Lecture 13: Logistic Regression

STAT GR5206 *Statistical Computing & Introduction to Data Science*

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Lecture Notes

Topics:

- Supervised vs. Unsupervised Learning
- Supervised Learning
- Simple Logistic Regression (Parametric Model)

Supervised & Unsupervised Learning

Supervised vs. Unsupervised Learning

Supervised Learning

- Have access to a set of p predictors $X_1, X_2, ..., X_p$ and a response Y both measured on the same n observations.
- The goal is to predict Y using $X_1, X_2, ..., X_p$ (usually by learning β parameters of a model).

Unsupervised Learning

- *Only* have access to a set of p predictors $X_1, X_2, ..., X_p$ measured on n observations.
- We are not interested in prediction, because we do not have an associated response variable Y.
- The goal is to discover interesting patterns about the measurements on the predictors $X_1, X_2, ..., X_p$.

Supervised vs. Unsupervised Learning

The questions fall into two categories: **supervised learning** and *unsupervised learning*.

Supervised learning:

- Predicting an output
- Understanding the relationship between an input and an output

Unsupervised learning:

- Summarizing the data
- Understanding underlying (hidden) factors

Note: Principle Component Analysis (PCA) is unsupervised learning.

Supervised Learning

Supervised Learning: Regression and Classification

Regression:

- Y has continuous values

$$
\begin{aligned}
X &= (X_1, X_2, \ldots, X_p) && \text{inputs} \\
Y & && \text{output} \\
Y &= f(X) + \epsilon && \text{relationship} \\
Y &= E[Y|X = x] + \epsilon
\end{aligned}
$$

Classification:

- Y has categorical values

$$
\begin{aligned}
X &= (X_1, X_2, \ldots, X_p) && \text{inputs} \\
Y & && \text{output} \\
p_k &= P(Y = y_k|X = x) && \text{relationship}
\end{aligned}
$$

Prediction and Inference

Why estimate f and p?

- Prediction
- Inference

Prediction:

- We have a new product with a set advertising budget (`TV`, `radio` and `newspaper`). What will its sales be?
- Alice has 16 years of education and 0 years of seniority. What will her income be?

Goal:

Accurately estimate output for new inputs.

Inference

Inference

We want to learn about relationships between inputs and outputs:

- How will increasing one input affect the output?
- Is a specific combination of inputs associated with an increase in the output?

Inference vs. Prediction

- Can you think of some inference questions?
- Prediction questions?
- What is the difference between the two?

Fitting f and p

How do I find $\hat{f}$ and $\hat{p}$ using $(x_1, y_1), \ldots, (x_n, y_n)$?

1. select a statistical model
2. select the model parameters using the data

What types of statistical models are there?

- **Parametric:** described by a finite number of parameters, say

$$\beta_1, \beta_2, \ldots, \beta_d$$

- **Non-parametric:** not described by a finite number of parameters

Parametric Models

Parametric Models

A **parametric model** is a statistical model described by a finite number of parameters. Examples include:

- a Gaussian distribution ($N(\mu, \sigma^2)$)
- a Bernoulli distribution (Bern(p))
- a *linear model*

$$Y = \beta_0 + \beta_1 X_d + \cdots + \beta_d X_d + \epsilon, \quad \epsilon \sim N(0, \sigma^2)$$

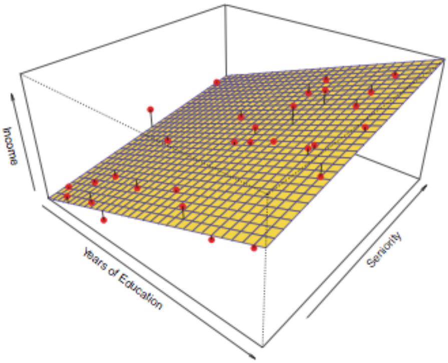
- a logistic model (this will be discussed today)

Parameters

- What are the parameters of the Gaussian?
- What are the parameters of a linear model?
- What are the parameters of a logistic model?

