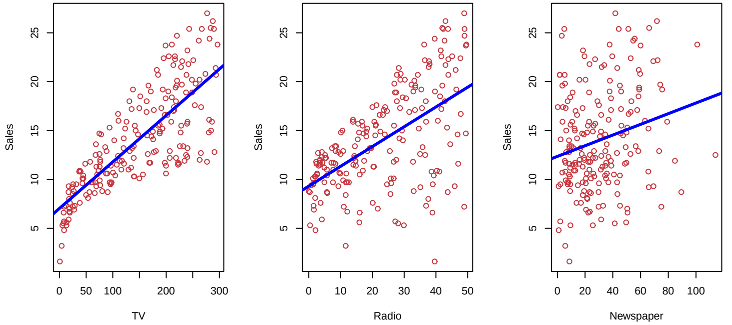
What is Statistical Learning?



Shown are Sales vs TV, Radio and Newspaper, with a blue linear-regression line fit separately to each.
Can we predict Sales using these three?
Perhaps we can do better using a model

$$\texttt{Sales} \approx f(\texttt{TV}, \texttt{Radio}, \texttt{Newspaper})$$

Notation

Here `Sales` is a *response* or *target* that we wish to predict. We generically refer to the response as Y.
`TV` is a *feature*, or *input*, or *predictor*; we name it X_1.
Likewise name `Radio` as X_2, and so on.
We can refer to the *input vector* collectively as

$$X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix}$$

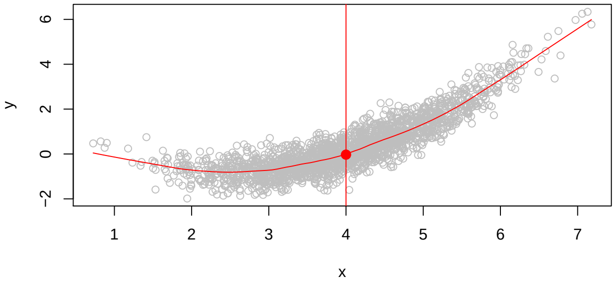
Now we write our model as

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

where ϵ captures measurement errors and other discrepancies.

What is $f(X)$ good for?

- With a good f we can make predictions of Y at new points $X = x$.
- We can understand which components of $X = (X_1, X_2, \ldots, X_p)$ are important in explaining Y, and which are irrelevant. e.g. `Seniority` and `Years of Education` have a big impact on `Income`, but `Marital Status` typically does not.
- Depending on the complexity of f, we may be able to understand how each component X_j of X affects Y.



Is there an ideal $f(X)$? In particular, what is a good value for $f(X)$ at any selected value of X, say $X = 4$? There can be many Y values at $X = 4$. A good value is

$$f(4) = E(Y|X = 4)$$

$E(Y|X = 4)$ means *expected value* (average) of Y given $X = 4$.

This ideal $f(x) = E(Y|X = x)$ is called the *regression function*.

The regression function $f(x)$

- Is also defined for vector X; e.g.
  $f(x) = f(x_1, x_2, x_3) = E(Y|X_1 = x_1, X_2 = x_2, X_3 = x_3)$

The regression function $f(x)$

- Is also defined for vector X; e.g. $f(x) = f(x_1, x_2, x_3) = E(Y|X_1 = x_1, X_2 = x_2, X_3 = x_3)$
- Is the *ideal* or *optimal* predictor of Y with regard to mean-squared prediction error: $f(x) = E(Y|X = x)$ is the function that minimizes $E[(Y - g(X))^2|X = x]$ over all functions g at all points $X = x$.

The regression function $f(x)$

- Is also defined for vector X; e.g. $f(x) = f(x_1, x_2, x_3) = E(Y|X_1 = x_1, X_2 = x_2, X_3 = x_3)$
- Is the *ideal* or *optimal* predictor of Y with regard to mean-squared prediction error: $f(x) = E(Y|X = x)$ is the function that minimizes $E[(Y - g(X))^2|X = x]$ over all functions g at all points $X = x$.
- $\epsilon = Y - f(x)$ is the *irreducible* error — i.e. even if we knew $f(x)$, we would still make errors in prediction, since at each $X = x$ there is typically a distribution of possible Y values.

