Lecture 17: Smoothing splines, Local Regression, and GAMs

Reading: Sections 7.5-7

STATS 202: Data mining and analysis

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Cubic splines

- Define a set of knots $\xi_1 < \xi_2 < \cdots < \xi_K$.
- We want the function f in the model $Y = f(X) + \epsilon$ to:
  1. Be a cubic polynomial between every pair of knots ξ_i, ξ_{i+1}.
  2. Be continuous at each knot.
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- It turns out, we can write f in terms of $K + 3$ basis functions:

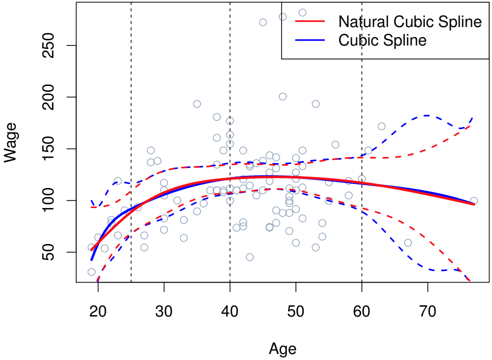
$$f(X) = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \beta_4 h(X, \xi_1) + \cdots + \beta_{K+3} h(X, \xi_K)$$

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 $X < \xi_1$, $X > \xi_K$.

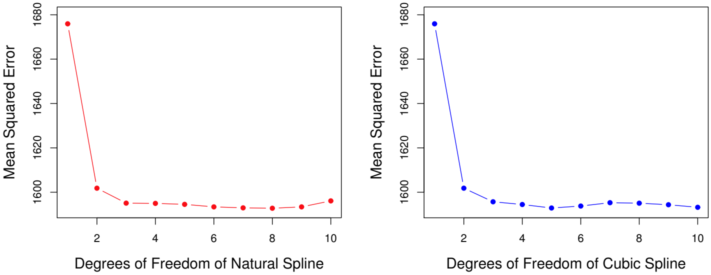


The predictions are more stable for extreme values of X.

Choosing the number and locations of knots

The locations of the knots are typically quantiles of X.

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



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 sample point $x_1, \ldots, x_n$.
- Obtaining $\hat{f}$ is similar to a Ridge regression.

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Deriving a smoothing spline

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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.

$$f(x) = \beta_0 + \beta_1 f_1(x) + \ldots \beta_{n+3} f_{n+3}(x)$$

Deriving a smoothing spline

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

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

where $\Omega_{\mathbf{N}}(i,j) = \int f_i''(t) f_j''(t) dt$.

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

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

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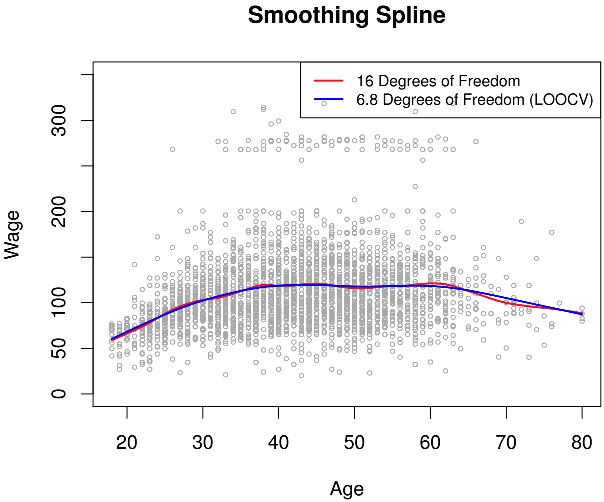
$$\begin{aligned} RSS_{\mathsf{loocv}}(\lambda) &= \sum_{i=1}^{n} (y_i - \hat{f}_\lambda^{(-i)}(x_i))^2 \\ &= \sum_{i=1}^{n} \left[\frac{y_i - \hat{f}_\lambda(x_i)}{1 - \mathbf{S}_\lambda(i,i)} \right]^2 \end{aligned}$$

Choosing the regularization parameter λ



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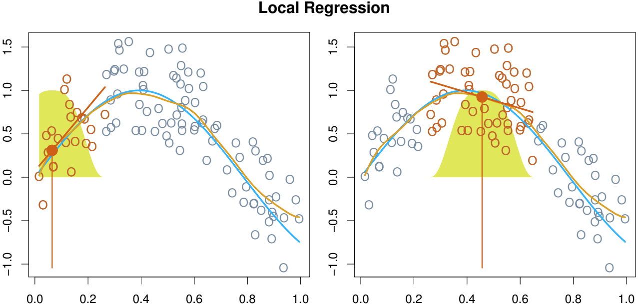
Local linear regression



The **span** is the fraction of training samples used in each regression.

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2. Perform a weighted least squares regression; i.e. find (β_0, β_1) which minimize

$$\hat{\beta}(x) = \mathrm{argmin}_{(\beta_0,\beta_1)} \sum_{i=i}^{n} K_i(x)(y_i - \beta_0 - \beta_1 x_i)^2.$$

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3. Predict $\hat{f}(x) = \hat{\beta}_0(x) + \hat{\beta}_1(x)x$.

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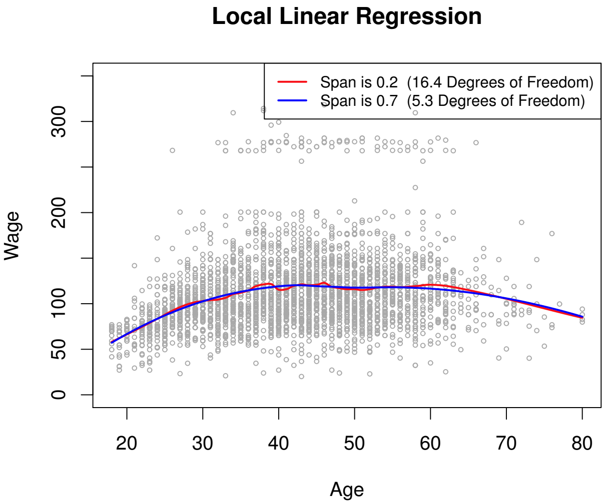
4. Common choice for $K_i(x) = \exp(-\|x - x_i\|^2/2\lambda)$ – smoother than nearest neighbors.

Local linear regression



The *span*, k/n, is chosen by cross-validation.

Generalized Additive Models (GAMs)

Extension of non-linear models to multiple predictors:

$$\texttt{wage} = \beta_0 + \beta_1 \times \texttt{year} + \beta_2 \times \texttt{age} + \beta_3 \times \texttt{education} + \epsilon$$

$$\longrightarrow \quad \texttt{wage} = \beta_0 + f_1(\texttt{year}) + f_2(\texttt{age}) + f_3(\texttt{education}) + \epsilon$$

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The functions $f_1, \ldots, f_p$ can be polynomials, natural splines, smoothing splines, local regressions...

Fitting a GAM

- If the functions f_1 have a basis representation, we can simply use least squares:
  - Natural cubic splines
  - Polynomials
  - Step functions

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