Parametric Regression Model

$$\texttt{income} \approx \beta_0 + \beta_1 \times \texttt{years of education} + \beta_2 \times \texttt{seniority}$$



Is this model good for prediction? What can it tell us for inference?

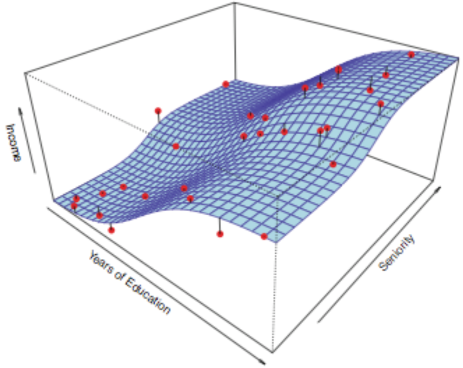
Nonparametric Models

Nonparametric Models:

- Nonparametric models are not described by a finite number of parameters.
- So, what does that mean?
- Nonparametric models assume less about the population.
- In the model
$$Y = f(X) + \epsilon,$$
we let the data decide what the function f looks like.

Nonparametric Model

$$\texttt{income} \approx f(\texttt{years of education}, \texttt{seniority})$$



Is this model good for prediction? What can it tell us for inference?

Problem Types (Generally)

	Continuous	**Categorical**
Supervised	Regression Parametric Linear reg,... Nonparametric kNN,..	Classification Parametric Logistic,... Nonparametric kNN,..
Unsupervised	Dimension Reduction PCA,..	Clustering k-means,..

Parametric Classification

Logistic Regression

Logistic Regression

Question:

How do we define a simple (one covariate) regression model that allows for a categorical (binary) response variable?

- To answer this question, first recall the Bernoulli random variable.
- Any rv whose possible values are 0 and 1 is called a **Bernoulli random variable**.
- Also recall that the **expected value** (or true mean) of a Bernoulli random variable is its success probability. That is, if $Y \sim Bern(p)$, then

$$E[Y] = p$$

Answer:

Regress a sigmoidal function $p = f(x)$ on covariate x.

- A sigmoidal function has an s shape and is bounded between 0 and 1 $(0 < f(x) < 1)$.

Simple Logistic Regression

The Simple Logistic Regression Model

Let $Y_1, Y_2, \ldots, Y_n$ be independently distributed Bernoulli random variables with respective success probabilities $p_1, p_2, \ldots, p_n$. Then the **logistic regression model** is:

$$E[Y_i] = p_i = F_L(\beta_0 + \beta_1 x_i) = \frac{e^{(\beta_0+\beta_1 x_i)}}{1 + e^{(\beta_0+\beta_1 x_i)}}, \quad i = 1, 2, \ldots, n.$$

The Estimated Simple Logistic Model

$$\hat{p}_i = \frac{e^{(\hat{\beta}_0+\hat{\beta}_1 x_i)}}{1 + e^{(\hat{\beta}_0+\hat{\beta}_1 x_i)}}, \quad i = 1, 2, \ldots, n.$$

- The quantities $\hat{\beta}_0$ and $\hat{\beta}_1$ are the estimated intercept and slope.
- Maximum likelihood estimation is used to estimate the logistic model parameters β_0 and β_1.

Maximum Likelihood

- Usually we think of parameters, θ, as fixed and consider the probability of different outcomes $f(x, \theta)$ with θ constant and x changing.
- **Likelihood** of a parameter value is given by $L(\theta)$: what probability does θ give the data?
  - For continuous variables, use the probability density.
  - Calculate $f(x, \theta)$ letting θ change with data constant.
  - *Not* the probability of θ.
- **Maximum likelihood** is the guess that the parameter is whatever makes the data most likely.
- Most likely parameter value is the **maximum likelihood estimate** or the **MLE**.

