Introduction to Machine Learning and Data Science

4. Supervised learning framework

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Table of contents

Table of contents

Input and output variables

The **input variables**[1] are typically denoted using the symbol X. If we observe p different variables, we write $X = (X_1, X_2, \ldots, X_p)$. The inputs belong to an *input space* $\mathcal{X}$.

- Examples: $\mathcal{X} \subseteq \mathbb{R}^p$ or $\mathcal{X} = \{0, 1\}^p$.

The **output variable**[2] is typically denoted using the symbol Y. The output belongs to an *output space* $\mathcal{Y}$.

- Regression: $\mathcal{Y} \subseteq \mathbb{R}$.
- Classification (with K categories): $\mathcal{Y} = \{\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_K\}$.
    - Binary classification ($K = 2$): $\mathcal{Y} = \{-1, 1\}$ or $\mathcal{Y} = \{0, 1\}$.

[1] also called *predictors*, *independent variables*, *features*, *variables*, or just *inputs*.
[2] also called the *response* or *dependent variable*.

Unknown joint distribution

We assume $(X, Y) \sim p_{X,Y}$ where $p_{X,Y}$ is a fixed *unknown* distribution which can be factorized as

$$p_{X,Y}(x, y) = p_X(x) p_{Y|X}(y \mid x),$$

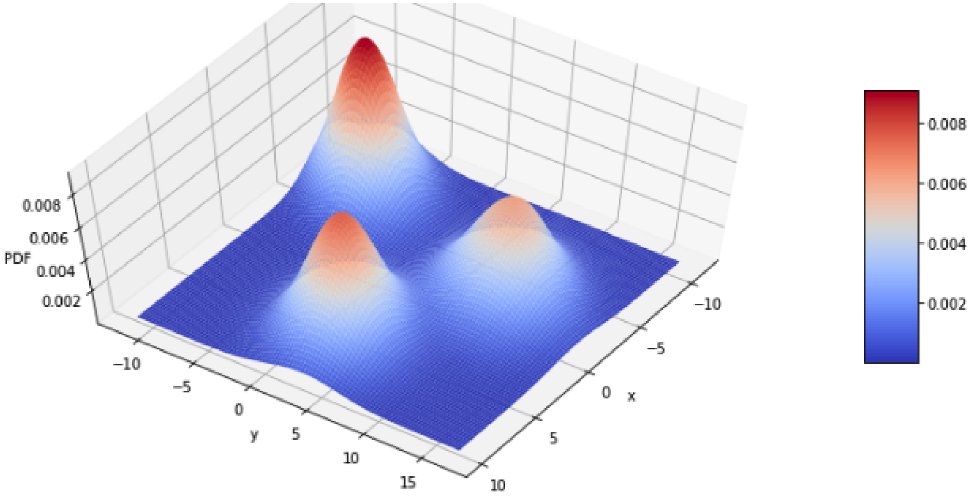
where

- the **marginal** distribution p_X models uncertainty in the sampling of the inputs.
- the **conditional** distribution $p_{Y|X}$ describes a stochastic (non-deterministic) relation between inputs and output.

Equivalently, we have

$$X \sim p_X \text{ and } Y \mid X = x \sim p_{Y|X}(\cdot \mid x).$$

Joint distribution



Optimal predictions

Define a **loss function** $L\colon \mathcal{Y} \times \mathcal{Y} \to [0, \infty)$. Given a prediction $\hat{y} \in \mathcal{Y}$ and the true (observed) value $y \in \mathcal{Y}$, $L(y, \hat{y})$ measures how far $\hat{y}$ is from y.

Examples include the *squared error loss* $L(y, \hat{y}) = (y - \hat{y})^2$, the *absolute error loss* $L(y, \hat{y}) = |y - \hat{y}|$, and the *zero-one loss* $L(y, \hat{y}) = \mathbb{1}\{y \neq \hat{y}\}$, where $\mathbb{1}\{\cdot\}$ is the indicator function.

The **optimal prediction function** which minimizes the **expected error** (or **expected risk**) is given by

$$f = \operatorname*{argmin}_{h:\mathcal{X}\to\mathcal{Y}} \mathbb{E}_{x,y}[L(y, h(x))].$$

In practice, we cannot compute f since we **do not know** $p_{X,Y}$.

