Statistical Learning and Prediction

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This Course

- New methodology for data analysis
- Same models, different focus
- Statistics and Machine Learning: Statistical Learning

Schedule

1. Tue, 11:00-13:00
   Introduction, bias-variance trade-off (MF).

2. Tue, 14:00-16:45
   Classification, resampling, cross validation (TW)

3. Tue, 17:00-18:15
   Regularization, model selection (TW)

4. Wed, 10:00-12:00
   Unsupervised learning (TW)

5. Wed, 13:00-18:00
   Non-linear methods (trees, splines, SVMs) (MF)

Statistical Learning

- Vast set of tools for understanding data.
  - Supervised: $Y \leftarrow f(X_1, \ldots, X_p)$; predict Y on the basis of X
  - Unsupervised: $X_1, \ldots, X_p$; finding structure in X (underlying dimensions/groups)

Statistical Learning

- The linear regression model

$$Y = f(X_1, \ldots, X_p) + \epsilon = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \epsilon$$

  can be used for explanation and/or prediction.

- Explanation: understanding how the X's are related to Y; possibly causally.

- Prediction: if we have new observations with known values of X's, what is the expected (predicted) value of Y and how accurate are these predictions?

Explanatory Regression

- Suppose we have data and obtained estimates:

$$\hat{y}_i = 2 + 0.5x_{i1} + 1.5x_{i2}$$

- Estimated coefficients indicate magnitude of the effects, standard errors indicate variability of estimates.

- Use statistical tests for deciding whether the explanatory variables really affect the response, given the other variables.

- Adequate estimation of coefficients ($\hat{\beta}$) is assumed crucial: Accurate estimates = unbiased estimates! That is:

$$\mathbb{E}[\hat{\beta}] = \beta$$

Explanatory Regression

- Unbiased estimates can be obtained with e.g., OLS:

$$\hat{\beta} = \arg\min_{\beta} \left(\sum_{i=1}^{N} (y_i - f(x_i, \beta))^2 \right)$$

- "From a Bayesian perspective, the principle of unbiasedness is reasonable in the limit of large samples, but otherwise it is potentially misleading" (Gelman et al., 1995)

Predictive Regression

- Suppose we have data and obtain estimates:

$$\hat{y}_i = 2 + 0.5x_{i1} + 1.5x_{i2}$$

- Suppose we have a new observation $x_i = [2 \quad 3]$
- With these values we can predict Y, i.e., $2 + 0.5 \times 2 + 1.5 \times 3 = 7.5$
- We do not care to recover parameters that generated the data, but want to obtain a model that yields as accurate as possible $\hat{Y}$.
- I.e., minimize

$$\mathbb{E}(\hat{Y} - Y)^2$$

Exercise 1: Bias can be beneficial

- Generate some training observations in `R`:

```
set.seed(1)
x <- runif(50, min = -3, max = 3)
epsilon <- rnorm(50)
y <- 0.1*x + epsilon
```

- Combine the observations into a training dataset:

```
train_dat <- data.frame(x, y)
```

- Estimate $\hat{\beta}_{OLS}$ on the training observations (exclude the intercept from the model):

```
beta_OLS <- coef(lm(y ~ 0 + x, data = train_dat))
```

- Generate 1,000 new observations from the same distributions as above. Combine the observations into a test dataset (`test_dat`).

- Generate a range of shrinkage factor values:
  ```
  s <- seq(0, 1, by = .1)
  ```

- Compute predictions for the test observations, but apply shrinkage to the OLS coefficient: $\hat{Y} = X \cdot s \cdot \hat{\beta}_{OLS}$
  - You thus generate predictions for the test observations 11 times: once for each value of the shrinkage factor s.

- For each value of s, compute MSE (mean squared prediction error) on the test observations.

- Plot the test MSE values as a function of shrinkage factor s. Is shrinkage beneficial for prediction?

