Supervised Learning

Feature space expansions

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Program

Morning session

Feature space expansions

Regression models form the core of statistical analysis. Most commonly used is the linear regression model $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p$. As the name suggests, this model assumes a linear relationship between the outcome variable y and each of the respective features $x_1, x_2, \ldots, x_p$. This linearity assumption, however, is a simplification of reality and may do a poor job in describing the true relationship between variables. Feature space expansion is a flexible tool for describing non-linear relationships between the outcome variable and the features. This session introduces expansion of the feature space with polynomials, splines, interactions and regression trees.

Course materials

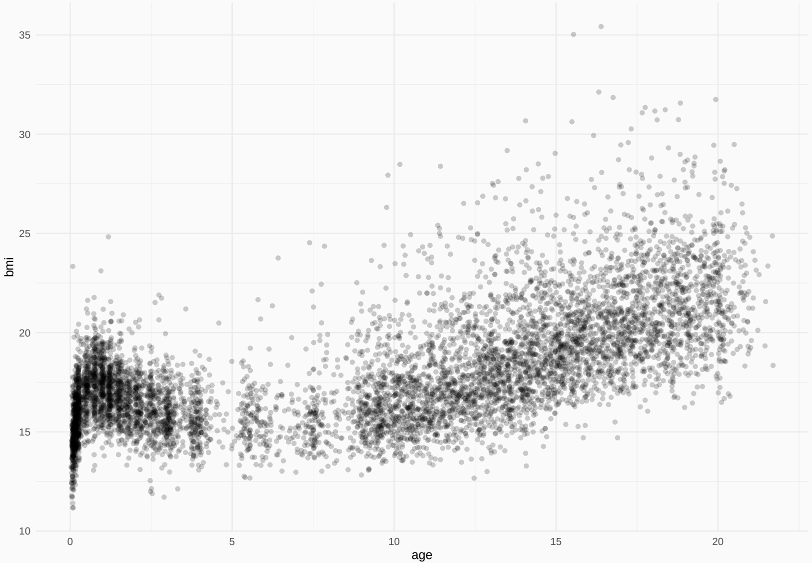
- Lecture sheets
- R lab
- R Markdown lab template

Recommended literature

- ISLR: 3 Linear regression; 7 Moving beyond linearity; 8 Tree-based methods

BMI Dutch boys

How to predict Body Mass Index from age?



Content

1. Linearity
2. Polynomials
3. Splines
4. Regression trees

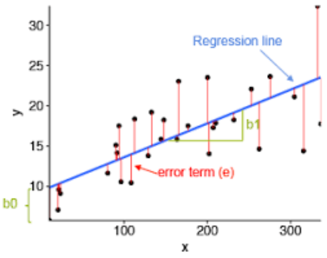
Linearity

Linearity assumption

Assumption of the linear regression model

$$y = \beta_0 + \beta x + \varepsilon, \qquad \varepsilon \sim N(0, \sigma^2)$$

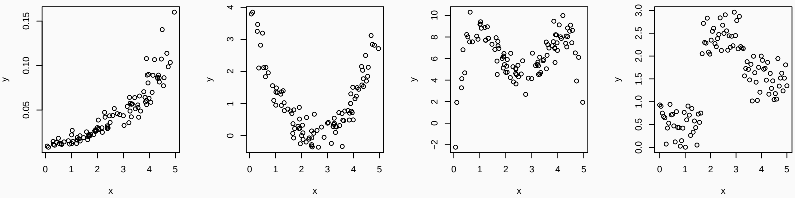
- predictions on straight regression line
- residuals normally distributed and homoscedastic



Non-linearity

Different shapes and forms

- model choice depends on shape and form



Accommodating non-linearity

Different models:

- polynomials

$$y = \beta_0 x^0 + \beta_1 x^1 + \beta_2 x^2 + \beta_3 x^3 + ...$$

- splines
    - fit polynomials to non-overlapping regions of X
- tree-based models
    - compute the mean in non-overlapping regions of X

