The Evaluation of Management Practices

6. Predictions and Machine Learning

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1. Introduction

What is Machine Learning?

It is hard to find one accepted definition of machine learning (ML).

- For our purposes, we will treat the terms machine learning and statistical learning as identical.
- In this respect, the goal is to cover methods that are able to predict an outcome of interest based on inputs.
  - Example: Predict a house's selling price based on the features of it.
  - Another example: Predict whether an employee will leave a company based on his/her age, wage,...
- Both of the examples are instances of what we call *supervised learning*. There are, however, other types of learning problems.

Types of Machine Learning

Supervised Learning

- The task of learning a function that maps an input to an output based on example input-output pairs.
- The learning method learns from a training sample consisting of a set of input-output observations.
- In general, there are two types of supervised learning problems: *regression* and *classification*.
- In a regression problem, the outcome is quantitative:
  - Example: Predict a house's selling price based on the features of it.
- In a classification problem, the outcome takes values in a finite unordered set.
  - Example: Predict whether an employee will leave a company based on his/her age, wage,...

Unsupervised Learning

- We observe inputs but no outputs
- We can seek to understand the relationship between the variables or between the observations
- For example, in a market segmentation study we might observe multiple characteristics for potential customers and attempt to see if customers can be clustered into groups based on these characteristics
- If we have high-dimensional data, we might use unsupervised methods to project our inputs onto a lower dimensional space
- This can be a pre-processing step for a supervised learning method
- We do not cover unsupervised learning here.

Starting point

- Dependent variable (output) Y.
  - In a regression problem, Y is quantitative (i.e.,$Y \in \mathbb{R}$).
  - In a classification problem, Y takes values in a finite unordered set.
- Independent variables (inputs) are denoted by the p-dimensional vector X.
- (X, Y) follows the joint distribution P. Furthermore, $P_{Y|X}$ denotes the conditional distribution of Y given X.
- We have a sample $\mathcal{D} = \{(x_1, y_1), \ldots, (x_N, y_N)\}$ of known observation drawn from P.
- Goal:
  - Estimate a function f that accurately predicts Y given X.
  - Understand which independent variables affects the dependent variable, and how.
  - Assess the quality of our predictions and make inferences.

2. Regression

Regression problem

- Note that one of our goals is to assess the quality of our predictions based on the function f that makes predictions of Y given X.
- To do this, we need some measurement of what a “good” and “bad prediction” is. Specifically, we need a “loss” function that penalizes “bad” predictions that are far away from the outcome.
- A common choice in a regression problem is to use the squared loss:

$$\ell(f(x), y) = (y - f(x))^2 \tag{1}$$

Suppose we knew $P_{Y|X}$. The following property follows:

CEF prediction property

Let $f(x) = E[Y|X = x]$, i.e., the conditional expectation function (CEF). Furthermore, let m be any function. It follows that the CEF solves:

$$f(x) = \underset{m(X)}{\arg\min}\, E[(Y - m(X))^2|X = x] \tag{2}$$

- Hence, if the squared loss is our measurement to which we evaluate the quality of our predictions, we can do no better than the CEF.
- That is, if we knew the CEF, we could make predictions on which values Y would take for different values of X.

In addition, recall the following property of the CEF:

CEF decomposition property

Let $f(x) = E[Y|X = x]$, i.e., the conditional expectation function (CEF). We can decompose Y as follows:

$$Y = f(x) + \epsilon \tag{3}$$

where

1. ϵ is mean independent of X: $E[\epsilon|X = x] = 0$.
2. ϵ is uncorrelated with any function of X.

- Hence, f captures all of the variation in Y that is predictable by X.
- However, usually "noise" remains which means that we cannot perfectly predict Y given X, even if we knew the CEF.

The irreducible error

Suppose we have estimated $f(x)$ by $\hat{f}(x)$ for $X = x$. Then we have

$$E[(Y - \hat{f}(X))^2 | X = x] = \underbrace{(f(x) - \hat{f}(x))^2}_{\text{reducible}} + \underbrace{Var[\epsilon]}_{\text{irreducible}} \tag{4}$$

- We focus on techniques for estimating f with the aim of minimizing the reducible error.
- The irreducible error provides an upper bound on the accuracy, but is almost always unknown.