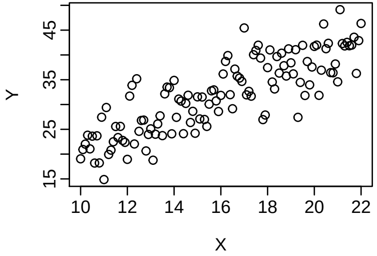
The dataset

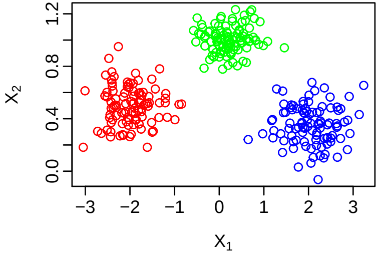
The **dataset**, also called *training set*, is a set of n input-output pairs

$$\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\} = \{(x_i, y_i)\}_{i=1}^{n},$$

where the data points (x_i, y_i) are assumed to be i.i.d. realizations of $p_{X,Y}$.

Each pair, also called an *example* or a *data point*, belongs to the *data space* $\mathcal{X} \times \mathcal{Y}$.





- Left figure: $\mathcal{X} \subseteq \mathbb{R}$ $(p = 1)$ and $\mathcal{Y} \subseteq \mathbb{R}$.
- Right figure: $\mathcal{X} \subseteq \mathbb{R}^2$ $(p = 2)$ and $\mathcal{Y} = \{R, G, B\}$.

The supervised learning problem

Let $\mathcal{H}$ be a **hypothesis set**, i.e., a set of prediction functions (hypotheses) under consideration. An example is the linear hypothesis set

$$\mathcal{H} = \{h(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p \mid \beta_0, \beta_1, \ldots, \beta_p \in \mathbb{R}\}.$$

Given a dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$, the goal of supervised learning is to learn a **prediction function** $h\colon \mathcal{X} \to \mathcal{Y}$ to map new/unseen examples with minimal expected **prediction error**.

We can compute the **in-sample error** or **training error**[3]

$$E_{\text{in}}(h) = \frac{1}{n}\sum_{i=1}^{n} L(y_i, h(x_i)),$$

and solve the following optimization problem:

$$g_{\mathcal{D}} = \underset{h \in \mathcal{H}}{\operatorname{argmin}}\; E_{\text{in}}(h).$$

[3]Also called the **empirical risk**.

The supervised learning problem

Ideally, we would like to select the hypothesis $h \in \mathcal{H}$ which minimizes the **out-of-sample error**

$$E_{\text{out}}(h) = \mathbb{E}_{x,y}[L(y, h(x))], \tag{1}$$

and compute

$$g^* = \underset{h \in \mathcal{H}}{\operatorname{argmin}}\ E_{\text{out}}(h).$$

In summary, there are three different prediction functions:

$$f = \underset{h\colon \mathcal{X} \to \mathcal{Y}}{\operatorname{argmin}}\ E_{\text{out}}(h),$$

$$g^* = \underset{h \in \mathcal{H}}{\operatorname{argmin}}\ E_{\text{out}}(h),$$

and

$$g_{\mathcal{D}} = \underset{h \in \mathcal{H}}{\operatorname{argmin}}\ E_{\text{in}}(h).$$

Summary

The **dataset** $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$ is composed of n input-output pairs (x_i, y_i), which are i.i.d. realizations from an **unknown joint distribution** $p_{X,Y}$ where $X \in \mathcal{X}$ and $Y \in \mathcal{Y}$.

The **loss function** $L\colon \mathcal{Y} \times \mathcal{Y} \to [0, \infty)$ allows us to measure the error we incur in predicting $\hat{y}$ in place of y.

The **hypothesis set** $\mathcal{H}$ is a set of prediction functions under consideration. Each hypothesis $h \in \mathcal{H}$ has an **in-sample error** $E_{\text{in}}(h)$, computed on $\mathcal{D}$, and an **out-of-sample error** $E_{\text{out}}(h)$ which depends on $p_{X,Y}$.

Given $\mathcal{H}$ and using $\mathcal{D}$, the **learning algorithm** $\mathcal{A}$ picks the best hypothesis g from $\mathcal{H}$ according to the loss function L.

Together, the hypothesis set and the learning algorithm are referred to as the **learning model**.

Table of contents

Linear models

Let us consider a regression problem where $x \in \mathbb{R}^p$.

