X) + \varepsilon \]

Motivations:

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

- **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:

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

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f(X) = X_1 \beta_1 + \cdots + X_p \beta_p
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with parameters \( \beta_1, \ldots, \beta_p \). Using the training data, we try to *fit* the parameters.
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- **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.
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Prediction error

Training data: \((x_1, y_1), (x_2, y_2) \ldots (x_n, y_n)\)

Predicted function: \(\hat{f}\).

Future data: \((x_0, y_0)\) having some distribution.

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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:

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

\[
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The circles are simulated data from the black curve by adding Gaussian noise.
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Three estimates $\hat{f}$ are shown:

1. Linear regression.
2. Splines (very smooth).
3. Splines (quite rough).
Red line: Test MSE.
Gray line: Training MSE.
The function $f$ is now almost linear.
When the noise $\varepsilon$ has small variance relative to $f$, 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:

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MSE(x_0) = E(y_0 - \hat{f}(x_0))^2 = Var(\hat{f}(x_0)) + [Bias(\hat{f}(x_0))]^2 + Var(\varepsilon_0).
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Irreducible error
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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 $f(x_0)$. 
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Implications of bias variance decomposition

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More flexibility ⇔ Higher variance ⇔ Lower bias.
Squiggly $f$, high noise  

Linear $f$, high noise  

Squiggly $f$, low noise

Figure 2.12
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:

\[
\begin{align*}
P(X, Y) & : \text{ joint distribution of } (X, Y), \\
P(Y \mid X) & : \text{ conditional distribution of } X \text{ given } Y, \\
\hat{y}_i & : \text{ prediction for } x_i.
\end{align*}
\]
There are many ways to measure the error of a classification prediction. One of the most common is the 0-1 loss:

\[ E(\mathbf{1}(y_0 \neq \hat{y}_0)) \]
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:

$$\frac{1}{n} \sum_{i=1}^{n} \mathbf{1}(y_i \neq \hat{y}_i)$$
In practice, we never know the joint probability $P$. However, we can assume that it exists.

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The Bayes classifier assigns:

$$\hat{y}_i = \arg\max_j P(Y = j \mid X = x_i)$$

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