## Module 2: Splines and Kernel Methods

# Regression Splines, Smoothing Splines

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# Backtrack a bit…

- Instead of just considering input variables *x* (potentially mult.), augment/replace with transformations = "input features"

- ***Linear basis expansions*** maintain linear form in terms of these transformations

$$f(x) = \sum_{m=1}^{M} \beta_m h_m(x)$$

← trans.

← linear in these transformations

- What transformations should we use?
  - $h_m(x) = x_m$ → linear model
  - $h_m(x) = x_j^2, \quad h_m(x) = x_j x_k$ → polynomial reg.
  - $h_m(x) = I(L_m \leq x_k \leq U_m)$ → piecewise constant
  - …

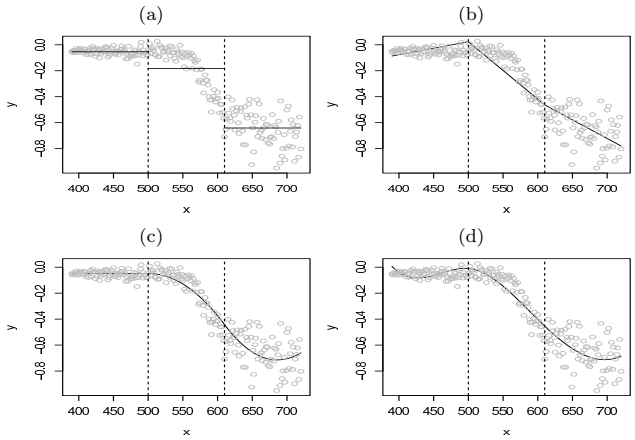
# Piecewise Polynomial Fits

- Again, assume *x* univariate
- Polynomial fits are often good locally, but not globally
  - Adjusting coefficients to fit one region can make the function go wild in other regions
- Consider ***piecewise polynomial*** fits
  - Local behavior can often be well approximated by low-order polynomials




# Piecewise Polynomial Fits

**LIDAR Data Example**

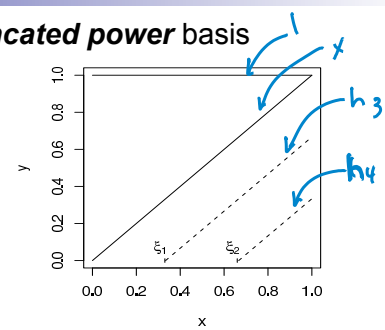



From Wakefield book

# Regression Splines – Linear

- More directly, we can use the ***truncated power*** basis

$$h_1(x) = 1$$
$$h_2(x) = x$$
$$h_3(x) = (x - \xi_1)_+$$
$$h_4(x) = (x - \xi_2)_+$$




From Wakefield book

- Resulting model:

$$f(x) = \beta_0 + \beta_1 x + \beta_2 (x - \xi_1)_+ + \beta_3 (x - \xi_2)_+$$

- Continuous at the knots because all prior basis functions are contributing to the fit up to any single *x*




# Regression Splines – Cubic

- Naively, extend as

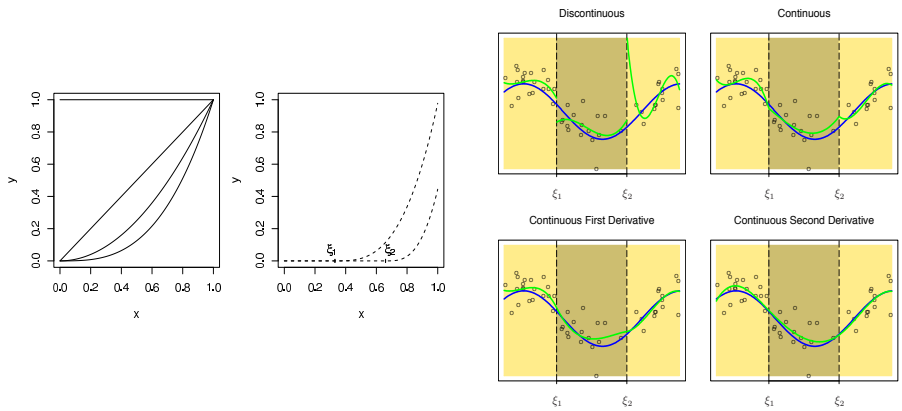
$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 (x - \xi_1)_+ + \beta_4 (x - \xi_1)_+^2 + \beta_5 (x - \xi_2)_+ + \beta_6 (x - \xi_2)_+^2$$