Estimating f with $\mathcal{D}$ - KNN regression

With our training data, we might attempt to directly apply the concept of $E[Y|X = x]$ by asking, at each point x, for the average y.

- Since we rarely have sufficient data points to do this, we can settle for:

  $$\hat{f}(x) = \frac{1}{K} \sum_{x_i \in N_K(x)} y_i \tag{5}$$

  Where $N_K(x)$ is a neighborhood containing the K "closest" known points of x in $\mathcal{D}$. Note:

- Expectation is approximated by averaging over sample data;
- Conditioning at a point is relaxed to conditioning on some region "close" to the target point.
- This approach is called K nearest neighbors (KNN) regression.

Estimating f with $\mathcal{D}$ - Linear regression

Another (parametric) approach is to assume that f (CEF) is approximately linear:

$$f(X) \approx \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p \tag{6}$$

- Although f is almost never linear, such an assumption is reasonable in many settings.
- Based on our sample $\mathcal{D}$ we thus estimate:

$$\hat{f}(x) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p \tag{7}$$

- See the previous lecture slides on regression for further details.

Parametric vs. Non-parametric methods

Broadly speaking, we can assign any of the regression (and classification) methods into one of the following two groups:

1. Parametric methods
   - We make an assumption about the functional form of f.
   - For example, if we assume f is linear, we only need to estimate $p + 1$ coefficients as opposed to an arbitrary p-dimensional function.
2. Non-parametric methods
   - No explicit assumptions about the functional for of f.
   - Attempts to give an estimate of f close to observed data points subject to pre-specified constraints.

Both methods have their pros and cons as we shall see.

Example

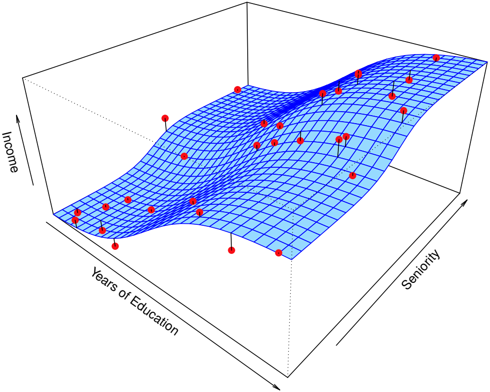


Figure: Simulated data: Income as a function of years of education and seniority. The blue surface represents the true underlying relationship (i.e. f). Red dots indicate observed values for 30 individuals (i.e. $\mathcal{D}$) (See ISLR p. 18)

Parametric estimation:

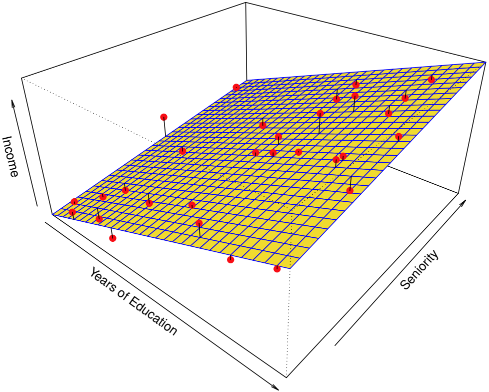


Figure: A linear model fit by least squares:
$\hat{f} = \hat{\beta}_0 + \hat{\beta}_1 * \textit{education} + \hat{\beta}_2 * \textit{seniority}$ (See ISLR p. 22)

Non-parametric estimation:

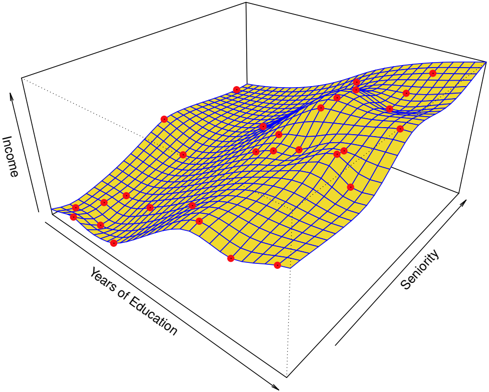


Figure: A rough thin-plate spline fit to the same income data (See ISLR p. 24)

Prediction Accuracy vs. Model Interpretability

Why would we ever choose to use more restrictive models instead of a very flexible approach?

