Lecture 13: Non-linear Regression

Reading: Section 5.2, 5.3, 5.4

GU4241/GR5241 Statistical Machine Learning

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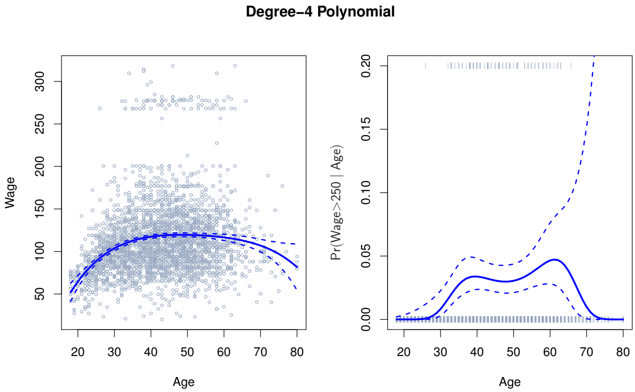
Non-linear regression

Problem: How do we model a non-linear relationship?



Left: Regression of wage onto age.
Right: Logistic regression for classes wage> 250 and wage≤ 250

Basis functions

Strategy:

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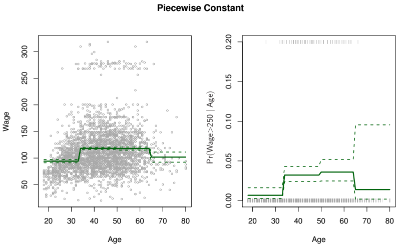
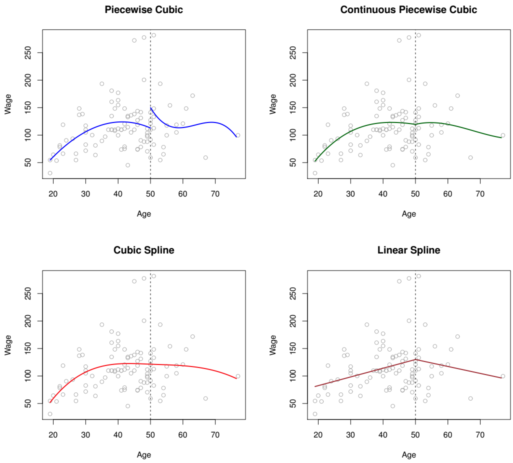
  1. Polynomials, $f_i(x) = x^i$.
  2. Indicator functions, $f_i(x) = \mathbf{1}(c_i \leq x < c_{i+1})$.



Basis functions

- Options for $f_1, \dots, f_d$:

  3. Piecewise polynomials:



Cubic splines

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- It turns out, we can write f in terms of $K + 4$ basis functions:

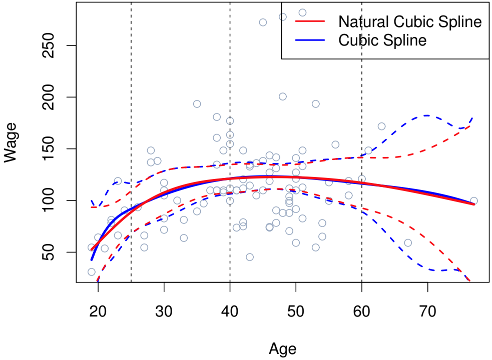
$$f(X) = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \beta_4 h(X, \xi_1) + \cdots + \beta_{K+3} h(X, \xi_K)$$

where,

$$h(x, \xi) = \begin{cases} (x - \xi)^3 & \text{if } x > \xi \\ 0 & \text{otherwise} \end{cases}$$

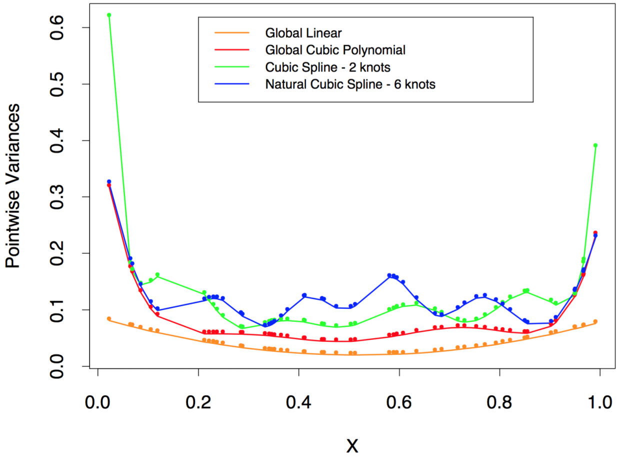
Natural cubic splines

Spline which is linear instead of cubic for $X < \xi_1$, $X > \xi_K$.



The predictions are more stable for extreme values of X.

