MATH 637: Mathematical Techniques in Data Science Categorical data

Dominique Guillot

Departments of Mathematical Sciences University of Delaware

March 9, 2020

• So far, we developed methods for modelling *quantitative* or *continuous* outputs.

- So far, we developed methods for modelling *quantitative* or *continuous* outputs.
- We will now discuss techniques to model *categorical* or *discrete* outputs.

- So far, we developed methods for modelling *quantitative* or *continuous* outputs.
- We will now discuss techniques to model *categorical* or *discrete* outputs.
- Examples of problems:
 - **1** You receive an email. Is it spam or not? (binary response).

- So far, we developed methods for modelling *quantitative* or *continuous* outputs.
- We will now discuss techniques to model *categorical* or *discrete* outputs.
- Examples of problems:
 - **1** You receive an email. Is it spam or not? (binary response).
 - Web browsing analysis: link clicked or not clicked?

- So far, we developed methods for modelling *quantitative* or *continuous* outputs.
- We will now discuss techniques to model *categorical* or *discrete* outputs.
- Examples of problems:
 - You receive an email. Is it spam or not? (binary response).
 - Web browsing analysis: link clicked or not clicked?
 - Solution Handwritten digits recognition $(Y \in \{0, \ldots, 9\})$.



ESL, Figure 1.2.

- So far, we developed methods for modelling *quantitative* or *continuous* outputs.
- We will now discuss techniques to model *categorical* or *discrete* outputs.
- Examples of problems:
 - You receive an email. Is it spam or not? (binary response).
 - Web browsing analysis: link clicked or not clicked?
 - Solution Handwritten digits recognition $(Y \in \{0, \ldots, 9\})$.



ESL, Figure 1.2.

• We begin with two very simple approaches: linear regression and nearest neighbors.

Linear regression

- We are given $X \in \mathbb{R}^{n \times 2}$ and $Y \in \{0, 1\}^n$.
- Think of y_i as x_i 's label (red/blue say).

Linear regression

- We are given $X \in \mathbb{R}^{n \times 2}$ and $Y \in \{0, 1\}^n$.
- Think of y_i as x_i 's label (red/blue say).





Linear regression

- We are given $X \in \mathbb{R}^{n \times 2}$ and $Y \in \{0, 1\}^n$.
- Think of y_i as x_i 's label (red/blue say).



We want to predict new points' category.

• Fit $Y = X\beta + \epsilon$ (linear decision boundary).

- Fit $Y = X\beta + \epsilon$ (linear decision boundary).
- Given $x = (x_1, x_2)^T$, use $x^T \beta$ to predict the label.

- Fit $Y = X\beta + \epsilon$ (linear decision boundary).
- Given $x = (x_1, x_2)^T$, use $x^T \beta$ to predict the label.
- Output is in $\{0,1\}$, but $x^T \beta \in \mathbb{R}$.

- Fit $Y = X\beta + \epsilon$ (linear decision boundary).
- Given $x = (x_1, x_2)^T$, use $x^T \beta$ to predict the label.
- Output is in $\{0,1\}$, but $x^T\beta \in \mathbb{R}$.

Use

$$\hat{y} = \begin{cases} 0 & \text{ if } x^T \beta < 0.5 \\ 1 & \text{ if } x^T \beta \ge 0.5 \end{cases}$$

Linear regression (cont.)

```
# X = 2*n by 2, Y = 2*n by 1 {0,1} labels
# Include an intercept
Xp = np.ones((2*n,3))
Xp[:,1:3] = X
# Use regression
beta = np.linalg.lstsq(Xp,Y)[0]
# Our decision boundary is
# beta[0] + beta[1] *x + beta[2]*y = 0.5,
# or y = (0.5-beta[0]-beta[1]*x)/beta[2]
```

Linear regression (cont.)

```
# X = 2*n by 2, Y = 2*n by 1 {0,1} labels
# Include an intercept
Xp = np.ones((2*n,3))
Xp[:,1:3] = X
# Use regression
beta = np.linalg.lstsq(Xp,Y)[0]
# Our decision boundary is
# beta[0] + beta[1] *x + beta[2]*y = 0.5,
# or y = (0.5-beta[0]-beta[1]*x)/beta[2]
```



Test error

- As usual, we split our data into train and test sets.
- Train model on training set.
- Compute classification error on test set.



In general, when working with k categories, can use a loss-function

 $(L(i,j))_{i,j=1}^k,$

where L(i, j) = costfor classifying i as j.

Nearest neighbors

Nearest neighbors: use closest observations in the training set to make predictions.

$$\hat{Y}(x) = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i.$$

Here $N_k(x)$ denotes the *k*-nearest neighbors of x (w.r.t. some metric, e.g. Euclidean distance).

Nearest neighbors

Nearest neighbors: use closest observations in the training set to make predictions.

$$\hat{Y}(x) = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i.$$

Here $N_k(x)$ denotes the *k*-nearest neighbors of x (w.r.t. some metric, e.g. Euclidean distance). Use a "majority vote" to determine final labels

$$\hat{G}(x) = \begin{cases} 0 & \text{if } \hat{Y}(x) < 0.5 \\ 1 & \text{if } \hat{Y}(x) \ge 0.5 \end{cases}$$



ESL, Fig. 2.2: 15 Nearest Neighbor classifier

Nearest neighbors

Reducing the number of neighbors leads to:

- A smaller training error (training error is 0 when using k = 1 neighbor).
- Can use train/test sets to choose k.
- Although a small k leads to a small training error, the model may not generalize well (large test error).



ESL, Fig. 2.3, 1 Nearest classifier

Example

from sklearn.neighbors import KNeighborsClassifier neigh = KNeighborsClassifier(n_neighbors=i)



A bias-variance tradeoff: Linear regression:

- Relies on the assumption that the decision boundary is linear.
- Decision boundary is smooth.

A bias-variance tradeoff: Linear regression:

- Relies on the assumption that the decision boundary is linear.
- Decision boundary is smooth.

Nearest neighbors:

- Adaptive, less assumptions on the data.
- A particular decision may depend only on a handful of points. Less robust.
- More wiggly and unstable.

A bias-variance tradeoff:

- Linear regression:
 - Relies on the assumption that the decision boundary is linear.
 - Decision boundary is smooth.

Nearest neighbors:

- Adaptive, less assumptions on the data.
- A particular decision may depend only on a handful of points. Less robust.
- More wiggly and unstable.

Each method has its own situations for which it works best

A bias-variance tradeoff:

Linear regression:

- Relies on the assumption that the decision boundary is linear.
- Decision boundary is smooth.

Nearest neighbors:

- Adaptive, less assumptions on the data.
- A particular decision may depend only on a handful of points. Less robust.
- More wiggly and unstable.

Each method has its own situations for which it works best Both methods can lead to very good predictions.

A bias-variance tradeoff:

Linear regression:

- Relies on the assumption that the decision boundary is linear.
- Decision boundary is smooth.

Nearest neighbors:

- Adaptive, less assumptions on the data.
- A particular decision may depend only on a handful of points. Less robust.
- More wiggly and unstable.

Each method has its own situations for which it works best Both methods can lead to very good predictions. Many strategies exist to improve these methods (as we will see later).