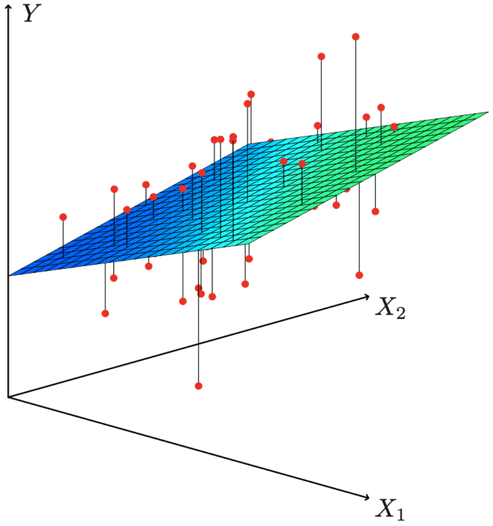
- The **hypothesis set** for linear models is given by

$$\mathcal{H} = \{h(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p \mid \beta_0, \beta_1, \ldots, \beta_p \in \mathbb{R}\}.$$

- One **learning algorithm** is the *(ordinary) least squares* method.

Linear models

Example with $p = 2$.



K-Nearest Neighbors (KNN) model

- **Input**: $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$, number of neighbors $K \leq n$, and new input x_*.
- **Classification** with M categories ($y \in \{C_1, \ldots, C_M\}$):
  - Find the K nearest points to x_* in $\mathcal{D}$; this set of points is denoted $\mathcal{N}_*$.
  - The predicted probability for each class is given by

$$\hat{p}(C_m \mid x = x_*) \approx \frac{1}{K} \sum_{i \in \mathcal{N}_*} \mathbb{1}\{y_i = C_m\} \quad (m = 1, 2, \ldots, M).$$

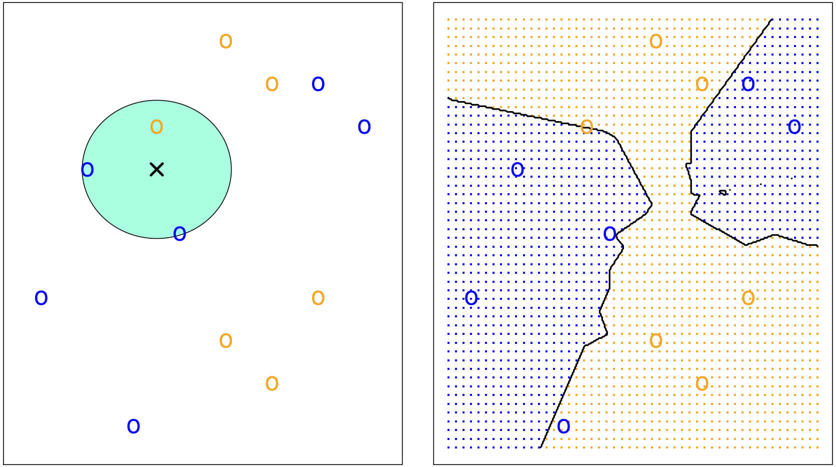
  - The predicted class is then

$$h(x_*) = C_{m^*} \text{ where } m^* = \operatorname{argmax}_m \hat{p}(C_m \mid x = x_*).$$

- **Regression**
  - Find the K nearest points to x_* in $\mathcal{D}$; this set of points is denoted $\mathcal{N}_*$.
  - Choose

$$h(x_*) = \frac{1}{K} \sum_{i \in \mathcal{N}_*} y_i.$$

K-Nearest Neighbors (KNN)



Picture: Classification problem, $K = 3$. Right: *decision boundary*.
K-Nearest Neighbors (KNN) is one of the simplest machine learning model for both classification and regression.

Parametric and non-parametric models

Two classes of models: **parametric** and **non-parametric**.

- In a **parametric model**, every hypothesis is uniquely defined by a **fixed number of parameters**. Example: $p + 1$ for linear regression with $\mathcal{X} = \mathbb{R}^p$.
- In a **non-parametric model**, we can not describe a hypothesis with a fixed number of parameters. Usually the number of "parameters" **grows with the size of the dataset**. Example: KNN, in which every prediction uses the whole dataset.
- Both parametric and non-parametric models have **hyper-parameters** (structural parameters), while parametric models also have **parameters**
  - For KNN, K is a **hyper-parameter**.
  - For linear models, p is a **hyper-parameter**, and the coefficients β_j are **parameters**.
- We also make a distinction between **linear** and **non-linear** models.