- But, 1st derivate is discontinuous (check this)
- Drop the truncated linear basis:
- Has continuous 1st derivative (check), but not 2nd
- Popular to consider ***cubic spline***:

$$\boxed{f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + b_1 (x - \xi_2)_+^3 + b_2 (x - \xi_2)_+^3}$$

- Has continuous 1st and 2nd derivatives
- Typically people stop here

# Cubic Spline Basis and Fit






# Cubic Splines as Linear Smoothers

- Cubic spline function with *K* knots:

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \sum_{k=1}^{K} b_k (x - \xi_k)_+^3$$

- Simply a linear model

- Estimator:

- Linear smoother:

# Natural Cubic Splines

- For polynomial regression, fit near boundaries is erratic.
  - Problem is worse for splines: each is fit locally so no global constraint
- ***Natural cubic splines*** enforce linearity beyond boundary knots
- Starting from a cubic spline basis, the natural cubic spline basis is

$$N_1(x) = 1 \qquad N_2(x) = x \qquad N_{k+2}(x) = d_k(x) - d_{K-1}(x)$$

$$d_k(x) = \frac{(x-\xi_k)_+^3 - (x-\xi_K)_+^3}{\xi_K - \xi_k}$$

- Derivation




# Regression Splines – Summary

- Definition:

  *An **order-M spline** with knots $\xi_1 < \xi_2 < \cdots < \xi_K$ is a piecewise M-1 degree polynomial with M-2 continuous derivatives as the knots*

  *A spline that is linear beyond the boundary knots is called a **natural spline***

- Choices:
  - Order of the spline
  - Number of knots
  - Placement of knots

# Return to Smoothing Splines

- Objective:

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

- Solution:
  - ***Natural cubic spline***
  - Place knots at every observation location $x_i$
- Proof: See Green and Silverman (1994, Chapter 2) or Wakefield textbook
- Notes:
  - Would seem to overfit, but penalty term shrinks spline coefficients toward linear fit
  - Will not typically interpolate data, and smoothness is determined by λ




# Smoothing Splines

- Model is of the form: $f(x) = \sum_{j=1}^n N_j(x)\beta_j$
- Rewrite objective:

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

- Solution:
- Linear smoother:

# Splines Intro – Summary

- **Regression splines:**
  Fewer number of knots and no regularization
- **Smoothing splines:**
  Knots at every observation and regularization (smoothness penalty) to avoid interpolators




## Module 2: Splines and Kernel Methods

# B-Splines

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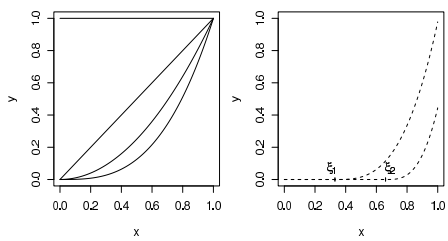
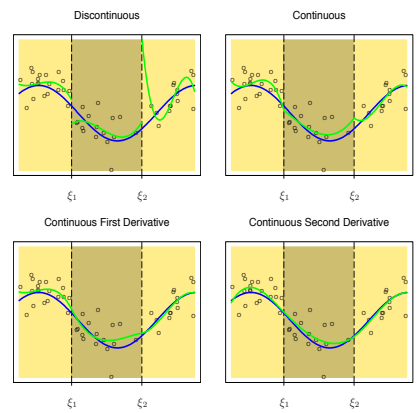
# Cubic Spline Basis and Fit

