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 $\xi_i, \xi_{i+1}$.
  2. Be continuous at each knot.
  3. Have continuous first and second derivatives 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.
Natural cubic splines vs. Smoothing splines

Natural cubic splines

- Fix the locations of $K$ knots at quantiles of $X$.

Smoothing splines

- Number of knots $K < n$.
- Find the natural cubic spline $\hat{f}$ which minimizes the RSS:
  \[ n \sum_{i=1}^{n} \left( y_i - f(x_i) \right)^2 \]
- Choose $K$ by cross validation.
- Put $n$ knots at $x_1, \ldots, x_n$.
- We could find a cubic spline which makes the RSS $= 0$ → Overfitting!
- Instead, we obtain the fitted values $\hat{f}(x_1), \ldots, \hat{f}(x_n)$ through an algorithm similar to Ridge regression.
- The function $\hat{f}$ is the only natural cubic spline that has these fitted values.
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<th>Smoothing splines</th>
</tr>
</thead>
<tbody>
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<td></td>
</tr>
<tr>
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<td></td>
</tr>
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<td></td>
</tr>
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Deriving a smoothing spline

1. Show that if you fix the values \( f(x_1), \ldots, f(x_n) \), the roughness

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\int f''(x)^2 \, dx
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is minimized by a natural cubic 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.

\[
f(x) = \beta_0 + \beta_1 f_1(x) + \cdots + \beta_{n+3} f_{n+3}(x)
\]
3. Letting $\mathbf{N}$ be a matrix with $\mathbf{N}(i, j) = f_j(x_i)$, we can write the objective function:

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

where $\Omega_N(i, j) = \int f_i''(t)f_j''(t)dt$. 

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

$$(y - N\beta)^T (y - N\beta) + \lambda \beta^T \Omega_N \beta,$$

where $\Omega_N(i, j) = \int f''_i(t)f''_j(t)dt$.

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

$$(y - N\beta)^T (y - N\beta) + \lambda \beta^T \Omega_N \beta,$$

are $\hat{\beta} = (N^T N + \lambda \Omega_N)^{-1} N^T y$. 
5. Note that the predicted values are a linear function of the observed values:

\[
\hat{y} = N(N^T N + \lambda \Omega_N)^{-1} N^T y \]

\[
\text{Trace}(S_\lambda) = S_\lambda(1,1) + S_\lambda(2,2) + \cdots + S_\lambda(n,n)
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6. The **degrees of freedom** for a smoothing spline are:

\[
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Choosing the regularization parameter $\lambda$

- We typically choose $\lambda$ through cross validation.
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$$RSS_{loocv}(\lambda) = \sum_{i=1}^{n} (y_i - \hat{f}^{(\lambda)}(x_i))^2$$
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- There is a shortcut for LOOCV:

\[
RSS_{loocv}(\lambda) = \sum_{i=1}^{n} (y_i - \hat{f}_\lambda^{(-i)}(x_i))^2 = \sum_{i=1}^{n} \left[ \frac{y_i - \hat{f}_\lambda(x_i)}{1 - S_\lambda(i,i)} \right]^2
\]
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![Smoothing Spline](image)

- 16 Degrees of Freedom
- 6.8 Degrees of Freedom (LOOCV)
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Local linear regression

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

To predict the regression function $f$ at an input $x$:

1. Assign a weight $K_i(x)$ to the training point $x_i$, such that:
   - $K_i(x) = 0$ unless $x_i$ is one of the $k$ nearest neighbors of $x$.
   - $K_i(x)$ decreases when the distance $d(x, x_i)$ increases.

2. Perform a weighted least squares regression; i.e. find $(\hat{\beta}_0, \hat{\beta}_1)$ which minimize
   
   $$\hat{\beta}(x) = \arg\min_{(\beta_0, \beta_1)} \sum_{i=1}^n K_i(x)(y_i - \beta_0 - \beta_1 x_i)^2.$$ 

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Local linear regression: generalized nearest neighbors

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

The span, $k/n$, is chosen by cross-validation.
Generalized Additive Models (GAMs)

Extension of non-linear models to multiple predictors:

\[ \text{wage} = \beta_0 + \beta_1 \times \text{year} + \beta_2 \times \text{age} + \beta_3 \times \text{education} + \epsilon \]

\[ \rightarrow \quad \text{wage} = \beta_0 + f_1(\text{year}) + f_2(\text{age}) + f_3(\text{education}) + \epsilon \]
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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

\[
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\]