- More complex models require more data.
- Recall that one of our goals is to understand how the independent variables vary with Y.
  - Some of the models become so complex that understanding how any individual input is associated with the output becomes difficult
- We might overfit with highly flexible methods. We will see this shortly.

Assessing Model Accuracy

Why introduce many different methods?

- No Free Lunch: No one method dominates all others over all possible data sets.

Hence an important task is deciding on the best method for a given data set. To decide on a method, we need a metric to evaluate the quality of the predictions.

- We could compute the mean squared error directly in our sample $\mathcal{D}$:

$$MSE_{\mathcal{D}} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{f}(x_i))^2 \tag{8}$$

- However, as $Y = f(x) + \epsilon$, this will in most cases be a biased estimate of the expected squared error.
- Specifically, it may substantially underestimate the error of complex models that are fitting the "noise".

- Instead, a better approach is to have a designated hold-out or test set $\mathcal{D}_{Te} = \{(x_1, y_1), \ldots, (x_M, y_M)\}$ to estimate it:

$$MSE_{\mathcal{D}_{Te}} = \frac{1}{M}\sum_{i=1}^{M}(y_i - \hat{f}(x_i))^2 \tag{9}$$

- This test MSE will then serve as a unbiased estimate of the expected squared error.
- However, notice that this cannot be done without a cost:
  - To construct a test set, we need to split our sample $\mathcal{D}$ into a training set $\mathcal{D}_{Tr}$ on which we fit our model, and a test set $\mathcal{D}_{Te}$ on which we evaluate its predictions.
- Let us consider some simulated examples to understand why this is necessary.

Example

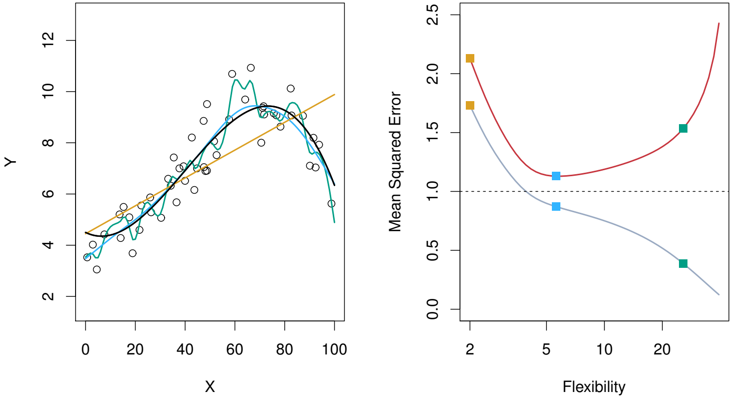


Figure: Simulated data: true f (black), linear regression line (orange), and two smoothing splines (blue and green) (See ISLR p. 31)

Example

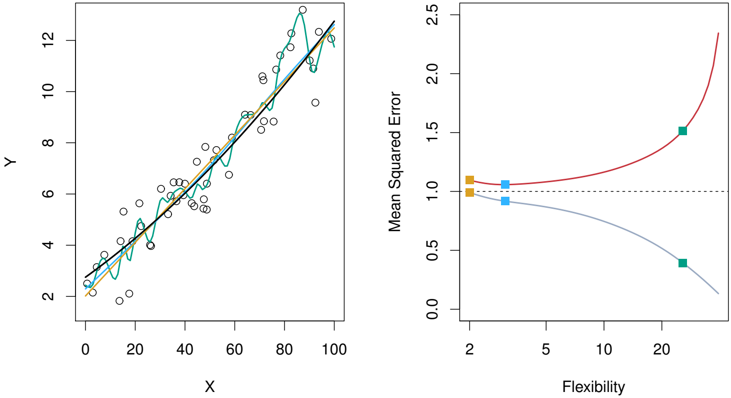


Figure: Simulated data: true *f* (black), linear regression line (orange), and two smoothing splines (blue and green) (See ISLR p. 33)

