Winter Course Statistical Learning

Splines and Generalized Additive Models

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Modeling non-linearity

- Can use polynomial regression, e.g., cubic:

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \epsilon_i$$

- More generally, of degree d:

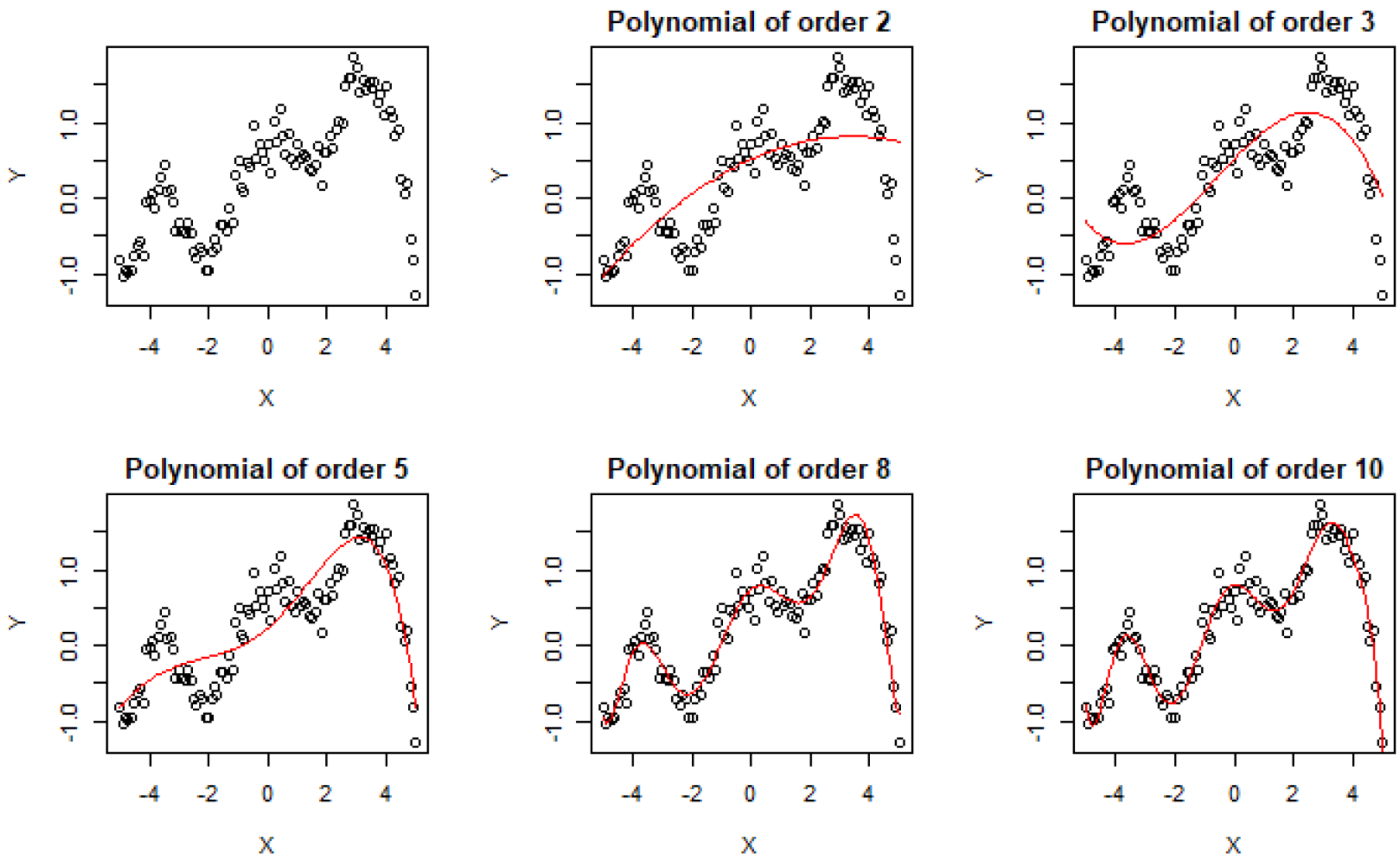
$$y_i = \beta_0 + \sum_{j=1}^{d} \beta_j x_i^j + \epsilon_i$$

