Statistical methods for bioinformatics
Beyond linearity: case study (de Vijver et al.)

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1 Exercise 1

1.1 Part a

This is straightforward by taking the coefficients $a_1 = \beta_0, b_1 = \beta_1, c_1 = \beta_2, d_1 = \beta_3$

1.2 Part b

Since we are looking at $x > \xi$, we have the form:

- $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 (x - \xi)^3$

We can distribute the cube and get:

- $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 (x^3 - 3x^2\xi + 3x\xi^2 - \xi^3)$

The expression can be re-arranged to highlight the predictors coefficients' values:

- $f(x) = (\beta_0 - \beta_4\xi^3) + (\beta_1 + 3\beta_4\xi^2)x + (\beta_2 - 3\beta_4\xi)x^2 + (\beta_3 + \beta_4)x^3$

Combining with the answer of Part a, we now see that $f(x)$ is a piecewise polynomial

1.3 Part c

Showing that the 2 pieces are connected continuously can be done by solving both in ξ:

- $f_1(\xi) = \beta_0 + \beta_1\xi + \beta_2\xi^2 + \beta_3\xi^3$
- $f_2(\xi) = (\beta_0 - \beta_4\xi^3) + (\beta_1 + 3\beta_4\xi^2)\xi + (\beta_2 - 3\beta_4\xi)\xi^2 + (\beta_3 + \beta_4)\xi^3$

When distributing the terms in $f_2(\xi)$, one obtains that the terms in β_4 cancel each other, and that $f_2(\xi) = \beta_0 + \beta_1\xi + \beta_2\xi^2 + \beta_3\xi^3 = f_1(\xi)$

1.4 Part d

For this, we need the first order derivatives of $f_1(x)$ and $f_2(x)$

- $f_1'(x) = \beta_1 + 2\beta_2 x + 3\beta_3 x^2$
- $f_2'(x) = \beta_1 + 3\beta_4 x^2 + 2(\beta_2 - 3\beta_4 x)x + 3(\beta_3 + \beta_4)x^2$

Solving the equations above for $x = \xi$:

- $f_1'(\xi) = \beta_1 + 2\beta_2\xi + 3\beta_3\xi^2$
- $f_2'(\xi) = \beta_1 + 3\beta_4\xi^2 + 2(\beta_2 - 3\beta_4\xi)\xi + 3(\beta_3 + \beta_4)\xi^2$
- $f_2'(\xi) = \beta_1 + 3\beta_4\xi^2 + 2\beta_2\xi - 6\beta_4\xi^2 + 3\beta_3\xi^2 + 3\beta_4\xi^2$
- $f_2'(\xi) = \beta_1 + 2\beta_2\xi + 3\beta_3\xi^2 + 3\beta_4\xi^2 + 3\beta_4\xi^2 - 6\beta_4\xi^2$
- $f_2'(\xi) = \beta_1 + 2\beta_2\xi + 3\beta_3\xi^2$

Hence, $f_1'(\xi) = \beta_1 + 2\beta_2\xi + 3\beta_3\xi^2 = f_2'(\xi)$

1.5 Part e

We can take the second order derivatives of $f_1(x)$ and $f_2(x)$, and solve in ξ to verify if the transition is continuous:

- $f_1''(x) = 2\beta_2 + 6\beta_3 x$
- $f_2''(x) = 2(\beta_2 - 3\beta_4 x) + 6(\beta_3 + \beta_4)x = 2\beta_2 + 6\beta_3 x$

Hence, $f_1''(\xi) = 2\beta_2 + 6\beta_3\xi = f_2''(x)$

Combining this with the previous parts, we have shown that $f(x)$ is indeed a cubic spline, where the piecewise functions $f_1(x)$ and $f_2(x)$ are indeed connected, and where the first order and second order derivatives are smoothly connected.

2 Exercise 9

2.1 part a

2.2 part b

2.3 part c

2.4 part d

2.5 part e

2.6 part f