Table of contents

How does E_{out} relates to E_{in}?

Observe that

$$E_{\text{out}}(h) = E_{\text{in}}(h) + [E_{\text{out}}(h) - E_{\text{in}}(h)].$$

To obtain a small $E_{\text{out}}(h)$, we thus want

1. small $E_{\text{in}}(h)$, and

2. small $[E_{\text{out}}(h) - E_{\text{in}}(h)]$.

Selecting the best hypothesis by minimizing $E_{\text{in}}(h)$ only can be misleading.

For example, a (stupid) model that remembers all training data and returns the right value for a training example but a random value otherwise will have a $E_{\text{in}}(h) = 0$ but a very high $E_{\text{out}}(h)$!

This is not a reasonable choice for a model. But how to select the "best" hypothesis set? What we care about is the *accuracy of the predictions that we obtain when we apply our method to previously unseen data*.

Training and test errors in regression

Let us consider multiple hypothesis sets $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_M$, and define

$$g_m = \underset{h \in \mathcal{H}_m}{\operatorname{argmin}}\ E_{\text{in}}(h) = \underset{h \in \mathcal{H}_m}{\operatorname{argmin}}\ \frac{1}{n} \sum_{i=1}^{n} (y_i - h(x_i))^2, \tag{2}$$

for $m = 1, 2, \ldots, M$. Here, we consider the *mean squared error* (MSE) loss.

Let $\mathcal{D}_{\text{test}} = \{(x'_i, y'_i)\}_{i=1}^{n'}$ be **another** sample (**independent** of $\mathcal{D}$) where $(x'_i, y'_i) \overset{\text{i.i.d.}}{\sim} p_{X,Y}$. We define the **testing/test error** of a hypothesis h as

$$E_{\text{test}}(h) = \frac{1}{n'} \sum_{i=1}^{n'} (y'_i - h(x'_i))^2.$$

Note that the test set **is not involved** in the learning process, and is **only used to evaluate the hypothesis** h.

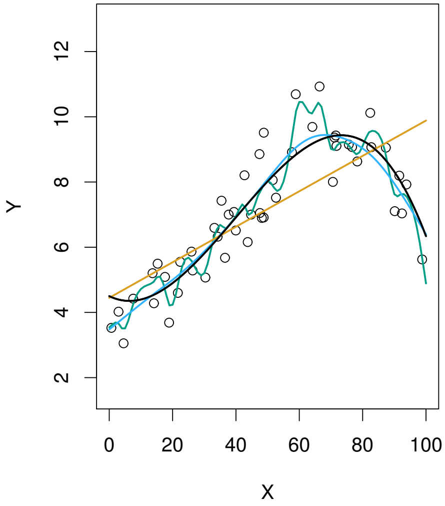
Training and test errors in regression (1/6)

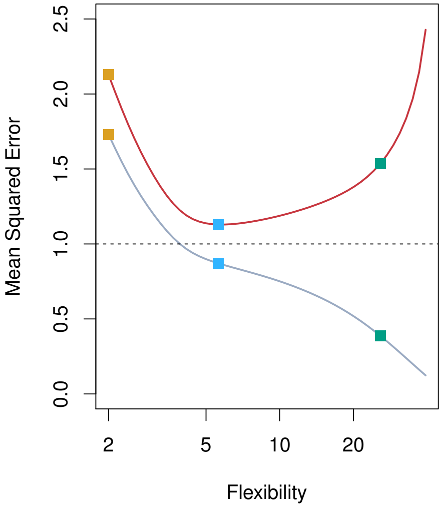
Let us compare $E_{\text{in}}(g_m)$ and $E_{\text{test}}(g_m)$ for $m = 1, 2, \ldots, M$ on an example (with $M = 3$).

We start from a function f which we know. We generate datasets $\mathcal{D}$ and $\mathcal{D}_{\text{test}}$ from f by sampling points and adding a small amount of noise (with mean 0). We then find the hypothesis g_m that minimizes the training error for each hypothesis set $\mathcal{H}_m$.

Obviously, in general, we do not know the "true" function f; this is just for illustration purposes.