$$\mathbb{E}(y_i|x_i) = \beta_0 + \sum_{j=1}^{d} \beta_j x_i^j$$

- Can generalize as usual within the GLM, e.g., for binary outcome:

$$\log\left(\frac{\pi_i}{1-\pi_i}\right) = \beta_0 + \sum_{j=1}^{d} \beta_j x_i^j$$

Flexibility may been needed, but ...



Why splines?

- Splines *localize* the fitted model $\hat{f}(x)$ while enforcing *smoothness*.
- This critically improves on the main drawback of polynomial functions, where an observation on one end of the range of x may heavily influence the fitted curve on the opposite.
- The *smoother* $\hat{f}(x)$, the less change there is in the *derivatives* w.r.t. x of $\hat{f}(x)$.
- Question: What is the derivative of $\hat{f}(x)$ w.r.t. x in a linear model? Does it change as a function of x?

Polynomial regression, generalized additive models

- Interest in inference and in flexible approximation of shape of association; no interest in individual coefficients (difficult to interpret).

- Model selection and hypothesis testing through:

  1. Statistical tests (t and/or F tests, ANOVA, likelihood ratio tests)
  2. Information criteria (AIC, BIC)
  3. Cross validation

Step functions

- Define cut points $\xi_1, \xi_2, \ldots, \xi_K$ and with these, step functions:

$$\begin{aligned} h_0(X) &= I(X < \xi_1) \\ h_1(X) &= I(\xi_1 \leq X < \xi_2) \\ &\ldots \\ h_{K-1}(X) &= I(\xi_{K-1} \leq X < \xi_K) \\ h_K(X) &= I(\xi_K \leq X) \end{aligned}$$

- Can use $h_k(X)$ as predictors in a regression:

$$y_i = \beta_0 + \sum_{k=1}^{K} \beta_k h_k(x_i) + \epsilon_i$$

Basis functions

- Polynomials and step functions are *basis functions* of the predictors.
- We can define basis functions of each predictor X_j: $h_{j,1}(X_j), h_{j,2}(X_j), \ldots, h_{j,K_j}(X_j)$
- Generalized Additive Model: Use basis functions instead of original X_j as predictors in a (G)LM:

$$f(x_i) = \beta_0 + \sum_{j=1}^{p} \sum_{k_j=1}^{K_j} \beta_{k_j} h_{k_j}(x_{ij}) = \beta_0 + \sum_{j=1}^{p} f_j(x_{ij})$$

- If functions h_{k_j} are known in advance, parameters can be estimated 'as usual' (with OLS, ML, ...).
- Better: Precise shape is unknown in advance, so use penalized estimation (i.e., smoothing splines).