- Cubic spline function with *K* knots:

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \sum_{k=1}^{K} b_k (x - \xi_k)_+^3$$






# B-Splines

- Alternative basis for representing polynomial splines
- Computationally attractive…Non-zero over limited range
- As before:
  - Knots
  - Domain
  - Number of basis functions =
- Step 1: Add knots
- Step 2: Define auxiliary knots $\tau_j$

$$\tau_1 \leq \tau_2 \leq \cdots \leq \tau_M \leq \xi_0$$
$$\tau_{j+M} = \xi_j$$
$$\xi_{K+1} \leq \tau_{K+M+1} \leq \cdots \leq \tau_{K+2M}$$

# B-Splines

- For 1st order B-spline


From Hastie, Tibshirani, Friedman book



# B-Splines

- For 2nd order B-spline

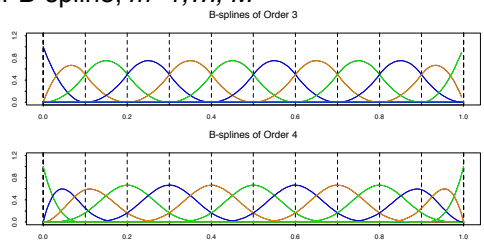

From Hastie, Tibshirani, Friedman book

- Modify 1st order basis:

- Convention: If divide by 0, set basis element to 0

# B-Splines

- For m[th] order B-spline, *m=1,…, M*




From Hastie, Tibshirani, Friedman book

- Modify (m-1)[th] order basis:

$$B_j^m(x) = \frac{x - \tau_j}{\tau_{j+m-1} - \tau_j} B_j^{m-1} + \frac{\tau_{j+m} - x}{\tau_{j+m} - \tau_{j+1}} B_{j+1}^{m-1}$$

  - B-spline bases are non-zero over domain spanned by at most M+1 knots
  - Only subsets $\{B_i^m \mid i = M - m + 1, \ldots, M + K\}$ are needed for basis of order *m* with knots $\xi$



# Cubic Splines as Linear Smoothers

- Cubic spline function with *K* knots:

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \sum_{k=1}^{K} b_k (x - \xi_k)_+^3$$

- Simply a linear model $f(x) = E[Y|c] = c\gamma$

$$C = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & (x_1-\xi_1)_+^3 & \cdots & (x_1-\xi_K)_+^3 \\ \vdots & & & & & & \\ 1 & x_n & x_n^2 & x_n^3 & (x_n-\xi_1)_+^3 & \cdots & (x_n-\xi_K)_+^3 \end{bmatrix} \qquad \gamma = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \\ b_1 \\ \vdots \\ b_K \end{bmatrix}$$

- Estimator: $\hat{\gamma} = (C^T C)^{-1} C^T Y$
- Linear smoother: $\hat{f} = \underbrace{C(C^T C)^{-1} C^T}_{L} Y$

# Cubic B-Splines

- Cubic B-spline with *K* knots has basis expansion:
- Simply a linear model
- Computational gain:



# Return to Smoothing Splines

- Objective:

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

- Solution:
  - ***Natural cubic spline***
  - Place knots at every observation location $x_i$
- Proof: See Green and Silverman (1994, Chapter 2) or Wakefield textbook
- Notes:
  - Would seem to overfit, but penalty term shrinks spline coefficients toward linear fit
  - Will not typically interpolate data, and smoothness is determined by λ

# Smoothing Splines

- Model is of the form: $f(x) = \sum_{j=1}^{n} N_j(x)\beta_j$

  # of obs.

  natural cubic spline basis

- Rewrite objective:

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

$[N]_{ij} = N_j(x_i)$

$[\Omega_N]_{jk} = \int N_j''(t) N_k''(t)\, dt$

- Solution: $\hat{\beta} = (N^T N + \lambda\Omega_N)^{-1} N^T y$ as in ridge

- Linear smoother:

$$\hat{f} = \underbrace{N(N^T N + \lambda\Omega_N)^{-1} N^T}_{L_\lambda} y$$

"smoothing matrix"