Example

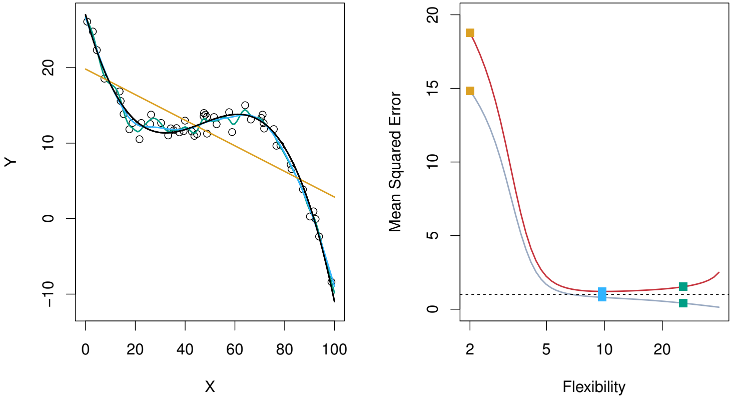


Figure: Simulated data: true f (black), linear regression line (orange), and two smoothing splines (blue and green) (See ISLR p. 33)

The Bias-Variance Tradeoff

We saw that the test MSE tends to be U-shaped

- The shape is the result of two competing forces
- More formally, given we draw a test observation (x_0, y_0) from P, the expected squared prediction error is given by

$$E[(y_0 - \hat{f}(x_0))^2] = \underbrace{Var[\epsilon]}_{\text{irreducible error of } f} + \underbrace{Var[\hat{f}(x_0)]}_{\text{variance of } \hat{f}} + \underbrace{[f(x_0) - E[\hat{f}(x_0)]]^2}_{\text{bias}^2 \text{ of } \hat{f}}$$

- $E[(y_0 - \hat{f}(x_0))^2]$ is the expected squared error
  - i.e. the average test MSE if we repeatedly estimated f using a large number of training sets, and tested each at (x_0, y_0)

A comparison of bias and variance in the three cases :

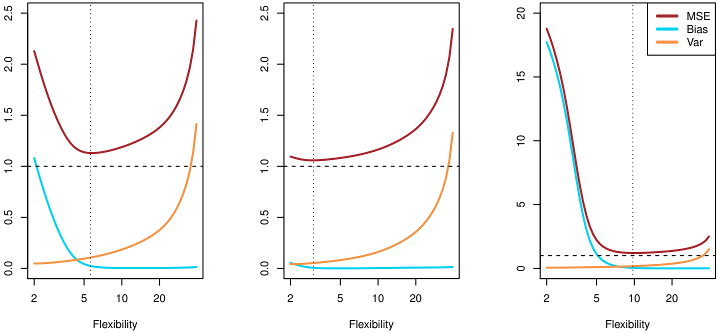


Figure: Squared bias (blue), variance (orange), $Var(\varepsilon)$ (dashed), and test MSE (red) for the three data sets (See ISLR p. 36)

Python - Scikit-Learn

- Suppose we have a dataframe *df* consisting of two columns *a* and *b*.
- We wish to apply a model that predicts *b* based on *a*.
- To do this, we first define *y* as a vector and *X* as a matrix:

```
y = df[‘b’]
X = df[[‘a’]]
```

- To perform a linear regression using Scikit-Learn, we can do as follows:

```
from sklearn.linear_model import LinearRegression
lr = LinearRegression().fit(X,y)
```

- Suppose we want to make a prediction at *X=[[1]]*:

```
pred = lr.predict([[1]])
```

- To perform e.g., 10NN regression in Scikit-Learn, we can do as follows:

```
from sklearn.neighbors import KNeighborsRegressor
knn = KNeighborsRegressor(n_neighbors=10).fit(X,y)
```

- Predictions can be made in the same manner as for linear regression.

Your task - The Bias-Variance Tradeoff

- Write a script that generates a fictitious data set with 10,000 observations:

  ```
  n=10000
  df = pd.DataFrame(index=range(n))
  ```

- Generate a uniformally distributed random variable *age* with 18 and 70 as the lower and upper boundary, respectively:

  ```
  df[‘age’] = np.random.uniform(18,70,size=n)
  ```

- Generate a random variable *income* (yearly, in 1,000s) as a function of *age*:

  ```
  d[‘income’]=(2*df[‘age’]-0.002*df[‘age’]**2+
  np.random.normal(0,10,size=n)
  ```

- Note that in this setting, $Y =$ `df[‘income’]`.