Training and test errors in regression (2/6)

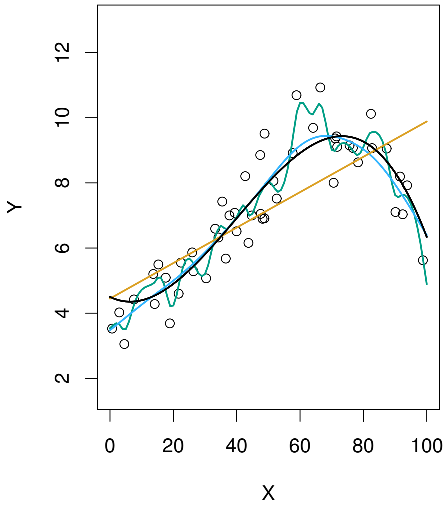


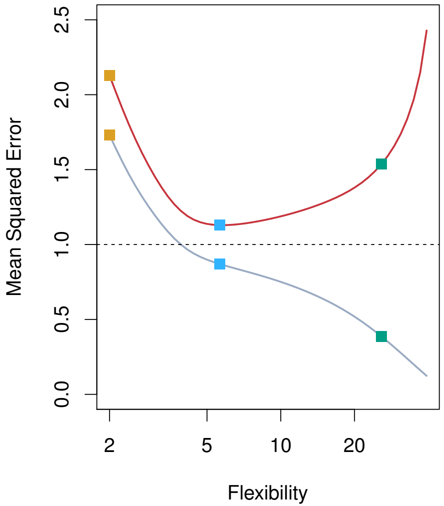


Black: true curve f
Orange: linear regression
Blue/green: nonlinear regressions

Grey: Training MSE
Red: Test MSE
Dashed: Minimum test MSE

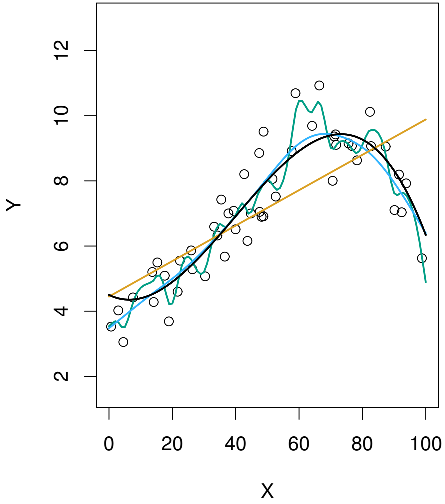
Training and test errors in regression (2/6)

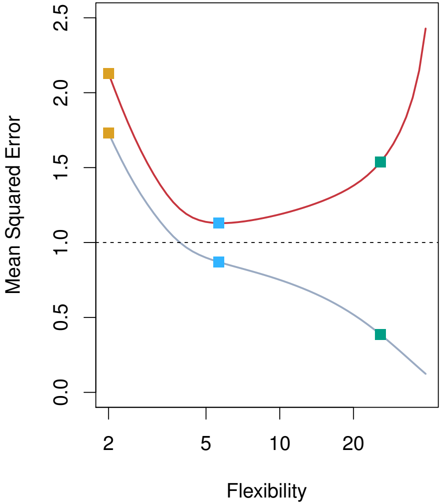




Here, **flexibility** refers to the "degrees of freedom" of the hypothesis set. For example, two parameters for linear regression, and more for nonlinear regression. The dashed line represents the **theoretical minimum test error** due to noise (called *irreducible error*).

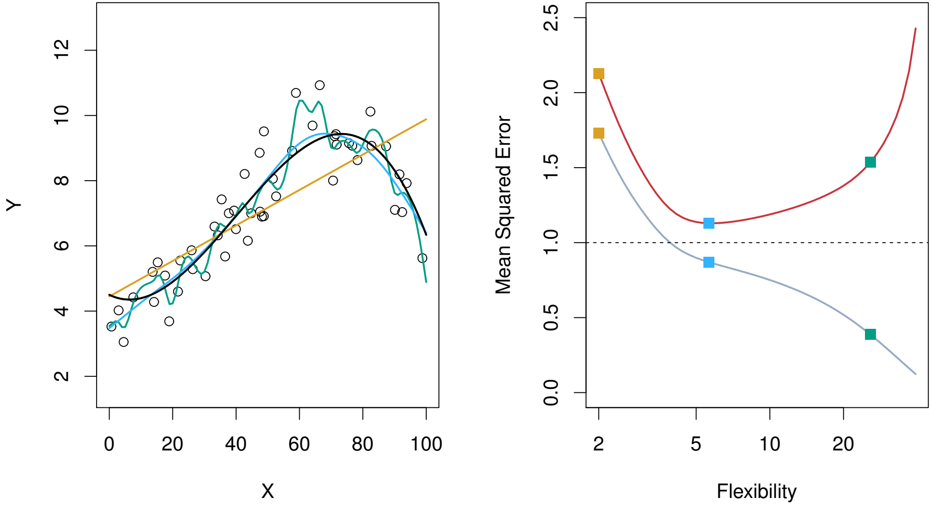
Training and test errors in regression (2/6)