The regression function $f(x)$

- Is also defined for vector X; e.g. $f(x) = f(x_1, x_2, x_3) = E(Y|X_1 = x_1, X_2 = x_2, X_3 = x_3)$
- Is the *ideal* or *optimal* predictor of Y with regard to mean-squared prediction error: $f(x) = E(Y|X = x)$ is the function that minimizes $E[(Y - g(X))^2|X = x]$ over all functions g at all points $X = x$.
- $\epsilon = Y - f(x)$ is the *irreducible* error — i.e. even if we knew $f(x)$, we would still make errors in prediction, since at each $X = x$ there is typically a distribution of possible Y values.
- For any estimate $\hat{f}(x)$ of $f(x)$, we have

$$E[(Y - \hat{f}(X))^2|X = x] = \underbrace{[f(x) - \hat{f}(x)]^2}_{\textit{Reducible}} + \underbrace{\mathrm{Var}(\epsilon)}_{\textit{Irreducible}}$$

Parametric and structured models

The *linear* model is an important example of a parametric model:

$$f_L(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots \beta_p X_p.$$

- A linear model is specified in terms of $p + 1$ parameters $\beta_0, \beta_1, \dots, \beta_p$.
- We estimate the parameters by fitting the model to training data.
- Although it is *almost never correct*, a linear model often serves as a good and interpretable approximation to the unknown true function $f(X)$.

Assessing Model Accuracy

Suppose we fit a model $\hat{f}(x)$ to some training data $\mathsf{Tr} = \{x_i, y_i\}_1^N$, and we wish to see how well it performs.

- We could compute the average squared prediction error over Tr:

$$\mathrm{MSE}_{\mathsf{Tr}} = \mathrm{Ave}_{i \in \mathsf{Tr}}[y_i - \hat{f}(x_i)]^2$$

This may be biased toward more overfit models.

- Instead we should, if possible, compute it using fresh *test* data $\mathsf{Te} = \{x_i, y_i\}_1^M$:

$$\mathrm{MSE}_{\mathsf{Te}} = \mathrm{Ave}_{i \in \mathsf{Te}}[y_i - \hat{f}(x_i)]^2$$

Bias-Variance Trade-off

Suppose we have fit a model $\hat{f}(x)$ to some training data Tr, and let (x_0, y_0) be a test observation drawn from the population. If the true model is $Y = f(X) + \epsilon$ (with $f(x) = E(Y|X = x)$), then

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

The expectation averages over the variability of y_0 as well as the variability in Tr. Note that $\text{Bias}(\hat{f}(x_0))] = E[\hat{f}(x_0)] - f(x_0)$.

Typically as the *flexibility* of $\hat{f}$ increases, its variance increases, and its bias decreases. So choosing the flexibility based on average test error amounts to a *bias-variance trade-off.*

The Supervised Learning Problem

Starting point:

- Outcome measurement Y (also called dependent variable, response, target).
- Vector of p predictor measurements X (also called inputs, regressors, covariates, features, independent variables).
- In the *regression problem*, Y is quantitative (e.g price, blood pressure).
- In the *classification problem*, Y takes values in a finite, unordered set (survived/died, digit 0-9, cancer class of tissue sample).
- We have training data $(x_1, y_1), \ldots, (x_N, y_N)$. These are observations (examples, instances) of these measurements.

Objectives

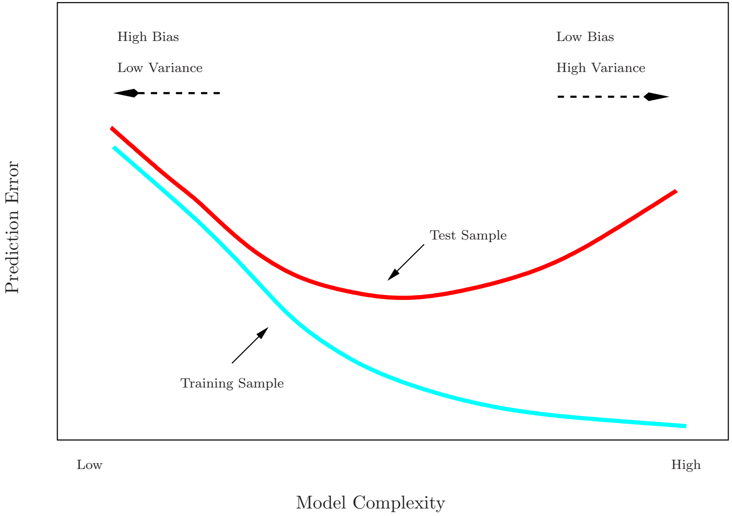
On the basis of the training data we would like to:

- Accurately predict unseen test cases.
- Understand which inputs affect the outcome, and how.
- Assess the quality of our predictions and inferences.