Coding the Likelihood Function

- With independent data points $x_1, x_2, \ldots, x_n$ the likelihood is

$$L(\theta) = \prod_{i=1}^{n} f(x_i, \theta).$$

- Multiplying lots of small numbering is bad, so we usually take the log:

$$\ell(\theta) = \sum_{i=1}^{n} \log f(x_i, \theta).$$

- Note the maximizer is the same for both (though the maximum value will be different).

Maximum Likelihood Logistic

Recall the Bernoulli pmf

$$f(x|p) = P(X = x) = p^x(1-p)^{1-x}$$

Joint pmf

$$f(x_1, x_2, \ldots, x_n | p_1, p_2, \ldots, p_n) = \prod_{i=1}^{n} p_i^{x_i}(1-p_i)^{1-x_i}$$

The objective function is:

$$\ell(\beta_0, \beta_1) = \sum_{i=1}^{n} Y_i(\beta_0 + \beta_1 x_i) - \sum_{i=1}^{n} \log(1 + \exp(\beta_0 + \beta_1 x_i)).$$

Log-odds and the Logit Link

Odds

$$\frac{p_i}{1-p_i} = e^{\beta_0+\beta_1 x_i}, \quad i = 1, 2, \ldots, n.$$

- The equation above relates the *odds* of event $\{Y = 1\}$ occurring to a deterministic *exponential function*.

Logit-Link and Log-Odds

$$F_L^{-1}(p_i) = \log\left(\frac{p_i}{1-p_i}\right) = \beta_0 + \beta_1 x_i, \quad i = 1, 2, \ldots, n.$$

- The link function "links" the mean ($E[Y] = p$) to a linear function.

Example

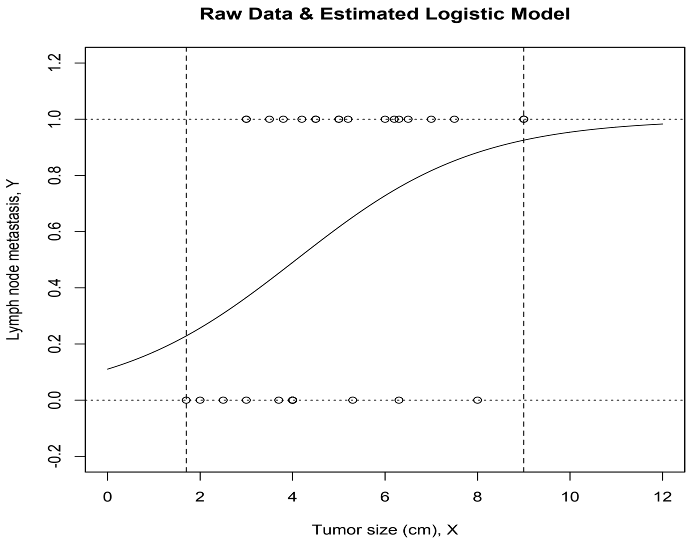
Esophageal cancer is a serious and very aggressive disease. Scientists conducted a study of 31 patients with esophageal cancer in which they studied the relationship between the size of the tumor that a patient had and whether or not the cancer had spread (metastasized) to the lymph nodes of the patient. In this study the response variable is dichotomous: $Y = 1$ if the cancer had spread to the lymph nodes and $Y = 0$ if not. The predictor variable is the size (recorded as the maximum dimension, in cm) of the tumor found in the esophagus.

```
> cancer <- read.table("logistic.txt")
```

Data Table

Patient number	Tumor Size (cm), X	Lymph node metastasis, Y
1	6.5	1
2	6.3	0
3	3.8	1
4	7.5	1
5	4.5	1
6	3.5	1
7	4.0	0
8	3.7	0
9	6.3	1
10	4.2	1
$\vdots$	$\vdots$	$\vdots$
30	3	1
31	1.7	0