$v_\lambda = tr(L_\lambda)$



# Smoothing Splines

- Model is of the form: $f(x) = \sum_{j=1}^{n} N_j(x)\beta_j$
- Using B-spline basis instead:
- Solution: $\hat{\beta} = (B^T B + \lambda\Omega_B)^{-1} B^T y$
- Penalty implicitly leads to natural splines
  - Objective gives infinite weight to non-zero derivatives beyond boundary

# Spline Overview (so far)

**Smoothing Splines**

- Knots at data points $x_i$
- Natural cubic spline
- O($n$) parameters
  - Shrunk towards subspace of smoother functions

**Regression Splines**

- $K < n$ knots chosen
- M$^{th}$ order spline = piecewise *M-1* degree polynomial with *M-2* continuous derivatives at knots

- Linear smoothers, for example using natural cubic spline basis:




**Module 2: Splines and Kernel Methods**

# Penalized Regression Splines

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# Penalized Regression Splines

- Alternative approach:
  - Use $K < n$ knots
  - How to choose $K$ and knot locations?
- Option #1:
  - Place knots at $n$ unique observation locations $x_i$ and do stepwise
  - Issue??
- Option #2:
  - Place many knots for flexibility
  - Penalize parameters associated with knots
- Note: Smoothing splines penalize complexity in terms of roughness. Penalized reg. splines shrink coefficients of knots.




# Penalized Regression Splines

- General spline model
- Definition: A ***penalized regression spline*** is $\hat{\beta}^T h(x)$ with
- Form of resulting spline depends on choice of
  - Basis
  - Penalty matrix
  - Penalty strength
- Still need to choose $K$ and associated locations. RoT (Ruppert et al 2003):

$$K = \min(\frac{1}{4} \times \ \# \text{ unique } x_i, 35) \qquad \xi_k \text{ at } \frac{k+1}{K+2} th \text{ points of } x_i$$

# PRS Example #1

$$\sum_{i=1}^{n}(y_i - \beta^T h(x_i))^2 + \lambda \beta^T D \beta$$

- Cubic B-spline basis + penalty
- For this penalty, the matrix *D* is given by
- Leads to




# PRS Example #2

$$\sum_{i=1}^{n}(y_i - \beta^T h(x_i))^2 + \lambda \beta^T D \beta$$

- B-spline basis + penalty
- For this penalty, the matrix *D* is given by
- Leads to

# PRS Example #3

$$\sum_{i=1}^{n}(y_i - \beta^T h(x_i))^2 + \lambda \beta^T D \beta$$

- Cubic spline using truncated power basis

  + penalty on truncated power coefficients

- For this penalty, the matrix *D* is given by




# A Brief Spline Summary

- ***Smoothing spline*** – contains *n* knots
- ***Cubic smoothing spline*** – piecewise cubic
- ***Natural spline*** – linear beyond boundary knots
- ***Regression spline*** – spline with $K < n$ knots chosen
- ***Penalized regression spline*** – imposes penalty (various choices) on coefficients associated with piecewise polynomial
- The # of basis functions depends on
  - # of knots
  - Degree of polynomial
  - A reduced number if a natural spline is considered (add constraints)

# Reading

- Hastie, Tibshirani, Friedman: 5.1-5.5 (skipping 5.3), Ch. 5 appendix
- Wakefield: 11.1.1-11.2.6




# What you should know…

- Regression splines
  - Cubic splines, natural cubic splines, …
  - Interpretation as a linear smoother
  - Degrees of freedom
- Smoothing splines
  - Arising from penalized regression setting with smoothness penalty
  - Cubic spline basis with knots at every data point
- Natural splines
  - Linear beyond boundary points
- B-splines
  - Basis functions with compact support
- Penalized regression splines
  - Choose knots as in regression splines, but penalize associated coefficients