Exercise 1 - Continued

- To eliminate effects due to chance fluctuations, repeat the above experiment 100 times, and plot the average MSE (over the 100 replications) as a function of shrinkage c.
- Plot the distribution of estimated coefficients against the values of s. (Hint: use function `boxplot`)
- Repeat above with increased training sample size: $N = 100$.
- Repeat above for twice as strong an effect (i.e., $Y = .2X + \epsilon$).
- Describe how optimal amount of shrinkage is affected by sample and effect size.

Predictive Regression

- Traditional statistical textbooks focus on obtaining *unbiased* estimates (e.g., OLS, ML).
- (Modern) statistical learning accepts biased parameter estimates as long as *variance* decreases more than *squared bias* increases:

Predictive perspective: Bias-variance trade-off

- We have a probability distribution P^*, from which we draw a sample $\mathcal{T}$ of size N
- Let f_B be Bayes optimal f (unknown, depends on P^*)
- Let $\bar{f}(X) = \mathbb{E}_{\mathcal{T}}[\hat{f}(X)]$
- Aim is to minimize *expected prediction error:*

$$\begin{aligned}\mathbb{E}_{\mathcal{T}}[\mathrm{EPE}(\hat{f})] = &\mathbb{E}_X[Var(Y|X)] + \\ &\mathbb{E}_X[(f_B(X) - \bar{f}(X))^2] + \\ &\mathbb{E}_{\mathcal{T}}\mathbb{E}_{X,Y}[(\hat{f}(X) - \bar{f}(X))^2]\end{aligned}$$

- EPE = irreducible error (or σ^2) + bias^2 + variance

Population: Non-linear Regression

Often we fit a linear model, assuming that the conditional means in the population lie on a straight line.

This assumption is most likely false! Why does it often work so well?

Excercise 2: Under- and overfitting with polynomial regression

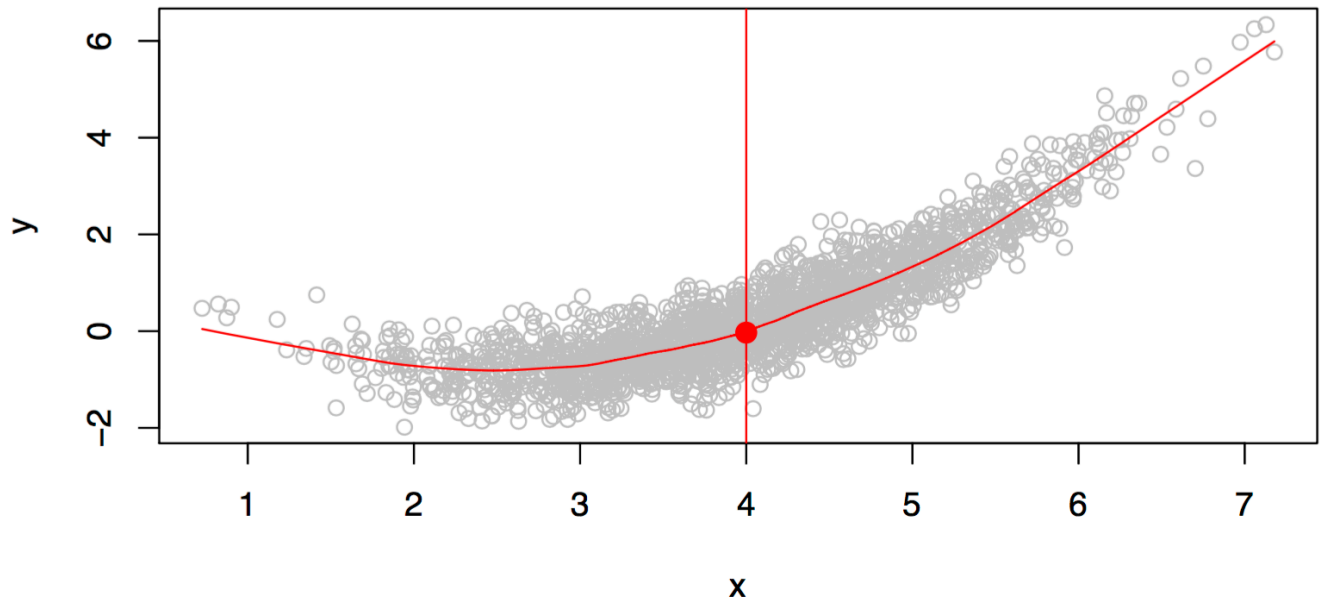
- Generate a training and test set, each with $n = 50$, with a single predictor which has a non-linear effect on the response:

```
set.seed(42)
n <- 50
x <- runif(n, min = -5, max = 5)
y <- x + 8*sin(x/2) + rnorm(n)
train <- data.frame(x, y)
x <- runif(n, min = -5, max = 5)
y <- xtest + 8*sin(xtest/2) + rnorm(n)
test <- data.frame(x, y)
```