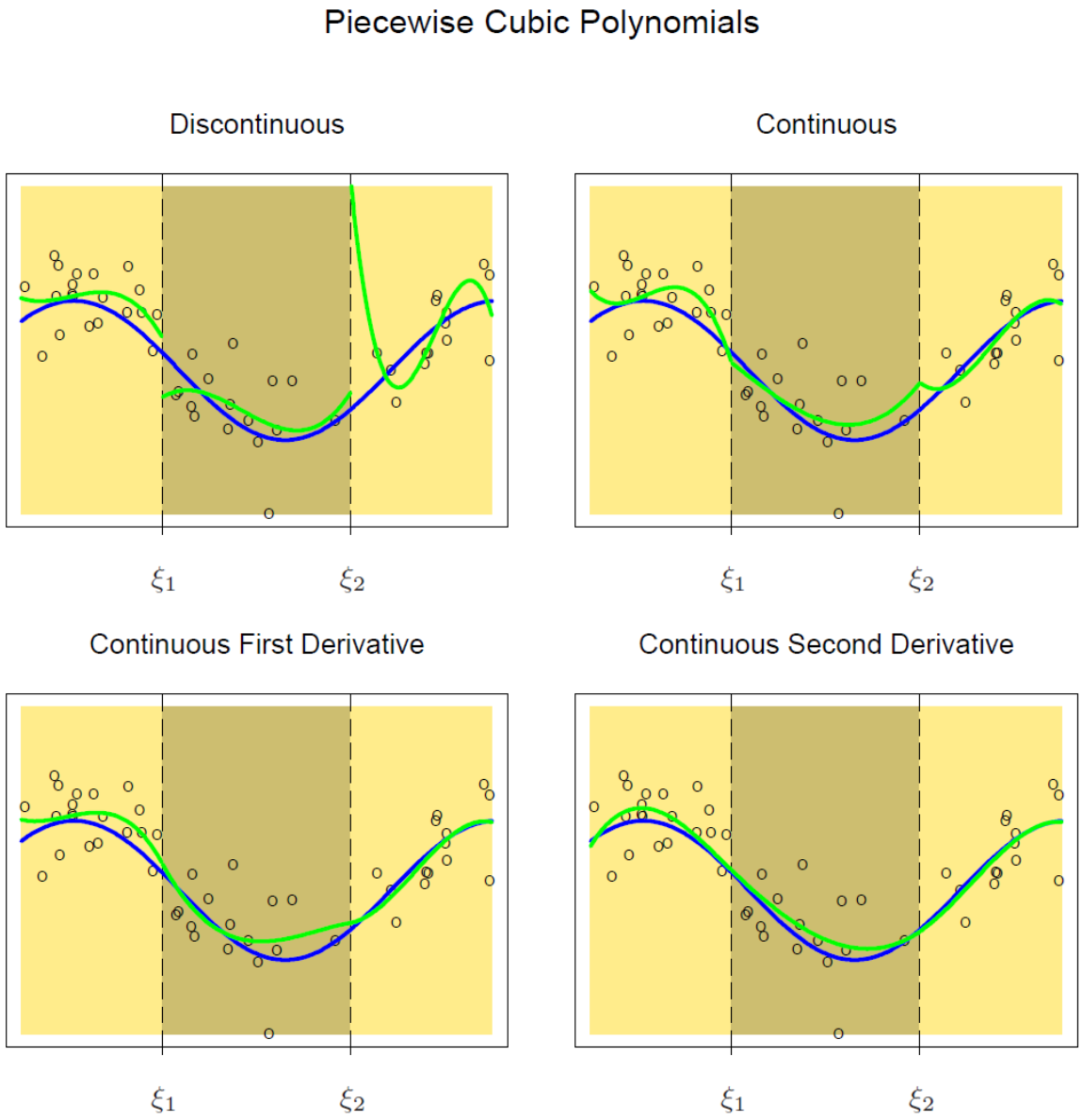
Piecewise polynomial

- Combine step idea with polynomial functions
- Create cutpoints ξ_1 through ξ_k:

$$\hat{y}_i = \begin{cases} \hat{\beta}_{01} + \hat{\beta}_{11} x_i + \hat{\beta}_{21} x_i^2 + \hat{\beta}_{31} x_i^3 \text{ if } x_i < \xi_1 \\ \hat{\beta}_{02} + \hat{\beta}_{12} x_i + \hat{\beta}_{22} x_i^2 + \hat{\beta}_{32} x_i^3 \text{ if } \xi_1 \leq x_i < \xi_2 \\ \hat{\beta}_{03} + \hat{\beta}_{13} x_i + \hat{\beta}_{23} x_i^2 + \hat{\beta}_{33} x_i^3 \text{ if } x_i \geq \xi_2 \end{cases}$$

- This is a *piecewise polynomial* with 2 knots (cutpoints).
- Can still give erratic behavior near boundaries:

Piecewise polynomial



Regression Splines

- We rather have a *smooth* curve, so we add constraints:
  - f should be continuous.
  - f' should be continuous.
  - f'' should be continuous.
- General definition:
  - A degree-d spline is a piecewise polynomial of degree d,
  - with continuity in the derivatives up to degree $d - 1$.
- It uses $d + 1 + K$ degrees of freedom. A cubic spline with K knots uses $K + 4$ degrees of freedom (see next slide!).

