

### Problem set 3

• **Problem 1 (4 pts)**

It was mentioned in the lecture that a cubic regression spline with two knots at  $\xi_1 < \xi_2$  can be represented as

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 (x - \xi_1)_+^3 + \beta_5 (x - \xi_2)_+^3$$

where

$$(x - \xi_k)_+^3 = \begin{cases} (x - \xi_k)^3 & \text{if } x > \xi_k \\ 0 & \text{otherwise} \end{cases}, \quad \forall k \in \{1, 2\}. \quad (0.1)$$

We now verify  $f(x)$  is indeed a cubic regression spline by proving:

1. **(1 pt)**  $f(x)$  can be written as three cubic polynomials for  $x \leq \xi_1$ ,  $\xi_1 < x \leq \xi_2$  and  $x > \xi_2$ .
2. **(1 pt)** the three polynomials have the same value at each knot.
3. **(1 pt)** the three polynomials have the same first order derivative at each knot.
4. **(1 pt)** the three polynomials have the same second order derivative at each knot.

**SOLUTION:**

1. According to the definition of  $f(x)$ , we have

$$f(x) = \begin{cases} f_1(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 & \text{if } x \leq \xi_1 \\ f_2(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 (x - \xi_1)^3 & \text{if } \xi_1 < x \leq \xi_2 \\ f_3(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 (x - \xi_1)^3 + \beta_5 (x - \xi_2)^3 & \text{if } x > \xi_2 \end{cases}$$

as desired.

2. This follows immediately from the previous part by letting  $x = \xi_1$  and  $x = \xi_2$ .
3. Since

$$\frac{df_1(x)}{dx} = \beta_1 + 2\beta_2 x + 3\beta_3 x^2,$$

$$\frac{df_2(x)}{dx} = \beta_1 x + 2\beta_2 x + 3\beta_3 x^2 + 3\beta_4 (x - \xi_1)^2,$$

$$\frac{df_3(x)}{dx} = \beta_1 x + 2\beta_2 x + 3\beta_3 x^2 + 3\beta_4 (x - \xi_1)^2 + 3\beta_5 (x - \xi_2)^2,$$

$f'_1(\xi_1) = f'_2(\xi_1)$  and  $f'_2(\xi_2) = f'_3(\xi_2)$  follow by taking  $x = \xi_1$  and  $x = \xi_2$ .

4. Since

$$\frac{d^2 f_1(x)}{dx^2} = 2\beta_2 + 6\beta_3 x,$$

$$\frac{d^2 f_2(x)}{dx^2} = 2\beta_2 + 6\beta_3 x + 6\beta_4 (x - \xi_1)$$

$$\frac{d^2 f_3(x)}{dx^2} = 2\beta_2 + 6\beta_3 x + 6\beta_4 (x - \xi_1) + 6\beta_5 (x - \xi_2),$$

taking  $x = \xi_1$  and  $x = \xi_2$  leads to  $f''_1(\xi_1) = f''_2(\xi_1)$  and  $f''_2(\xi_2) = f''_3(\xi_2)$ .

• **Problem 2 (7 pts)**

Consider the classification problem with the label of  $Y$  belong to  $\mathcal{C} := \{1, 2, \dots, K\}$  and any realization  $x$  of  $X \in \mathbb{R}^p$ . The Bayes classifier  $f^*$  at  $X = x$  is defined as

$$f^*(x) := \operatorname{argmin}_{f(x) \in \mathcal{C}} \mathbb{E} \left[ 1\{Y \neq f(X)\} \mid X = x \right].$$

1. **(2 pts)** Prove that

$$f^*(x) = \operatorname{argmax}_{k \in \mathcal{C}} \mathbb{P}(Y = k \mid X = x).$$

2. **(1 pt)** Prove that the Bayes error at  $X = x$  equals to

$$1 - \max_{k \in \mathcal{C}} \mathbb{P}(Y = k \mid X = x).$$

3. **(2 pts)** Consider that  $K = 3$ . For a fixed  $x_0$ , assume that

$$\mathbb{P}(Y = 1 \mid X = x_0) = 0.5$$

$$\mathbb{P}(Y = 2 \mid X = x_0) = 0.3$$

$$\mathbb{P}(Y = 3 \mid X = x_0) = 0.2.$$

State the Bayes classifier at  $X = x_0$  and compute its error at  $X = x_0$ .

4. **(2 pts)** Consider a naive classifier  $\hat{f}$ , called random guessing, which randomly picks one label from  $\mathcal{C} = \{1, 2, 3\}$  with equal probability. Compute its expected error rate at  $X = x_0$  and compare it with the Bayes error at  $X = x_0$  in part 3.