Excercise 2 - Continued

- Fit polynomial regression models to the training data of degree 1 trough 15, make predictions on the test set and compute the prediction error for each degree.
  - Hint: Use functions `lm`, `poly`, and a `for` loop. E.g.:
    ```
    lm(y ~ poly(x, degree = 3))
    ```
- Plot the test MSE as a function of the degree of the polynomial.
- If time permits, create a plot which shows the training observations, and fitted curves for the degree 1, 2, 3 and 15 polynomials.

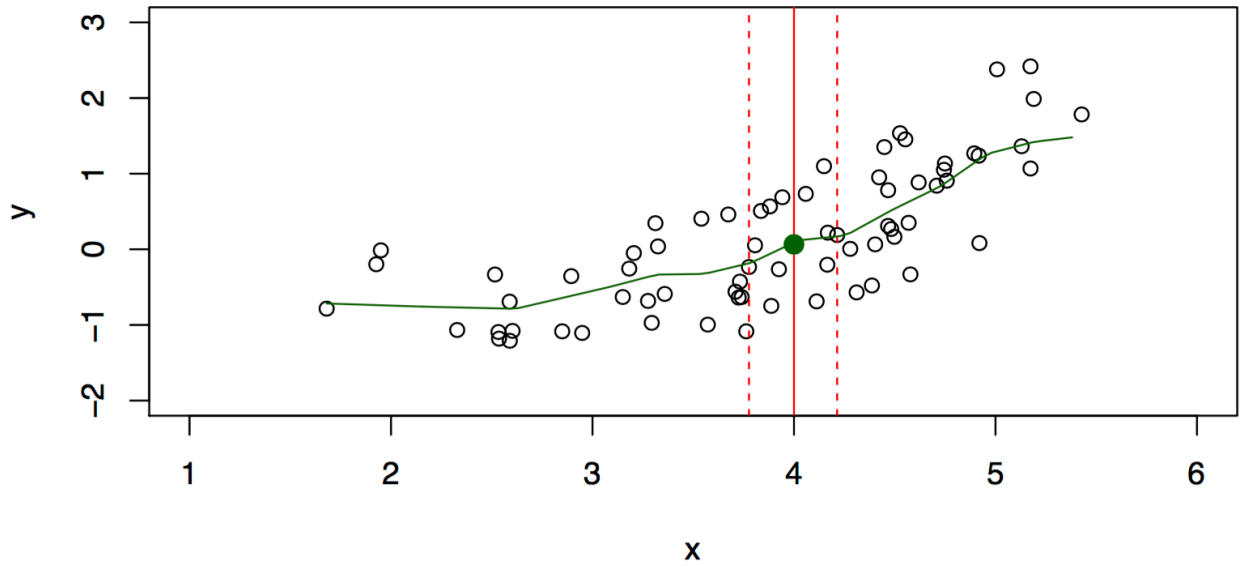
Population: Non-linear Regression



The regression line in the population combines the conditional means at each point x

Sample data

Using sample data, we want to obtain an estimate $\hat{f}(X)$ of $f(X)$.