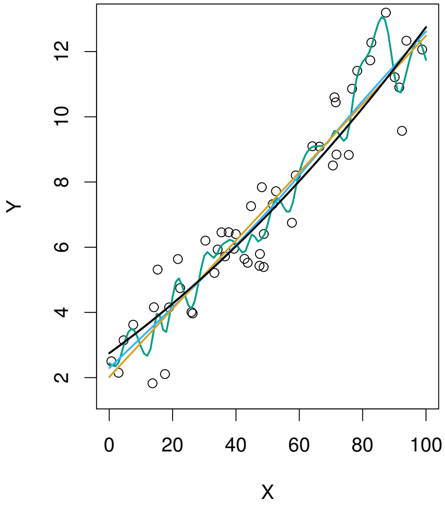
It is natural that the **training MSE decreases as the flexibility of the hypothesis set increases**, since we compute an argmin over a larger set. However, the test MSE may increase if the hypothesis set is too flexible.

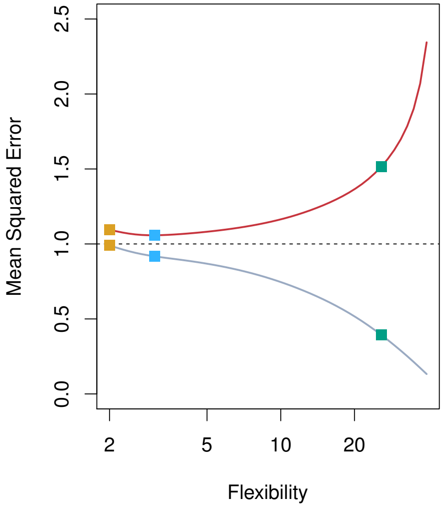
Training and test errors in regression (2/6)



Key takeaway: flexibility is not always better; *U-shaped* test error curve.

Training and test errors in regression: simpler f (3/6)

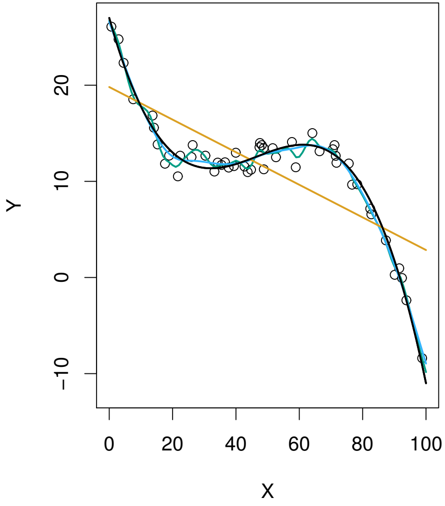


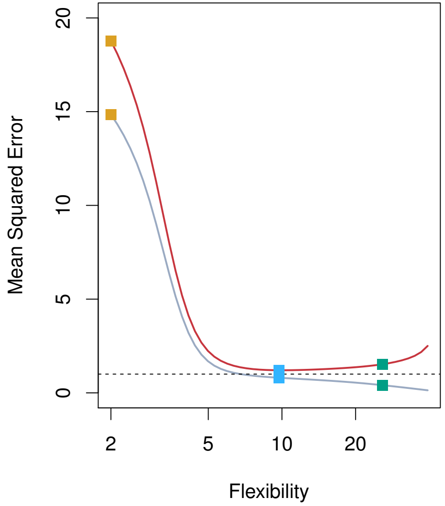


Black: true curve f
Orange: linear regression
Blue/green: nonlinear regression

Grey: Training MSE
Red: Test MSE
Dashed: Minimum test MSE

Training and test errors in regression: more complex f (4/6)