Cubic spline

- The basis functions are given by

$$
\begin{aligned}
h_1(X) &= X \\
h_2(X) &= X^2 \\
h_3(X) &= X^3 \\
h_{3+k}(X, \xi_k) &= (X - \xi_k)_+^3 = \begin{cases} (X - \xi_k)^3 & \text{if} \quad X > \xi_k \\ 0 & \text{otherwise} \end{cases}
\end{aligned}
$$

  for $k = 1, \ldots, K$

- The intercept uses up an additional degree of freedom.

Note: There are many equivalent ways to define splines. In line with the book, here the truncated power basis function approach is given. It is easiest to describe, but computationally inefficient and therefore rarely used in software implementations. However, the different approaches to define splines tend to give identical or highly similar results.

Natural spline

- The *natural spline* additionally constrains the function to be linear at the boundaries.

- Uses lower degrees of freedom: only linear effect at both boundaries.

$$
\begin{aligned}
h_1(X) &= X \\
h_2(X) &= X^2 \\
h_3(X) &= X^3 \\
h_{3+k}(X, \xi_k) &= (X - \xi_k)_+^3 = \begin{cases} (X - \xi_k)^3 & \text{if} \quad X > \xi_k \\ 0 & \text{otherwise} \end{cases}
\end{aligned}
$$

Smoothing Spline

- To avoid (mis)specification of number and location of knots, we simply place way too many and use penalization to obtain a smooth model.

- As in lasso and ridge regression, use a *fit + penalty* approach:

$$PRSS(f, \lambda) = \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \int f''(t)^2 dt$$

- The function f that minimizes this PRSS is known as a *smoothing spline*: A natural spline with a knot at every unique observed value x_i.

- The design matrix for the smoothing spline has n columns! With so many basis functions of x_j, it is heavily overparameterized!

- Penalty $\lambda \int f''(t)^2 dt$ shrinks coefficients of many columns towards zero (cf. ridge regression).

From univariate splines to GAMs

- Often we have multiple predictor variables: $X_1, \ldots, X_p$
- We can generalize the ideas:

$$y_i = \beta_0 + \sum_{j=1}^{p} f_j(x_{ij}) + \epsilon_i$$

- The f_j are estimated through minimizing 9.7 (p. 297):

$$PRSS = \sum_{i=1}^{N} \{y_i - \beta_0 - \sum_{j=1}^{p} f_j(x_{ij})\}^2 + \sum_{j=1}^{p} \left[\lambda_j \int f_j''(t_j)^2 dt_j \right]$$

- The f_j need not be smoothing splines. Can be linear functions (then 2nd derivative is 0, so penalty too) or unpenalized splines (then λ_j is fixed to 0).

Penalized likelihood estimation

- Current state-of-the-art: R package `mgcv` (Wood, 2004, 2011).
- Allows for using restricted maximum likelihood estimation: specify `method = "REML"` in the call to function `gam`).
- The *linear* basis function is estimated as a *fixed effect*, i.e., its parametric coefficient β_j is estimated in an unpenalized manner (cf. *PRSS* formula).
- The *non-linear* basis functions are treated as random effects, i.e., only the variance σ_b^2 of the coefficients is estimated; the coefficients of the non-linear functions are thereby estimated in a *penalized manner* (cf. *PRSS* formula).
- There is a one-to-one correspondence between λ (or λ_j) in the *PRSS* formula and the variance of the random effect σ_b: $\lambda = \frac{\sigma_\epsilon^2}{\sigma_b^2}$
- Random effects can also be included to account for *dependency* of observations! See `?mgcv::s` and `mgcv::?smooth.terms` to see how random effects can be specified using the `bs` argument of function `s()`.