Training Error versus Test error

- Recall the distinction between the *test error* and the *training error:*
- The *test error* is the average error that results from using a statistical learning method to predict the response on a new observation, one that was not used in training the method.
- In contrast, the *training error* can be easily calculated by applying the statistical learning method to the observations used in its training.
- But the training error rate often is quite different from the test error rate, and in particular the former can *dramatically underestimate* the latter.

Training- versus Test-Set Performance



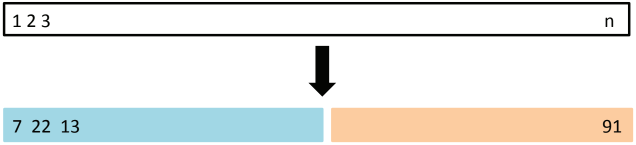
More on prediction-error estimates

- Best solution: a large designated test set. Often not available
- Some methods make a *mathematical adjustment* to the training error rate in order to estimate the test error rate. These include the *Cp statistic*, *AIC* and *BIC*. They are discussed elsewhere in this course
- Here we instead consider a class of methods that estimate the test error by *holding out* a subset of the training observations from the fitting process, and then applying the statistical learning method to those held out observations

Validation-set approach

- Here we randomly divide the available set of samples into two parts: a *training set* and a *validation* or *hold-out set*.
- 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 validation-set error provides an estimate of the test error. This is typically assessed using MSE in the case of a quantitative response and misclassification rate in the case of a qualitative (discrete) response.

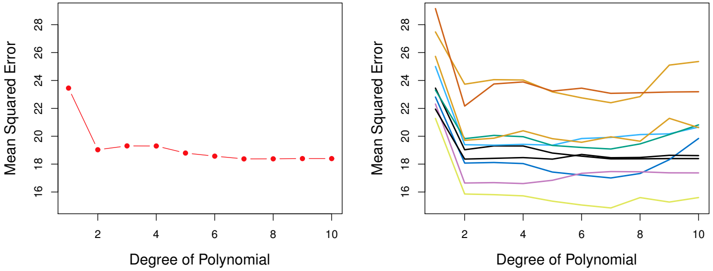
The Validation process



A random splitting into two halves: left part is training set, right part is validation set

Example: automobile data

- Want to compare linear vs higher-order polynomial terms in a linear regression
- We randomly split the 392 observations into two sets, a training set containing 196 of the data points, and a validation set containing the remaining 196 observations.



Left panel shows single split; right panel shows multiple splits

Drawbacks of validation set approach

- the validation estimate of the test error can be highly variable, depending on precisely which observations are included in the training set and which observations are included in the validation set.
- In the validation approach, only a subset of the observations — those that are included in the training set rather than in the validation set — are used to fit the model.
- This suggests that the validation set error may tend to *overestimate* the test error for the model fit on the entire data set.

Drawbacks of validation set approach

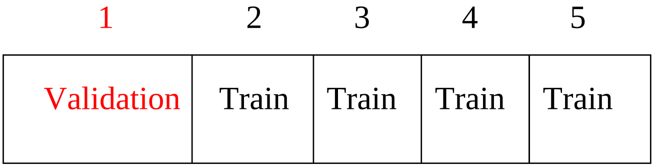
- the validation estimate of the test error can be highly variable, depending on precisely which observations are included in the training set and which observations are included in the validation set.
- In the validation approach, only a subset of the observations — those that are included in the training set rather than in the validation set — are used to fit the model.
- This suggests that the validation set error may tend to *overestimate* the test error for the model fit on the entire data set. *Why?*

K-fold Cross-validation

- *Widely used approach* for estimating test error.
- Estimates can be used to select best model, and to give an idea of the test error of the final chosen model.
- Idea is to randomly divide the data into K equal-sized parts. We leave out part k, fit the model to the other $K - 1$ parts (combined), and then obtain predictions for the left-out kth part.
- This is done in turn for each part $k = 1, 2, \ldots K$, and then the results are combined.

