STA 35C: Statistical Data Science III

Lecture 3: Statistical Learning

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Agenda

In the last lecture, we reviewed:

- Probability basics
- Conditional probability & Bayes' theorem
- Random variables
- Joint, marginal, and conditional distributions

Today, we will cover:

- More on probability with examples
- Statistical learning

Example: Expectation and variance

Example 1: Coin toss

$$p_X(x) = p(X = x) = \begin{cases} p & \text{if head } (x = 1), \\ 1 - p & \text{if tail } (x = 0). \end{cases}$$

- *Expectation:*

$$\begin{aligned} \mathbb{E}[X] &= \sum_x x \cdot p(x) \\ &= 0 \cdot (1 - p) + 1 \cdot p \\ &= p \end{aligned}$$

- *Variance:*

$$\begin{aligned} \mathrm{Var}(X) &= \mathbb{E}\left[(X - \mathbb{E}[X])^2\right] \\ &= \sum_x \left(x - p\right)^2 \cdot p(x) \\ &= (-p)^2 \cdot (1 - p) + (1 - p)^2 \cdot p \\ &= p(1 - p) \end{aligned}$$

- Alternatively:

$$\mathrm{Var}(X) = \mathbb{E}[X^2] - \mathbb{E}[X]^2 = p - p^2 = p(1 - p)$$

Example: Expectation and variance

Example 2: Gaussian random variable $X \sim N(0, \sigma^2)$

$$f_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}}$$

- *Expectation:*

$$\begin{aligned}
\mathbb{E}[X] &= \int_{-\infty}^{\infty} x \cdot f_X(x)\ dx \\
&= \int_{-\infty}^{0} x \cdot f_X(x)\ dx + \int_{0}^{\infty} x \cdot f_X(x)\ dx \\
&= \int_{0}^{\infty} (-x + x) \cdot f_X(x)\ dx \\
&= 0
\end{aligned}$$

- *Variance:*

$$\begin{aligned}
\mathrm{Var}(X) = \mathbb{E}[X^2] - \mathbb{E}[X]^2 &= \int_{-\infty}^{\infty} x^2 \cdot f_X(x)\ dx \\
&= \sigma^2 \int_{-\infty}^{\infty} f_X(x)\ dx = \sigma^2 P(X \in \mathbb{R}) \\
&= \sigma^2
\end{aligned}$$

- Integration by parts: for $a \neq 0$ ($a = \frac{1}{2\sigma^2}$),

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{x}{-2a}\ e^{-ax^2}\Big|_{-\infty}^{\infty} + \frac{1}{2a} \int_{-\infty}^{\infty} e^{-ax^2} dx$$

Example: Sum of random variables

Example 3: A mixture of two Gaussians

- Let $X \sim Bern(p)$, i.e., a Bernoulli random variable such that

$$p_X(x) = \begin{cases} p & \text{if head } (x = 1), \\ 1 - p & \text{if tail } (x = 0). \end{cases}$$

- Let $Y \sim N(0, \sigma^2)$, i.e., a Gaussian random variable with

$$f_Y(y) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{y^2}{2\sigma^2}}$$

We have seen that

- $\mathbb{E}[X] = p$ and $\mathrm{Var}(X) = p(1-p)$
- $\mathbb{E}[Y] = 0$ and $\mathrm{Var}(Y) = \sigma^2$

Suppose that $\mathrm{Cov}(X, Y) = 0$

Question: Compute

- $\mathbb{E}[cX + Y]$
- $\mathrm{Var}(cX + Y)$

Question: Draw the distribution of $X + Y$?