Conceptual questions:

1. What is the CEF f?
2. What is the irreducible error?
3. What is $f(age)$ for $age = 50$?

Your task - The Bias-Variance Tradeoff (cont'd)

Exercises:

1. Suppose you estimate f by $\hat{f} = \hat{\beta}_0 + \hat{\beta}_1 * age$. Attempt to estimate the (squared) bias and variance of $\hat{f}$ at $age = 50$, based on a sample size of 10,000 by resampling the data 100 times.
2. Suppose you estimate f by a 5NN regression. Attempt to estimate the (squared) bias and variance of $\hat{f}$ at $age = 50$, based on a sample size of 10,000 by resampling the data 100 times. Compare your result to 1. Which of the two has a higher bias and variance, respectively.

3. Classification

Classification problem

Now Y takes values in a finite and unordered set $\mathcal{Y}$.

- Suppoe $\mathcal{Y}$ contains K elements numbered $1, ..., K$
- Let $p_k(x) = Pr(Y = k|X = x)$, for $k = 1, ..., K$
- Suppose we knew these conditional probabilities.
- Then, the *Bayes optimal classifier* at x given by

$$f(x) = j \text{ if } p_j(x) = \max\{p_1(x), ..., p_K(x)\} \tag{10}$$

is optimal in the sense that it minimizes the expected misclassification rate:

$$E[\mathbb{1}_{\{Y \neq f(X)\}}] \tag{11}$$

Estimating f with $\mathcal{D}$ - KNN classification

Given our sample $\mathcal{D}$, we might attempt to apply a KNN once again to

1. approximate the conditional distribution of Y given X

$$\hat{p}_j(x) = \frac{1}{K} \sum_{x_i \in N_K} \mathbb{1}_{\{y_i = j\}} \tag{12}$$

2. predict that a given observation belongs to the class with highest estimated probability

$$\hat{f}(x) = j \text{ if } \hat{p}_j(x) = \max\{\hat{p}_1(x), ..., \hat{p}_K(x)\} \tag{13}$$

Thus, KNN gives an estimate for the conditional probabilities as well as for the decision boundary

Example

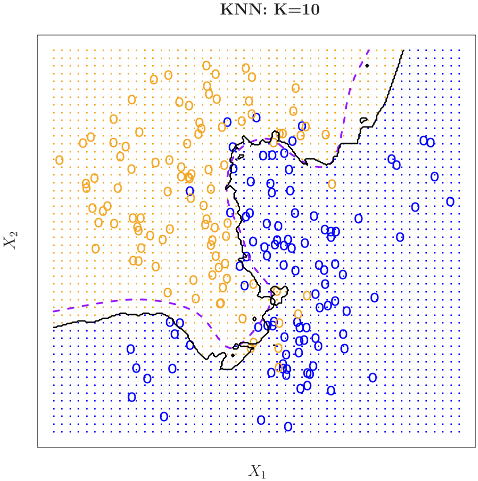


Figure: Bayes decision bounday (dashed), 10-NN decision boundary (black) (See ISLR p. 41)

Example

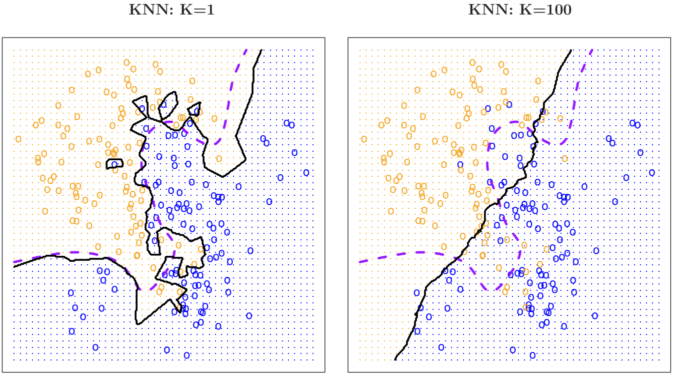


Figure: Bayes decision bounday (dashed), Left: 1-NN decision boundary (black), Right: 100-NN decision boundary (See ISLR p. 41)