K-fold Cross-validation in detail

Divide data into K roughly equal-sized parts ($K = 5$ here)



The details

- Let the K parts be $C_1, C_2, \dots C_K$, where C_k denotes the indices of the observations in part k. There are n_k observations in part k: if N is a multiple of K, then $n_k = n/K$.
- Compute

$$\mathrm{CV}_{(K)} = \sum_{k=1}^{K} \frac{n_k}{n} \mathrm{MSE}_k$$

where $\mathrm{MSE}_k = \sum_{i \in C_k} (y_i - \hat{y}_i)^2 / n_k$, and $\hat{y}_i$ is the fit for observation i, obtained from the data with part k removed.

The details

- Let the K parts be $C_1, C_2, \ldots C_K$, where C_k denotes the indices of the observations in part k. There are n_k observations in part k: if N is a multiple of K, then $n_k = n/K$.
- Compute

$$\mathrm{CV}_{(K)} = \sum_{k=1}^{K} \frac{n_k}{n} \mathrm{MSE}_k$$

  where $\mathrm{MSE}_k = \sum_{i \in C_k} (y_i - \hat{y}_i)^2 / n_k$, and $\hat{y}_i$ is the fit for observation i, obtained from the data with part k removed.
- Setting $K = n$ yields n-fold or *leave-one out cross-validation* (LOOCV).

A nice special case!

- With least-squares linear or polynomial regression, an amazing shortcut makes the cost of LOOCV the same as that of a single model fit! The following formula holds:

  $$\mathrm{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - h_i}\right)^2,$$

  where $\hat{y}_i$ is the ith fitted value from the original least squares fit, and h_i is the leverage (diagonal of the “hat” matrix; see book for details.) This is like the ordinary MSE, except the ith residual is divided by $1 - h_i$.

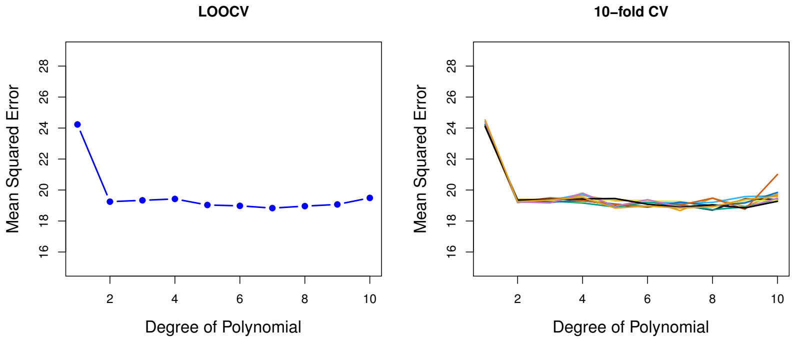
A nice special case!

- With least-squares linear or polynomial regression, an amazing shortcut makes the cost of LOOCV the same as that of a single model fit! The following formula holds:

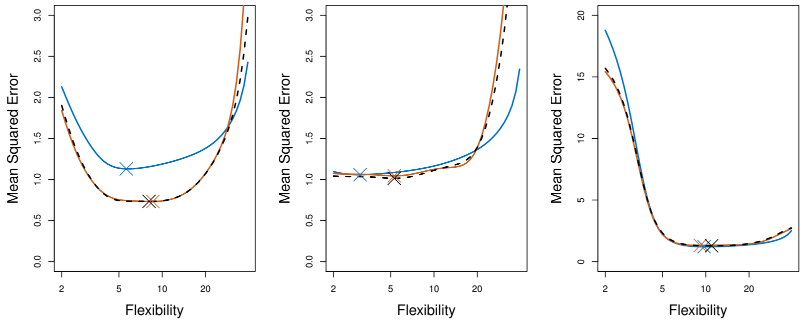
$$\mathrm{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - h_i}\right)^2,$$

  where $\hat{y}_i$ is the ith fitted value from the original least squares fit, and h_i is the leverage (diagonal of the "hat" matrix; see book for details.) This is like the ordinary MSE, except the ith residual is divided by $1 - h_i$.
- LOOCV sometimes useful, but typically doesn't *shake up* the data enough. The estimates from each fold are highly correlated and hence their average can have high variance.
- a better choice is $K = 5$ or 10.

Auto data revisited



True and estimated test MSE for the simulated data



Other issues with Cross-validation

- Since each training set is only $(K-1)/K$ as big as the original training set, the estimates of prediction error will typically be biased upward.