Example: Variance and covariance

Example 4: Consider a 2x2 contingency table as follows ($a \in [-1, 1]$)

X \ Y	-1	1	Marginal prob of X
1	(1 - a) / 4	(1 + a) / 4	1/2
-1	(1 + a) / 4	(1 - a) / 4	1/2
Marginal prob of Y	1/2	1/2	

- *Expectation of X:*

$$\mathbb{E}[X] = \sum_x x \cdot p_X(x) = (-1) \cdot \frac{1}{2} + 1 \cdot \frac{1}{2} = 0$$

- *Variance of X:*

$$\mathrm{Var}(X) = \mathbb{E}[X^2] = (-1)^2 \cdot \frac{1}{2} + 1^2 \cdot \frac{1}{2} = 1$$

- *Covariance between X and Y:*

$$\begin{aligned}
\mathrm{Cov}(X, Y) &= \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])] \\
&= \sum_{x,y} xy \cdot P_{X,Y}(x, y) \\
&= \frac{1+a}{2} - \frac{1-a}{2} \\
&= a
\end{aligned}$$

Example: Variance and covariance

Example 4: Consider a 2x2 contingency table as follows ($a \in [-1, 1]$)

X \ Y	-1	1	Marginal prob of X
1	(1 - a) / 4	(1 + a) / 4	1/2
-1	(1 + a) / 4	(1 - a) / 4	1/2
Marginal prob of Y	1/2	1/2	

- $\mathbb{E}[X] = \mathbb{E}[Y] = 0$
- $\mathrm{Var}(X) = \mathrm{Var}(Y) = 1$
- $\mathrm{Cov}(X, Y) = a$

Thus,

$$\rho_{X,Y} = \frac{\mathrm{Cov}(X, Y)}{\sqrt{\mathrm{Var}(X)}\sqrt{\mathrm{Var}(Y)}} = a$$

- Q: Are X and Y independent[a]?
  - Yes if and only if $a = 0$
  - If X and Y are independent, then $\rho_{X,Y} = 0$
  - However, $\rho_{X,Y} = 0$ does *not* imply X and Y are independent

[a] Random variables X, Y are independent if $P_{X,Y}(A, B) = P_X(A)P_Y(B)$ for all A, B

Example: Variance and covariance

Example 4: Consider a 2x2 contingency table as follows ($a \in [-1, 1]$)

X \ Y	-1	1	Marginal prob of X
1	(1 - a) / 4	(1 + a) / 4	1/2
-1	(1 + a) / 4	(1 - a) / 4	1/2
Marginal prob of Y	1/2	1/2	

- Q: Is observing X useful in predicting Y?
- Q: How would you estimate a, or $\mathrm{sign}(a)$, from data $\{(x_1, y_1), \ldots, (x_n, y_n)\}$?

Statistical learning

Let's begin with some examples

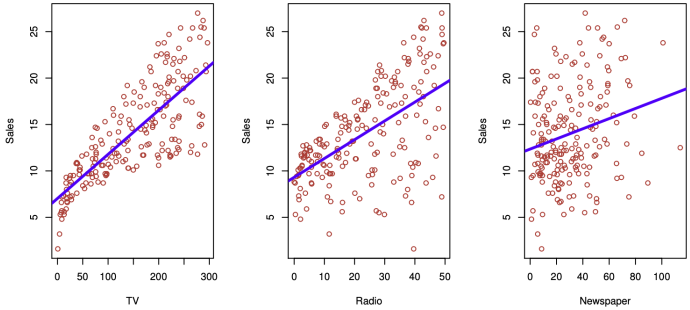


Figure: The Advertising data set shows Sales of a product in 200 different markets against advertising budgets for three media: TV, Radio, and Newspaper [JWHT21, Figure 2.1].

Want to know if there is an association between sales (Y) and advertising (X)
For example, can we predict Sales using TV, Radio, and Newspaper?

Statistical learning

Let's begin with some examples

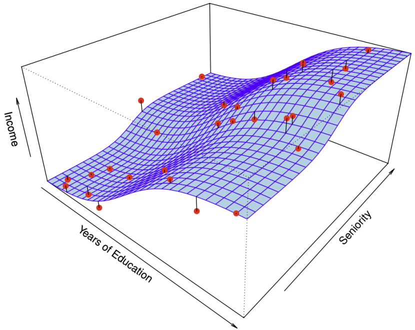


Figure: The simulated `Income` data set displays `Income` of 30 individuals as a function of `Years of education` and `Seniority` [JWHT21, Figure 2.3].