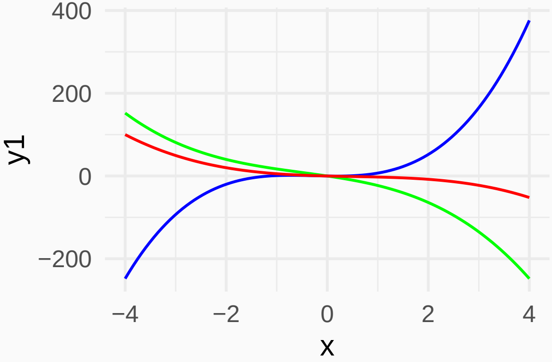
Polynomials

Basis expansion

Expand the feature space with polynomials of X, e.g.

- the cubic polynomial

$$\hat{y} = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$$



Making polynomials in R

The straightforward way

- use the function `I()` in the model formula
- `model.matrix()` creates the basis expansion

```r
(M <- model.matrix(~ I(x^1) + I(x^2) + I(x^3), data.frame(x = 1:4)))
```

```
  (Intercept) I(x^1) I(x^2) I(x^3)
1           1      1      1      1
2           1      2      4      8
3           1      3      9     27
4           1      4     16     64
attr(,"assign")
[1] 0 1 2 3
```

Multicollinearity

Potential problem with `I()`

- multicollinearity, i.e. high correlation between x, x^2, x^3, etc.

Correlations between polynomials:

```
round(cor(M[, -1]), 3)
```

```
       I(x^1) I(x^2) I(x^3)
I(x^1)  1.000  0.984  0.951
I(x^2)  0.984  1.000  0.991
I(x^3)  0.951  0.991  1.000
```

Orthogonal expansion

The function `poly(x, degree = 3)` creates on orthogonal basis

```
(P <- model.matrix( ~ poly(x, 3), data = data.frame(x = 1:4)))
```

```
  (Intercept) poly(x, 3)1 poly(x, 3)2 poly(x, 3)3
1           1  -0.6708204         0.5  -0.2236068
2           1  -0.2236068        -0.5   0.6708204
3           1   0.2236068        -0.5  -0.6708204
4           1   0.6708204         0.5   0.2236068
attr(,"assign")
[1] 0 1 1 1
```

Correlations

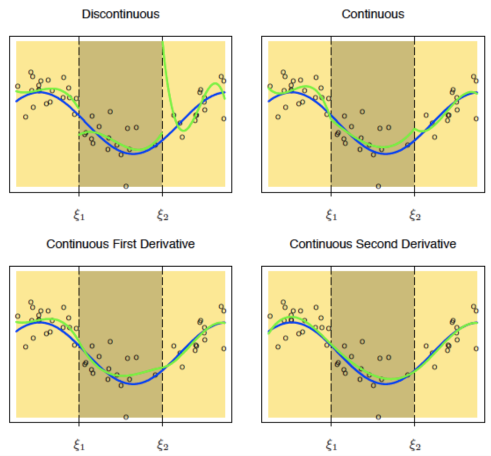
```
round(cor(P[, -1]), 3)
```

```
            poly(x, 3)1 poly(x, 3)2 poly(x, 3)3
poly(x, 3)1           1           0           0
poly(x, 3)2           0           1           0
poly(x, 3)3           0           0           1
```

Splines

B-splines

- Place a number of knots ξ that divide X in non-overlapping regions
- fit cubic polynomial to each region
- connect lines by equating 1st and 2nd derivative



Fitting cubic splines in R

Formula for generating B-spline basis matrix in R (package `splines`)

```
bs(x, df = NULL, knots = NULL, degree = 3) # cubic spline

ns(x, df = NULL, knots = NULL, degree = 3) # natural cubic spline
```