Example

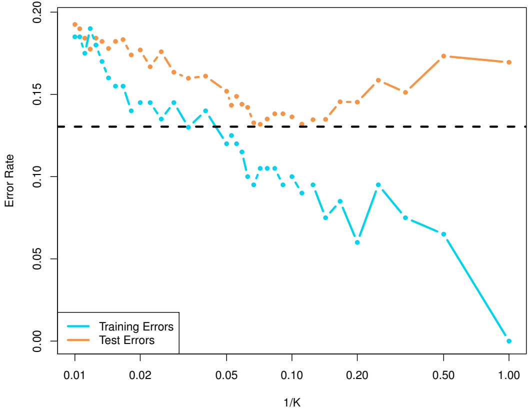


Figure: KNN training error rate (blue, 200 obs), test error rate (orange, 5,000 obs), Bayes error rate (dashed) (See ISLR p. 42)

Estimating f with $\mathcal{D}$ - Linear regression

- Suppose $\mathcal{Y} = \{0, 1\}$. In this case, we could consider using linear regression to estimate p_1.
- Since, in the population, we have $E[Y|X = x] = p_1(x) = Pr(Y = 1|X = x)$, regression seems to be good for this task.
- However, if the range of X is not limited, we will see probability estimates below zero and above one.
- If we are only concerned with classification, then the linear regression might still be fine.
- However, in the case of multiple unordered classes, there is no straightforward way of applying linear regression.

Estimating f with $\mathcal{D}$ - Logistic regression

- To avoid getting probability estimates outside $[0,1]$, we model $p(X)$ using a function which lies in the interval for all values of X.
- In the case of logistic regression, we use the logistic or sigmoid function.

$$\hat{p}_1(x) = \frac{exp(\hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p)}{1 + exp(\hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p)} \tag{14}$$

- To estimate (14) we use maximum likelihood.
- An additional benefit is that we can extend logistic regression to the case of multiclass classification.

Example

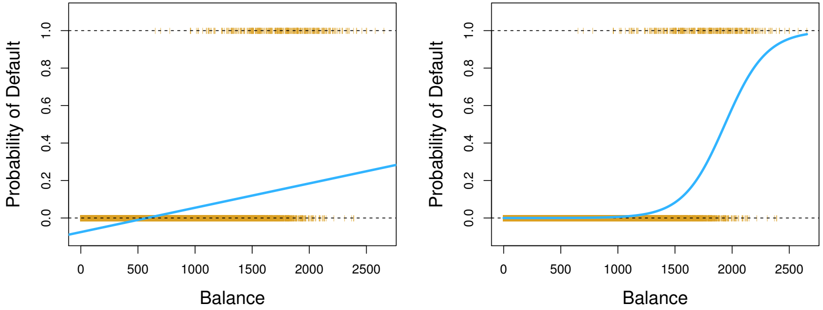


Figure: Left: Estimated probability of default using linear regression. Right: Same estimation using logistic regression (See ISLR p. 131)

- Some methods build structured models for $f(x)$.
  - e.g., support vector machines.
- Other methods, as we have seen here, build structured models for representing $p_k(x)$.
  - e.g., logistic regression.

Python - Scikit-Learn

- Suppose we have a training set (X_{train}, y_{train}) and a test set (X_{test}, y_{test}).
- To fit a logistic regression on the training set using Scikit-Learn, we can do as follows:

  ```
  from sklearn.linear_model import LogisticRegression
  logreg = LogisticRegression().fit(X_train,y_train)
  ```

- We can estimate the misclassification rate on the test set as follows:

  ```
  from sklearn.metrics import accuracy_score
  preds = logreg.predict(X_test)
  1-accuracy_score(y_test,preds)
  ```

- To make a probabilistic prediction at e.g., [[1]]:

  ```
  pred = logreg.predict_proba([[1]])
  ```

- To perform e.g., 10NN classification in Scikit-Learn, we can do as follows:

  ```
  from sklearn.neighbors import KNeighborsClassifier
  knn =
  KNeighborsClassifier(n_neighbors=10).fit(X_train,y_train)
  ```

- Making predictions and calculating the misclassification rate then follows in the same manner as for the logistic regression.