Want to know if there is an association between income (Y) and education/seniority (X)
For example, can we understand how `Years of education` affect `Income`?

Statistical learning: Terminology and notation

Response (dependent variable) Y**:**

- The output variable we want to predict (e.g., `Sales`)

Predictors (independent variables, features) X**:**

- Input variables used to predict Y (e.g., `TV`, `Radio`, `Newspaper`)
- Often multiple predictors are collectively denoted by $X = (X_1, X_2, \ldots, X_p)$

Assumption: There is some relationship between Y and X

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

where

- f is some fixed but ***unknown*** function.
- ϵ is a ***random*** error term, which has *mean zero*, and is *independent of* X.

Goal: Estimate f

Why estimate f?

Predicting Y:

- We often have input variables X but not the corresponding output Y
- With an estimate $\hat{f}$, we can *predict* Y at new points $X = x$ via $\hat{Y} = \hat{f}(x)$
- *Example:* $X =$ patient's blood sample, $Y =$ risk of a disease or adverse reactions

Identifying relevant predictors:

- We can determine *which* predictors among $X_1, \ldots, X_p$ are important in explaining Y, and which are irrelevant
- *Example:* Seniority and years of education heavily affect income, but marital status typically does not

Understanding how X affects Y:

- If f is not too complex, we can interpret *how* each predictor affects Y
- *Example:* Measuring how an increase in TV advertising changes sales

Two main reasons to estimate f

Prediction

- *Objective:* Make accurate prediction of Y given X
- $\hat{f}$ can be treated as a "black box," prioritizing predictive accuracy over exact form
- *Examples:*
  - Which individuals, based on demographics, are likely to respond positively to a mailer?
  - Based on blood sample, is a patient at high risk of a severe adverse drug reaction?

Inference

- *Objective:* Understand the association between Y and X
- We cannot treat $\hat{f}$ as a black box; we need to know its exact form
- *Examples:*
  - Which media are linked to higher sales?
  - Which medium generates the largest boost in sales?
  - How much of an increase in sales is attributable to a given increase in TV advertising?

What is the smallest prediction error we can hope for?

The predictive accuracy of $\hat{Y} = \hat{f}(X)$ depends on two sources of error

- **Reducible error:** If $\hat{f}$ is not a perfect estimate of f, any inaccuracy introduces error
- **Irreducible error:** Even if $\hat{f} = f$, there is variability from ϵ
  - ϵ may include *unmeasured* variables important for predicting Y.
  - ϵ may also reflect *inherent* fluctuations (e.g., day-to-day or manufacturing variation).

Mathematically,

$$\begin{aligned} \mathbb{E}(\hat{Y} - Y)^2 &= \mathbb{E}\big[(\hat{f}(X) - f(X) - \epsilon)^2\big] \\ &= \mathbb{E}\big[(\hat{f}(X) - f(X))^2\big] - 2\mathbb{E}\big[(\hat{f}(X) - f(X)) \cdot \epsilon)^2\big] + \mathbb{E}[\epsilon^2] \\ &= \underbrace{\big(\hat{f}(X) - f(X)\big)^2}_{\text{reducible}} + \underbrace{\mathrm{Var}(\epsilon)}_{\text{irreducible}} \end{aligned}$$

Goal: Estimate f that (1) minimizes the reducible error and (2) is interpretable

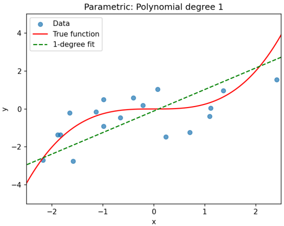
How do we estimate f?