- `degree = 3` for cubic polynomial (default)
- `df` number of knots (`df = degree + number of knots`)
- `knots` position of knots in percentiles
- natural cubic spline is linear beyond the boundary knots

Basis matrix cubic spline with `df = 4`

```r
bs(1:4, df = 4)
```

```
                1          2          3          4
[1,] 0.00000000 0.0000000 0.00000000 0.00000000
[2,] 0.51851852 0.3703704 0.07407407 0.00000000
[3,] 0.07407407 0.3703704 0.51851852 0.03703704
[4,] 0.00000000 0.0000000 0.00000000 1.00000000
attr(,"degree")
[1] 3
attr(,"knots")
50%
2.5
attr(,"Boundary.knots")
[1] 1 4
attr(,"intercept")
[1] FALSE
attr(,"class")
[1] "bs"     "basis"  "matrix"
```

Smoothing splines

Highly flexible spline

1. A *knot* ξ_i for each unique value x_i
2. `df` controls wiggliness (value between 1 and $\#\ x_i$)

Fitting smooth splines in R

```
smooth.spline(y ~ x, df = <nr>)
smooth.spline(y ~ x)
```

- 1st: user-specified `df`
- 2nd: optimal `df` determined with cross-validation

Regression trees

Binary recursive partioning algorithm

1. Partition the feature space in distinct, non-overlapping regions
2. Compute the mean of all observations within a region
3. Select the partition that minimizes the MSE
4. Continue partitioning until a stopping criterion is reached

Tree function `rpart()` from package `rpart`

```
reg_tree <- rpart(y ~ x, method = "anova")
plot(reg_tree)
text(reg_tree)
```

Warning: trees tend to overfit, more on this in classification

Example with one feature

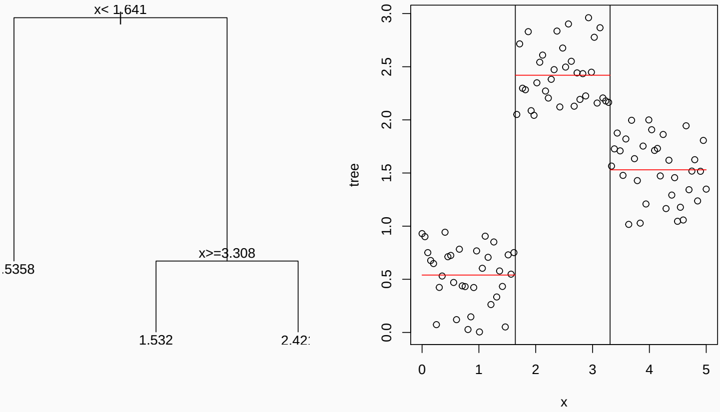


Figure 1: Tree representation (left) and its predictions (right)

Example with two features

Different way of looking at interactions

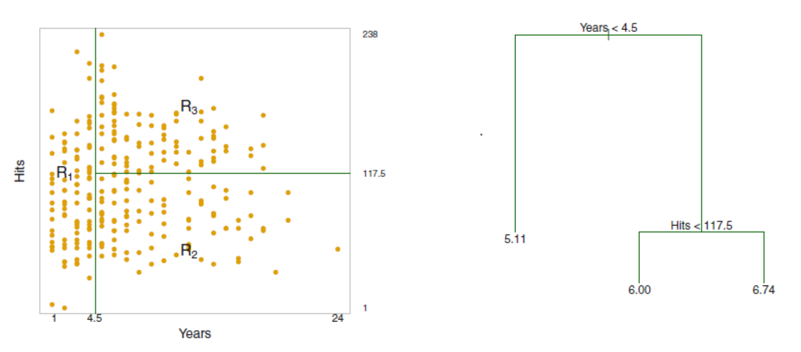


Figure 2: Salaries of baseball players (ISLR)

Preview Lab 2A

Topics

- polynomials
- splines
- trees

Next lab (Feature selection) features interactions