Plots



Raw Data & Estimated Logistic Model
Lymph node metastasis, Y
Tumor size (cm), X
-0.2
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
2
4
6
8
10
12

Estimating the Logistic Model - Gradient Descent

Process

- Define log-likelihood by:

$$\ell(\beta_0, \beta_1) = \sum_{i=1}^{n} Y_i(\beta_0 + \beta_1 x_i) - \sum_{i=1}^{n} \log(1 + \exp(\beta_0 + \beta_1 x_i)).$$

- Define negative-log-likelihood in R.

$$-\ell(\beta_0, \beta_1)$$

- Use `dbinom()` to set this up. Look up the argument `prob`. No need to define the neg-log-likelihood using the long expression from above.
- Use Newton's Method (Gradient Descent).
- Also try `nlm()`.

Maximum Likelihood Logistic

Set up the neg-log-likelihood in R

```
> logistic.NLL <- function(beta,data=cancer) {
+
+   beta_0 <- beta[1]
+   beta_1 <- beta[2]
+   y <- data$y
+   x <- data$x
+   linear.component <- beta_0 + beta_1*x
+   p.i <- exp(linear.component)/(1+exp(linear.component))
+   return(-sum(dbinom(y,size=1,prob=p.i,log=TRUE)))
+ }
> logistic.NLL(beta=c(-1,.5),data=cancer)
```

```
[1] 21.72804
```

nlm()

```
> nlm(logistic.NLL,p=c(-1,.5),data=cancer)
```

```
$minimum
[1] 18.50095

$estimate
[1] -2.0857732  0.5116513

$gradient
[1] 3.936344e-06 1.677591e-05

$code
[1] 1

$iterations
[1] 15
```

Interpretation of the slope parameter β_1

Consider a 1 unit increase in the covariate:

- The odds of event $\{Y = 1\}$ occurring when the covariate is fixed at x is

$$odds_1 = \frac{p_1}{1 - p_1} = e^{\beta_0 + \beta_1 (x)}$$

- The odds of event $\{Y = 1\}$ occurring when the covariate is fixed at $x + 1$ is

$$odds_2 = \frac{p_2}{1 - p_2} = e^{\beta_0 + \beta_1 (x+1)}$$

- Thus

$$\text{“odds ratio”} = \Theta = \frac{odds_2}{odds_1} = \frac{e^{\beta_0 + \beta_1 (x+1)}}{e^{\beta_0 + \beta_1 x}} = e^{\beta_1}$$

- Equivalently $odds_2 = e^{\beta_1} \cdot (odds_1)$

“The odds of event $\{Y = 1\}$ occurring are multiplied by $e^{\hat{\beta}_1}$ for every 1 unit increase in x.”

Estimation in R

glm function in R

```
> cancer <- read.table("logistic.txt")
> model <- glm(y~x,data=cancer,family=binomial(link="logit"))
> model
```

```
Call:  glm(formula = y ~ x, family = binomial(link = "logit"))

Coefficients:
(Intercept)            x
    -2.0858       0.5117

Degrees of Freedom: 30 Total (i.e. Null);  29 Residual
Null Deviance:          42.17
Residual Deviance: 37         AIC: 41
```

Estimation in R

Summary

```
> summary(model)
```

```
Call:
glm(formula = y ~ x, family = binomial(link = "logit"), data

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.0657  -1.1288   0.5657   0.9844   1.4185

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)  -2.0858     1.2256  -1.702   0.0888 .
x             0.5117     0.2561   1.998   0.0457 *
---
Signif. codes:
```

The `predict()` function in R

The `predict` function always predicts the "linear" component

.

$$\hat{\beta}_0 + \hat{\beta}_1 x$$

R code

```
> x.test <- data.frame(x=7)
> linear.pred <- predict(model,newdata = x.test)
> linear.pred
```

```
       1
1.495793
```

```
> exp(linear.pred)/(1+exp(linear.pred))
```

```
        1
0.8169462
```