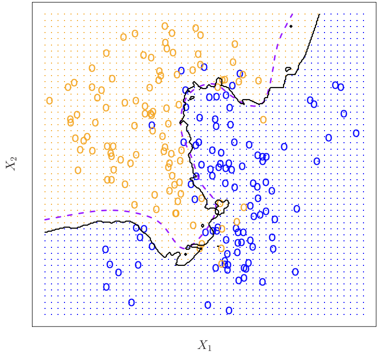




Black: true curve f
Orange: linear regression
Blue/green: nonlinear regression

Grey: Training MSE
Red: Test MSE
Dashed: Minimum test MSE

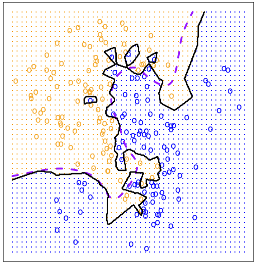
Training and test errors in classification (5/6)

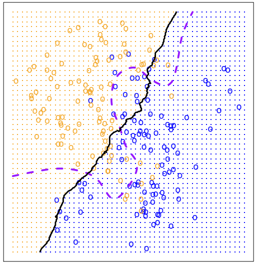


The same phenomenon occurs with classification: too much flexibility could lead to a increase in the test error.

Above: KNN with $K = 10$.
Bottom left: KNN with $K = 1$.
Bottom right: KNN with $K = 100$.

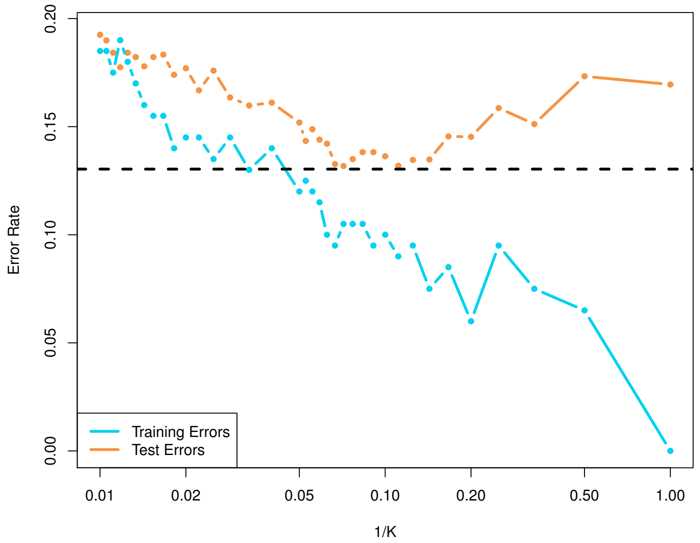
Observe that taking $K = 1$ leads to a training error of 0.



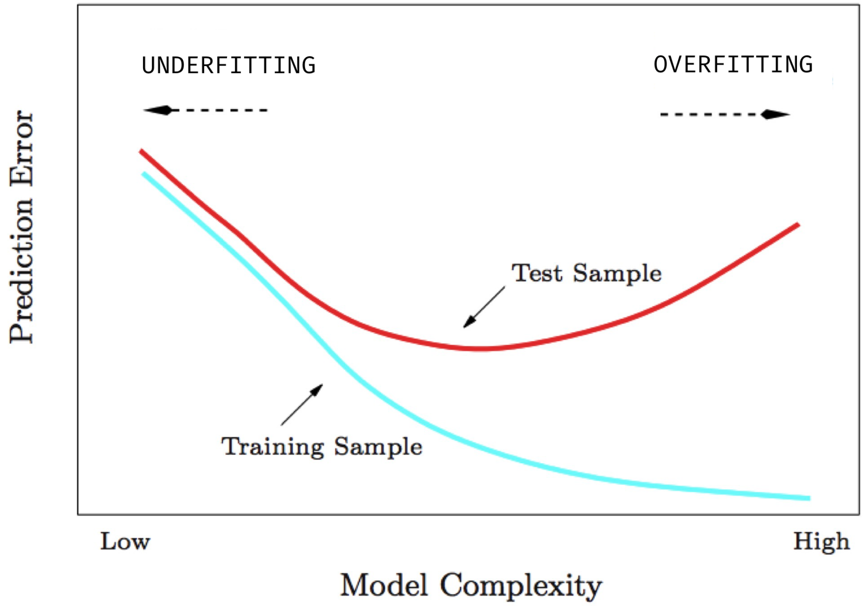


Training and test errors in classification (6/6)

The training and test errors of KNN as the flexibility increases (i.e., as K decreases). The dashed line represents the minimum test error.