Your task - Classification

- Import the *Default* data set:

```
path_to_df = ‘https://raw.githubusercontent.com/
armoutihansen/EEMP2021/main/datasets/Default.csv’
df = pd.read_csv(path_to_df)
```

- Let X consist only of the variable *balance* and let y be a binary indicator that equals 1 if the customer defaulted on his debt and 0 otherwise:

```
X=df[[‘balance’]]
y=(df[‘default’]==‘Yes’)*1
```

Exercises:

1. Fit the linear regression: $\hat{f}(balance) = \hat{\beta}_0 + \hat{\beta}_1 * balance$ on X, y. What is the estimated probability of default given a balance of 200? Is this estimate sensible?
2. Now fit a logistic regression on X, y and once again estimate the probability of default given a balance of 200. Is this a more sensible estimate?

Your task - Classification (cont'd)

- Now split the sample into a training set and test set:

  ```
  from sklearn.model_selection import train_test_split
  X_train, X_test, y_train, y_test =
  train_test_split(X,y,test_size=0.5)
  ```

3. Fit a 1NN classifier on the training set. Now calculate the misclassification rate on the training set and test set, respectively. Why is there a difference between these two estimates?
4. Fit a logistic regression on the training set and calculate the misclassification rate on the test set. Does this imply that the logistic regression is better or worse than the 1NN classifier in this problem? Why do you think that is?

4. Model selection and assessment

Motivation

- Assessment of the general performance of our model is what we truly care about.

- The *generalization performance* refers to a model's prediction capability on independent test data.
  - Or, more generally, its capability in the population.

- If we know methods generalization performance, we
  1. can select the best of our considered models;
  2. know the best model's performance on unseen test data.

Definitions

- Based on our choice of ℓ, we would like to know our model's general performance
- The *generalization error* is the error over an independent sample

$$Err_{\mathcal{D}} = E[\ell(Y, \hat{f}(X))|\mathcal{D}] \tag{15}$$

  i.e. the expected error of our model, given that (X, Y) are drawn from their joint distribution P, conditional on being trained on $\mathcal{D}$.

- Estimation of $Err_{\mathcal{D}}$ is our goal, however it turns out that our tools for estimation better estimate the *expected generalization error*

$$Err = E[\ell(Y, \hat{f}(X))] = E[E[\ell(Y, \hat{f}(X))|\mathcal{D}]] = E[Err_{\mathcal{D}}] \tag{16}$$

  i.e. the expected error over everything that is random – including the sample $\mathcal{D}$.

- The *training error* is simply the average loss in $\mathcal{D}$

$$\bar{err} = \frac{1}{N}\sum_{i=1}^{N}\ell(y_i, \hat{f}(x_i)) \tag{17}$$

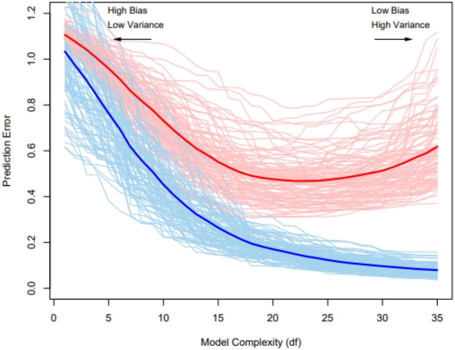


Figure: Light blue curves show $\bar{err}$ while light red curves show $Err_{\mathcal{D}}$ for 100 samples of size 50, as model complexity is increased. The solid curves show $E[\bar{err}]$ and Err, respectively (See ESL p. 220)

Goals

- Often our model will have a hyper/tuning parameter or parameters.
  - e.g. # of neighbors for the KNN method.
- We wish to find the parameter(s) that minimizes the generalization error.
- However, we do in fact have two separate goals in mind:

1. **Model selection**: estimating the performance of different models in order to choose the best one.
2. **Model assessment**: having chosen a final model, estimating its prediction error (generalization error).

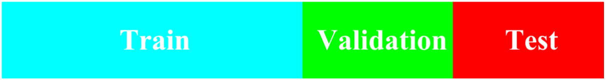
Validation-set approach (without model selection)

Idea: Estimate the generalization error by holding out a subset of the training observations from the fitting process, and then evaluate our model's predictions on those held out observations.