Natural cubic splines vs. cubic splines



Choosing the number and locations of knots

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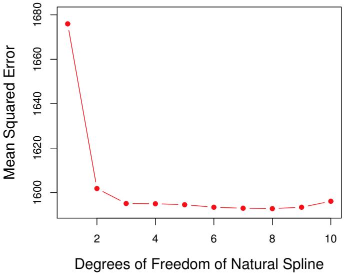
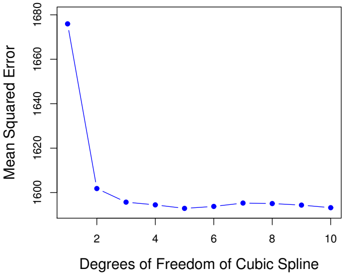
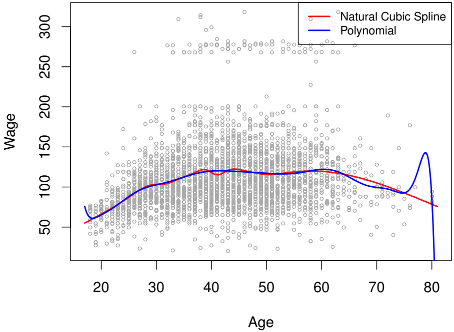
The number of knots, K, is chosen by cross validation:





Natural cubic splines vs. polynomial regression

- Splines can fit complex functions with few parameters.
- Polynomials require high degree terms to be flexible.
- High-degree polynomials can be unstable at the edges.



Smoothing splines

Find the function f which minimizes

$$\sum_{i=1}^{n}(y_i - f(x_i))^2 + \lambda \int f''(x)^2 dx$$

- The RSS of the model.
- A penalty for the roughness of the function.

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Facts:

- The minimizer $\hat{f}$ is a natural cubic spline, with knots at each unique sample point $x_1, \ldots, x_n$.
- Obtaining $\hat{f}$ is similar to a Ridge regression.

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- The function $\hat{f}$ is the only natural cubic spline that has these fitted values.

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2. Deduce that the solution to the smoothing spline problem is a natural cubic spline, which can be written in terms of its basis functions.

$$f(x) = \beta_1 N_1(x) + \dots \beta_n N_n(x)$$

Deriving a smoothing spline

3. Letting $\mathbf{N}$ be a matrix with $\mathbf{N}(i,j) = N_j(x_i)$, we can write the objective function:

$$(y - \mathbf{N}\beta)^T(y - \mathbf{N}\beta) + \lambda\beta^T\Omega_{\mathbf{N}}\beta,$$

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4. By simple calculus, the coefficients $\hat{\beta}$ which minimize

$$(y - \mathbf{N}\beta)^T(y - \mathbf{N}\beta) + \lambda\beta^T\Omega_{\mathbf{N}}\beta,$$

   are $\hat{\beta} = (\mathbf{N}^T\mathbf{N} + \lambda\Omega_{\mathbf{N}})^{-1}\mathbf{N}^Ty$.

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5. Note that the predicted values are a linear function of the observed values:

$$\hat{y} = \underbrace{\mathbf{N}(\mathbf{N}^T\mathbf{N} + \lambda\Omega_{\mathbf{N}})^{-1}\mathbf{N}^T}_{\mathbf{S}_\lambda} y$$

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6. The **degrees of freedom** for a smoothing spline are:

$$\text{Trace}(\mathbf{S}_\lambda) = \mathbf{S}_\lambda(1,1) + \mathbf{S}_\lambda(2,2) + \cdots + \mathbf{S}_\lambda(n,n)$$

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$$
\begin{aligned}
RSS_{\mathsf{loocv}}(\lambda) &= \sum_{i=1}^{n} (y_i - \hat{f}_\lambda^{(-i)}(x_i))^2 \\
&= \sum_{i=1}^{n} \left[\frac{y_i - \hat{f}_\lambda(x_i)}{1 - \mathbf{S}_\lambda(i,i)} \right]^2
\end{aligned}
$$

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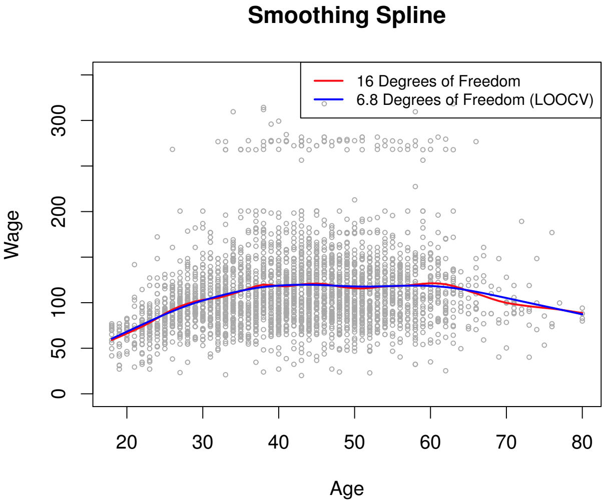

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