Other issues with Cross-validation

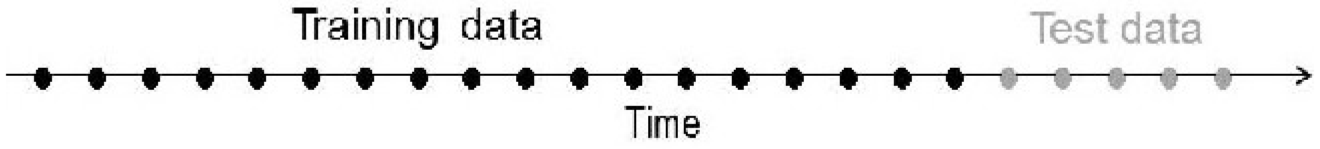
- Since each training set is only $(K-1)/K$ as big as the original training set, the estimates of prediction error will typically be biased upward. *Why?*

Other issues with Cross-validation

- Since each training set is only $(K-1)/K$ as big as the original training set, the estimates of prediction error will typically be biased upward. *Why?*
- This bias is minimized when $K = n$ (LOOCV), but this estimate has high variance, as noted earlier.
- $K = 5$ or 10 provides a good compromise for this bias-variance tradeoff.

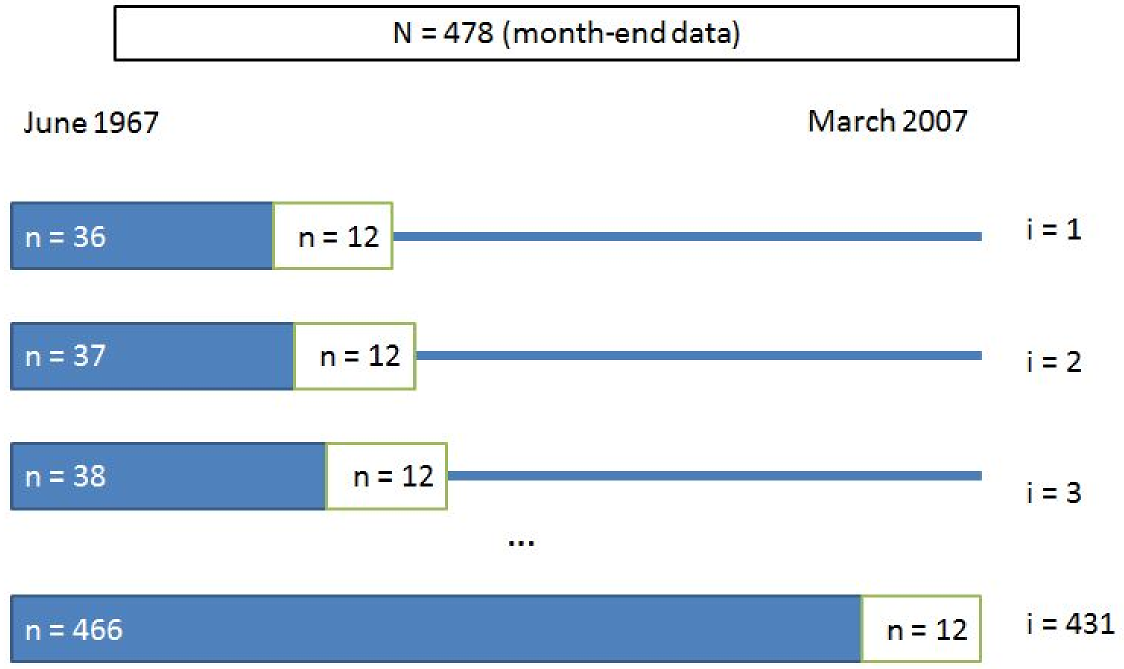
The validation set approach for time series data

- When using time series data, we cannot select the training set and the validation set in a random fashion.
- A splitting of the data in (e.g.) the first ¾ and in the remaining ¼. The first part is the training set and second one is the validation set:



Cross-validation for time series data

- Suppose we have a total of (e.g.) 478 observations, and we use *at least* (e.g.) 36 observations for training and (e.g.) 12 observations for evaluation. The cross-validation procedure would go as follows:



N = 478 (month-end data)
June 1967
March 2007
n = 36
n = 12
i = 1
n = 37
n = 12
i = 2
n = 38
n = 12
i = 3
...
n = 466
n = 12
i = 431