- Randomly divide the sample $\mathcal{D}$ into two parts: a training set $\mathcal{D}_{Tr}$ and a test (or validation) set $\mathcal{D}_{Te}$.
- The model is fit on the training set, and the fitted model is used to predict the responses for the observations in the validation set.
- The resulting test error provides an estimate of the expected generalization error.

Validation-set approach (with model selection)

- Best approach: randomly divide $\mathcal{D}$ into three parts:



Train

Validation

Test

- We
  - fit our methods on the training data $\mathcal{D}_{Tr}$ ($\sim 50\%$)
  - estimate error for model selection on the validation data $\mathcal{D}_{val}$ ($\sim 25\%$)
  - estimate the expected generalization error for our best model on the test data $\mathcal{D}_{Te}$ ($\sim 25\%$)
- If we use the test data for both model selection and assessment, we will usually underestimate the true test error of the best model

K-fold CV

- The error estimates of the validation approach may heavily depend on the splits of the sample.
- An approach of dealing with this is to instead use *K-fold Cross Validation* (CV).

1. Randomly split the data into K roughly equal parts
2. For each $k = 1, ..., K$:
   - leave the kth part out and fit the model using the other $K - 1$ parts: $\hat{f}^{-k}(x)$
   - calculate the error of $\hat{f}^{-k}(x)$ on the held out kth part
3. Average the k errors
   - Define the index function $\kappa : \{1, ..., N\} \rightarrow \{1, ..., K\}$ (allocating membership)
   - Then, the K-fold cross validation estimate of *Err* is:

$$CV(\hat{f}) = \frac{1}{N} \sum_{i=1}^{N} \ell(y_i, \hat{f}^{-\kappa(i)}(x_i)) \tag{18}$$

What value should we choose for K?

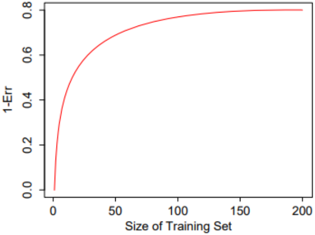


Figure: Hypothetical learning curve for a classifier on a given task: a plot of $1 - Err$ versus the size of the training set N (See ESL p. 243)

- The optimal choice of K depends on the slope of the learning curve
- In general, 5- or 10-fold CV are recommended as a good compromise between bias and variance.

Choosing hyper parameters with CV

- Often we consider models with hyper parameter(s) α
  - e.g. number of neighbors in KNN regression or classification.
- Denote by $\hat{f}^{-k}(x, \alpha)$ the αth model fit with the kth part of data removed
- Then, we have

$$CV(\hat{f}, \alpha) = \frac{1}{N} \sum_{i=1}^{N} \ell(y_i, \hat{f}^{-\kappa(i)}(x_i, \alpha)) \tag{19}$$

- Usually, instead of choosing the $\hat{\alpha}$ which minimizes (19), we apply the "one standard error rule":

choose the most parsimonious model with error no more than one standard error above the best error

Example - Classification

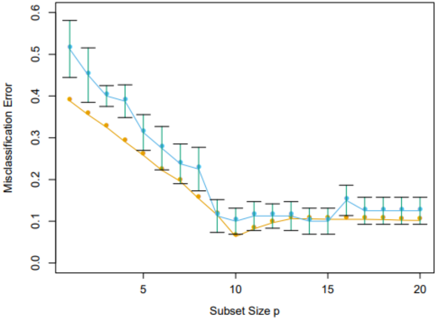


Figure: Test error (orange) and 10-fold CV curve (blue) from a single training set (See ESL p. 244)

- Which model would be chosen here?

CV for both model selection and assessment

- Recall that in the validation set approach:
    - If we use the test data for both model selection and assessment, we will risk underestimating the true test error of the best model
- The same holds with cross validation
- To deal with this problem, two approaches are used in practice:
    1. Leave out a test (or validation) set, use CV for model selection and estimate the generalization error on the test set.
    2. Nested K-fold CV: Model selection on inner CV and model assessment on outer cv.
- Here we opt for option 1.

References

James, G., Witten, D., Hastie, T., & Tibshirani, R. (2013). An introduction to statistical learning (Vol. 112). **Chapter 2,4,5**

Friedman, J., Hastie, T., & Tibshirani, R. (2001). The elements of statistical learning (Vol. 1, No. 10). **Chapters 2,7**