A fundamental picture: overfitting vs. underfitting



Training and test errors

Consider

$$f = \operatorname*{argmin}_{h\colon \mathcal{X}\to\mathcal{Y}} E_{\text{out}}(h),$$

$$g^* = \operatorname*{argmin}_{h\in\mathcal{H}} E_{\text{out}}(h),$$

and

$$g = \operatorname*{argmin}_{h\in\mathcal{H}} E_{\text{in}}(h).$$

How different are $E_{\text{out}}(g)$ and $E_{\text{out}}(f)$?

The approximation-generalization tradeoff

The difference between the out-of-sample error of g and f can be decomposed as follows

$$E_{\text{out}}(g) - E_{\text{out}}(f) = \underbrace{\left[E_{\text{out}}(g^*) - E_{\text{out}}(f)\right]}_{\text{Approximation error}} + \underbrace{\left[E_{\text{out}}(g) - E_{\text{out}}(g^*)\right]}_{\text{Estimation error}}.$$

- **Approximation error** is how far the entire hypothesis set is from f. Larger hypothesis sets have lower approximation error.
- **Estimation error** is how good g is with respect to the best function in the hypothesis set. Larger hypothesis sets have higher estimation error because it is harder to find a good prediction function based on limited data.

This is called the **approximation-generalization** tradeoff.

Table of contents

E_{in} for MLE

Recall that, given a set of possible distributions

$$\mathcal{H} = \{p(y;\boldsymbol{\theta}) \mid \boldsymbol{\theta} \in \boldsymbol{\Theta}\},$$

and a dataset $y_1, y_2, \ldots, y_n$, the maximum log-likelihood estimator is given by

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}\in\boldsymbol{\Theta}}{\operatorname{argmax}} \sum_{i=1}^{n} \log\, p(y_i;\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}\in\boldsymbol{\Theta}}{\operatorname{argmin}} \underbrace{\frac{1}{n}\sum_{i=1}^{n} -\log\, p(y_i;\boldsymbol{\theta})}_{E_{\text{in}}(\boldsymbol{\theta})}. \tag{3}$$

Since each hypothesis h is completely characterized by $\boldsymbol{\theta}$, this is equivalent to

$$g = \underset{h\in\mathcal{H}}{\operatorname{argmin}}\ E_{\text{in}}(h).$$

E_{out} for MLE

By the (strong) law of large numbers,

$$\frac{1}{n}\sum_{i=1}^{n} -\log p(y_i;\boldsymbol{\theta}) \overset{n\to\infty}{\longrightarrow} \mathbb{E}[-\log p(y;\boldsymbol{\theta})].$$

In other words, we can think of maximum likelihood estimation as trying to minimize

$$E_{\text{out}}(\boldsymbol{\theta}) = \mathbb{E}[-\log p(y;\boldsymbol{\theta})].$$

E_{out} for MLE

$$\begin{aligned}
\underset{\boldsymbol{\theta}\in\boldsymbol{\Theta}}{\operatorname{argmin}}\ E_{\text{out}}(\boldsymbol{\theta}) &= \underset{\boldsymbol{\theta}\in\boldsymbol{\Theta}}{\operatorname{argmin}}\ \mathbb{E}[-\log p(y;\boldsymbol{\theta})] \\
&= \underset{\boldsymbol{\theta}\in\boldsymbol{\Theta}}{\operatorname{argmin}}\ \mathbb{E}\left[\log p(y) - \log p(y;\boldsymbol{\theta})\right] \\
&= \underset{\boldsymbol{\theta}\in\boldsymbol{\Theta}}{\operatorname{argmin}}\ \mathbb{E}\left[\log\left(\frac{p(y)}{p(y;\boldsymbol{\theta})}\right)\right] \\
&= \underset{\boldsymbol{\theta}\in\boldsymbol{\Theta}}{\operatorname{argmin}}\ \int \log\left(\frac{p(y)}{p(y;\boldsymbol{\theta})}\right) p(y)\ \mathrm{d}y \\
&= \underset{\boldsymbol{\theta}\in\boldsymbol{\Theta}}{\operatorname{argmin}}\ \mathrm{KL}(p_\theta, p),
\end{aligned}$$

where $KL(q, p)$ is the **Kullback-Leibler divergence** between two distributions q and p, which measures the discrepancy between the two distributions. It is also called *relative entropy*. Note that KL-divergence is not a distance measure (it is not symmetric).
You can compare this general formula with the expression we found for the MLE of the logistic regression.