**SOLUTION:**

1. **Proof.** We have

$$\begin{aligned} \mathbb{P}(Y = f(X) \mid X = x) &= \sum_{k \in \mathcal{C}} \mathbb{P}(Y = f(X) = k \mid X = x) \\ &= \sum_{k \in \mathcal{C}} \mathbb{P}(Y = k \mid X = x) 1\{f(x) = k\} \\ &\leq \max_{k \in \mathcal{C}} \mathbb{P}(Y = k \mid X = x). \end{aligned}$$

Moreover, the maximal value is achieved when  $f(x) = k^*$  for

$$k^* = \operatorname{argmax}_{k \in \mathcal{C}} \mathbb{P}(Y = k \mid X = x).$$

This proves the first claim. □

2. **Proof.** Regarding the second claim, by similar reasoning,

$$\begin{aligned} \mathbb{P}(Y \neq f^*(X) \mid X = x) &= 1 - \mathbb{P}(Y = f^*(X) \mid X = x) \\ &= 1 - \sum_{k \in \mathcal{C}} \mathbb{P}(Y = k \mid X = x) 1\{f^*(x) = k\} \\ &= 1 - \max_{k \in \mathcal{C}} \mathbb{P}(Y = k \mid X = x). \end{aligned}$$

□

3. The Bayes classifier assigns  $x_0$  to 1 and the Bayes error at  $x_0$  is 0.5.
4. The expected error rate of  $\hat{f}$  at  $x_0$  is

$$\begin{aligned}\mathbb{E}\left[1\{\hat{f}(X) \neq Y\} \mid X = x_0\right] &= \mathbb{P}(\hat{f}(X) \neq Y \mid X = x_0) \\ &= 1 - \mathbb{P}(\hat{f}(X) = Y \mid X = x_0) \\ &= 1 - \sum_{c \in \mathcal{C}} \mathbb{P}(Y = c \mid X = x_0) \mathbb{P}(\hat{f}(X) = c \mid X = x_0) \\ &= 1 - \sum_{c \in \mathcal{C}} \mathbb{P}(Y = c \mid X = x_0) \mathbb{P}(\hat{f}(X) = c) \\ &= 1 - \frac{1}{3} \sum_{c \in \mathcal{C}} \mathbb{P}(Y = c \mid X = x_0) \\ &= 1 - \frac{1}{3}[0.5 + 0.3 + 0.2] = \frac{2}{3},\end{aligned}$$

which is greater than the Bayes error.

• **Problem 3 (7 pts)**

We will prove that a random guessing classifier for binary classification has the area under the curve (AUC) equal to  $1/2$ . Suppose  $Y \in \{0, 1\}$  with  $Y = 1$  meaning *true*, and *false* otherwise. Consider the following random guessing classifier at any  $X = x$

$$\hat{f}(x) = \begin{cases} 1, & \text{with prob. equal to } p \\ 0, & \text{with prob. equal to } 1 - p \end{cases}$$

with any  $p$  chosen from  $[0, 1]$ .

1. (**3 pts**) Prove that the expected AUC of this random classifier with  $p$  varying within  $[0, 1]$  is  $1/2$ . [Hint: the expected False Positive Rate is  $\mathbb{P}(\hat{f}(X) = 1 \mid Y = 0)$ ]
2. (**2 pts**) Let  $\eta(x) := \mathbb{P}(Y = 1 \mid X = x)$  for any  $x$ . Write the expected error rate of  $\hat{f}$  at  $X = x$  in terms of  $\eta(x)$  and  $p$ .
3. (**2 pts**) If you have the flexibility of choosing  $p$  in your expression of part 2, which choice minimizes the expected error rate of  $\hat{f}$  at  $X = x$ ? Is the resulting classifier equivalent to the Bayes classifier? State your explanation.

**SOLUTION:**

1. The expected FPR is

$$\mathbb{P}(\hat{f}(X) = 1 \mid Y = 0) = \mathbb{P}(\hat{f}(X) = 1) = p$$

while the expected FNR is

$$\mathbb{P}(\hat{f}(X) = 0 \mid Y = 1) = \mathbb{P}(\hat{f}(X) = 0) = 1 - p.$$

Note that the expected TPR is  $1 - \mathbb{P}(\hat{f}(X) = 0 \mid Y = 1) = p$ . Therefore, the AUC of  $\hat{f}$  is

$$\int_0^1 p dp = \frac{1}{2}.$$

2. The expected error rate at  $X = x$  equals to

$$\begin{aligned} & \mathbb{P}(Y \neq \hat{f}(x) \mid X = x) \\ &= \mathbb{P}(Y = 1, \hat{f}(x) = 0 \mid X = x) + \mathbb{P}(Y = 0, \hat{f}(x) = 1 \mid X = x) \\ &= \mathbb{P}(Y = 1 \mid X = x)\mathbb{P}(\hat{f}(x) = 0 \mid X = x) + \mathbb{P}(Y = 0 \mid X = x)\mathbb{P}(\hat{f}(x) = 1 \mid X = x) \\ &= \mathbb{P}(Y = 1 \mid X = x)\mathbb{P}(\hat{f}(x) = 0) + \mathbb{P}(Y = 0 \mid X = x)\mathbb{P}(\hat{f}(x) = 1) \\ &= \eta(x)(1 - p) + (1 - \eta(x))p. \end{aligned}$$

3. We choose

$$p = \begin{cases} 1 & \text{if } \eta(x) \geq 1/2 \\ 0 & \text{otherwise} \end{cases}$$

The resulting classifier only equals to the Bayes classifier at this point but not in general. Indeed, to match the Bayes classifier for all  $x$ , we need to allow  $p = p(x)$  being a function that depends on  $x$ .