- Due to sparsity, cannot estimate a conditional mean at all points $X = x$.

- Thus, take a small neighbourhood around $X = x$ and take

neighbourhood mean as predicted value, i.e. *nearest neighbour averaging*.

- The larger the neighbourhood, the larger the bias and the smaller the variance.

Bias-variance trade-off: kNN

- For kNN, assuming a fixed sample T, the variance is simply the variance of an average over k observations:

$$\begin{aligned}\mathrm{EPE}(\hat{f}_{kNN}) = \sigma^2 + & \\ & (f_B(X) - \bar{f}(X))^2 + \\ & \frac{\sigma^2}{k}\end{aligned}$$

Multiple Predictor Variables

With multiple predictors the observations are further spread out through the space:

- Nearest neighbours might not be near at every point
- Flexible models become very wild
- This is known as the *curse of dimensionality*
- More structure in f is needed
- *How can we impose structure?*

Exercise 3: Curse of dimensionality

- Generate a dataset with $p = 10,000$, $N = 100$ and $X \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$:

```
p <- 10000
N <- 100
set.seed(42)
X <- matrix(rnorm(p*N), ncol = p, nrow = N)
```

- Create a histogram of the Euclidian distances between all points in the dataset. First, only use the first column of X to compute the distances (i.e., $p = 1$), then use the first two columns (i.e., $p = 2$), and so on for $p \in \{1, 2, 10, 100, 1000, 10000\}$.
  - Hint: use functions `dist` to compute the distances of the observations in `X`, use function `hist` to create a histogram.

Specify argument `xlim` for each histogram, to make sure the value of 0 is included on the x-axis.

- Are the nearest neighbours near in 1-dimensional space? In 2-dimensional space? In 10-, 100-, 1000-, 10000-dimensional space?

Evaluating predictive accuracy: Numeric outcome

- Mean squared error (MSE):

$$\frac{1}{N_{test}} \sum_{i=1}^{N_{test}} (y_i - \hat{y}_i)^2$$

- Mean absolute error (MAE):

$$MAE = \frac{1}{N_{test}} \sum_{i=1}^{N_{test}} |y_i - \hat{y}_i|$$

Classification

Response variable Y may be a categorical variable with categories $\mathcal{C} = 1, \ldots, k, \ldots, K$.

Again, we want to predict response Y based on predictors X:

- Can directly construct a classifier $\hat{f}(X) = C(X)$ that assigns a predicted category from C based on X.
- Can construct a function $\hat{f}(X)$ that provides conditional probabilities: $\hat{p}_k(X) = Pr(Y = k|X = x)$.

  Then Bayes classifier assigns $C(X) = k$ if $\hat{p}_k(x) = \max\{\hat{p}_1(x), \ldots, \hat{p}_K(x)\}$

Evaluating predictive accuracy: Classification

- Misclassification rate:

$$\frac{1}{N_{test}} \sum_{i=1}^{N_{test}} I(y_i \neq \hat{y}_i)$$

- Brier score:

$$\frac{1}{N_{test}} \sum_{i=1}^{N_{test}} (y_i - \hat{y}_i)^2$$

- Cross-entropy:

$$-\frac{1}{N_{test}} \sum_{i=1}^{N_{test}} [y_i \cdot \log(\hat{y}_i) + (1 - y_i) \cdot \log(1 - \hat{y}_i)]$$

Exercise 4: Flexibility and predictive performance

For each of parts (a) through (d), indicate whether we would generally expect the performance of a flexible statistical learning method to be better or worse than an inflexible method:

a) Sample size N is extremely large, and the number of predictors p is small.

b) The number of predictors p is extremely large, and the number of observations N is small.

c) The relationship between the predictors and response is highly non-linear.

d) The variance of the error terms, $\sigma^2 = Var(\epsilon)$, is extremely high.