- We will explore multiple approaches to estimate f from data
- We use *training data* $\{(x_1, y_1), \ldots, (x_n, y_n)\}$ to fit $\hat{f}$
- Our goal: ensure $\hat{f}$ generalizes well to future data (X, Y)
- Most statistical learning methods are either **parametric** or **non-parametric**
  - **Parametric (model-based) approach:**
    - Step 1: Assume a functional form (model) of f (e.g., linear $Y = \alpha + \beta X$)
    - Step 2: Use the training data to fit model parameters
  - **Non-parametric approach:**
    - Make no explicit assumption about the functional form of f
    - Instead, seek an $\hat{f}$ that fits data closely while remaining sufficiently smooth

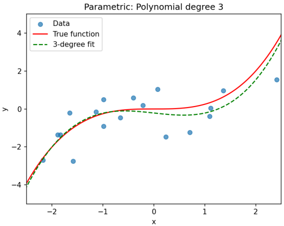
Illustration of parametric methods

Suppose that $Y = f(X) + \epsilon$ where $f(x) = \frac{1}{4}x^3$

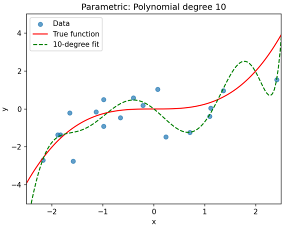
Parametric methods: e.g., polynomial regression $\hat{f}(x) = \sum_{j=0}^{d} \beta_j x^j$ (e.g., $\hat{f}(x) = \beta_0 + \beta_1 x$)



(a) Linear regression (deg 1)



(b) Polynomial regression (deg 3)



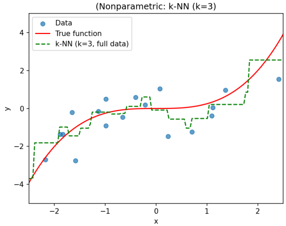
(c) Polynomial regression (deg 10)

- (Good) Estimating parameters $\beta_0, \ldots, \beta_d$ is easier than estimating an arbitrary function f
- (Bad) The assumed model may not match the true functional form of f
- (Ugly) Choosing a more flexible model can reduce bias but risks *overfitting*

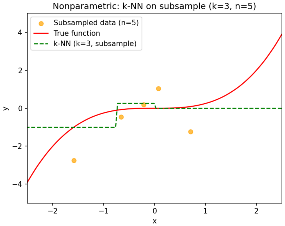
Illustration of non-parametric methods

Suppose that $Y = f(X) + \epsilon$ where $f(x) = \frac{1}{4}x^3$

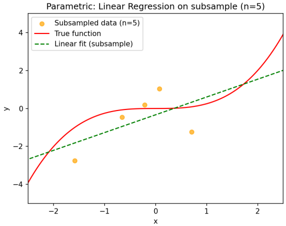
Non-parametric methods: e.g., k-nearest neighbors (k-NN)



(a) k-nearest neighbor ($k = 3$)



(b) k-NN ($k = 3$, subsampled)



(c) Linear regression (subsampled)

- (Good) Highly flexible; avoids the danger of using a wrong functional form
- (Bad) Requires more data to accurately estimate f & interpretation is more difficult
- (Ugly) Greater flexibility can increase the overfitting risk & computation can explode at query

Tradeoff: Prediction accuracy vs. model interpretability

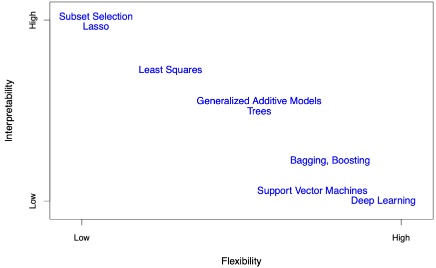


Figure: A representation of the tradeoff between flexibility and interpretability [JWHT21, Figure 2.7].

While more flexible methods can capture a much wider range of shapes to estimate f, we may still prefer more restrictive approaches because of:

- **Interpretability:** Restrictive (parametric) models are typically easier to interpret
- **Sample complexity:** Flexible models often requires more observations
- **Risk of overfitting:** Very flexible methods can fit noise ϵ rather than true f

References

Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani.
An Introduction to Statistical Learning: with Applications in R, volume 112 of *Springer Texts in Statistics*.
Springer, New York, NY, 2nd edition, 2021.