- **Problem 4 (14 pts)**

This question uses the variables `dis` (the weighted mean of distances to five Boston employment centers) and `nox` (nitrogen oxides concentration in parts per 10 million) from the `Boston` data in the library `MASS`. We will treat `dis` as the predictor and `nox` as the response. For drawing the fitted lines below, let's use the following code to generate a grid of `dis`

```
dislims<-range(Boston$dis)
dis.grid<-seq(from=dislims[1],to=dislims[2],length.out=100)
```

1. **(2 pt)** Use the `poly()` function to fit a polynomial regression with degree equal to 10 to predict `nox` using `dis`. Plot the data, the polynomial fit and its 95% confidence band. Comment on the width of the confidence band.
2. **(2 pts)** Plot the polynomial fits for a range of different polynomial degrees, from  $\{1, 3, 5, 7, 10\}$ , and report the associated residual sum of squares (RSS). What's your finding and how to explain it?
3. **(2 pts)** Perform 10-fold cross-validation to select the best degree of the polynomial from  $\{1, 3, 5, 7, 10\}$ .
4. **(2 pts)** Use the `bs()` function to fit a regression spline with 7 degrees of freedom to predict `nox` using `dis`. Specify how the knots are chosen and plot the resulting fit and its 95% confidence band. Comment on the width of confidence band.
5. **(2 pts)** Use the `ns()` function to fit a natural regression spline with the same knots specified in the previous part. (You may find the `nox` function and `Boundary.knots` useful). Plot the resulting fit and its 95% confidence band. Comparing to the previous plot, comment on the difference.
6. **(2 pts)** Now fit natural cubic splines for a range of degrees of freedom, from  $\{5, 10, 15, 20\}$  (specified via `df` in `ns()` function), and plot the resulting fits and report the resulting RSS. Comment on what you observe.
7. **(2 pts)** Perform 10-fold cross-validation to select the best degrees of freedom for a natural regression spline from  $\{5, 10, 15, 20\}$ .

• **Problem 5 (18 pts)**

You will implement different local regression approaches in this problem. Let's set the seed to `set.seed(20231101)`. For  $n = 300$  training data, let's generate  $(x_i, y_i)$  for  $1 \leq i \leq n$  from

$$x_i \stackrel{i.i.d.}{\sim} N(3, 1), \quad \epsilon_i \stackrel{i.i.d.}{\sim} N(0, 1),$$

$$y_i = 0.5 + 0.1x_i + 0.2x_i^2 + \epsilon_i.$$

Let's generate another  $m = 300$  test data points by the same generating mechanism. Set a grid of the training data as `x_grid=seq(0,6,by=0.02)`

1. **(5 pts)** Implement the  $k$ -nearest-neighbor, that is, for any given  $x_0$ , use the averaged responses of its  $k$  nearest neighbors to predict, namely,

$$\hat{y}_1(x_0) = \frac{1}{k} \sum_{i \in N_k(x_0)} y_i$$

with  $N_k(x_0)$  denoting the index set of  $k$  nearest neighbors of  $x_0$  among  $\{x_1, \dots, x_n\}$ .

Use your function to predict at each value of `x_grid`. Plot the training data points and add on the lines of your fitted values for  $k \in \{5, 20, 50, 100\}$ . Make sure you label each line correctly in your plot. Comment on your findings for different choices of  $k$ .

2. **(5 pts)** Repeat step 1 for the weighted  $k$ -nn, that is, for any given  $x_0$ , predict by

$$\hat{y}_2(x_0) = \sum_{i \in N_k(x_0)} w(x_0, x_i) y_i.$$

Here we choose the so-called *tricubic weights* as

$$w(x_0, x_i) = \frac{\tilde{w}(x_0, x_i)}{\sum_{i \in N_k(x_0)} \tilde{w}(x_0, x_i)}, \quad \forall i \in N_k(x_0) \quad (0.2)$$

with

$$\tilde{w}(x_0, x_i) = \left( 1 - \left( \frac{|x_i - x_0|}{\max_{i \in N_k(x_0)} |x_i - x_0|} \right)^3 \right)^3, \quad (0.3)$$

3. **(5 pts)** Repeat step 1 for the weighted local linear regression, that is, for any given  $x_0$ ,

$$\hat{y}_3(x_0) = \hat{\beta}_0 + \hat{\beta}_1 x_0$$

with

$$(\hat{\beta}_0, \hat{\beta}_1) = \operatorname{argmin}_{\beta_0, \beta_1} \sum_{i \in N_k(x_0)} w(x_0, x_i) (y_i - \beta_0 - \beta_1 x_i)^2.$$

Here  $w(x_0, x_i)$  is the same as in (0.2) – (0.3). For implementing the above weighted least squares, you might use the `lm` function by specifying the `weights` argument.

4. **(3 pts)** Use the test data to choose the best one among the above three procedures for  $k \in \{5, 20, 50, 100\}$ .