Nonlinear effects and generalized additive models

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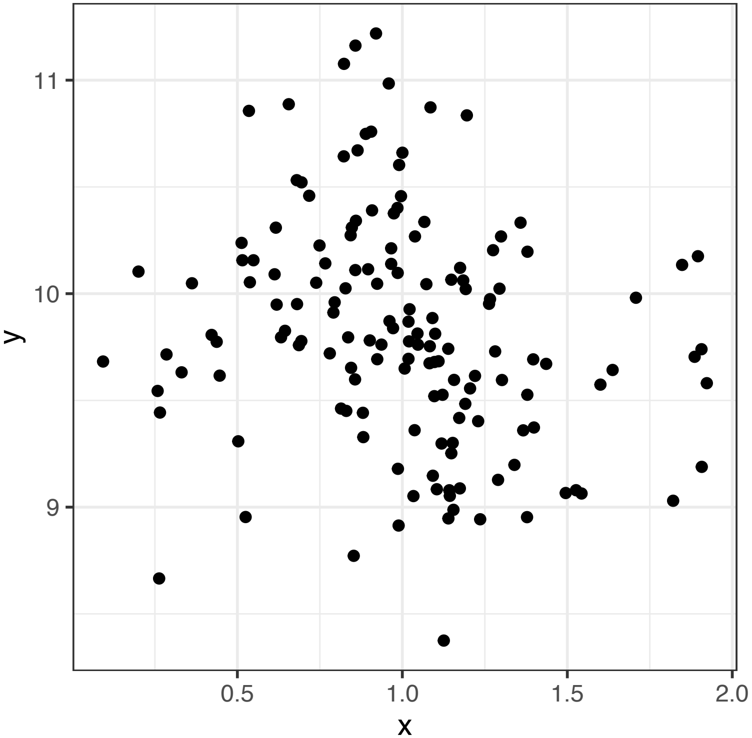
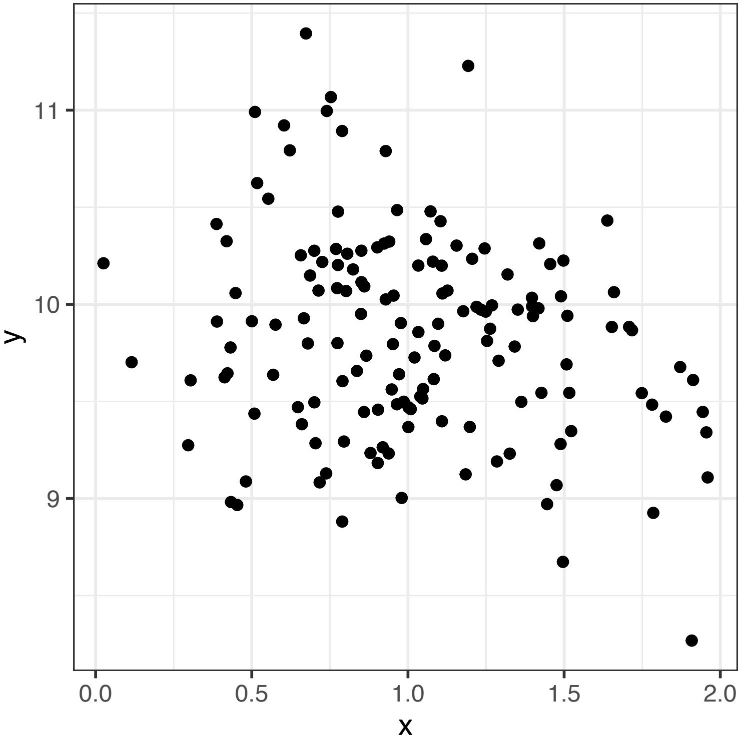
Inferring the trend





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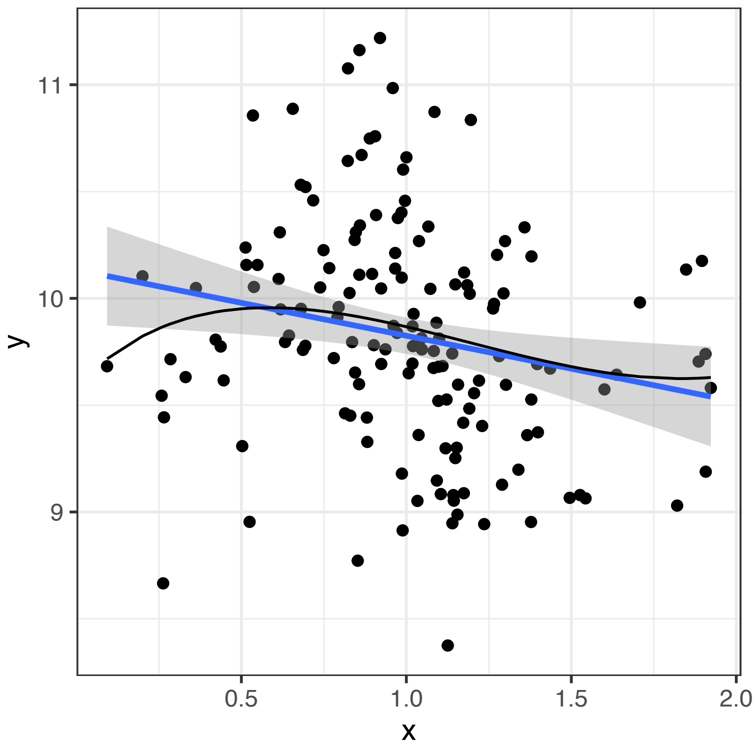
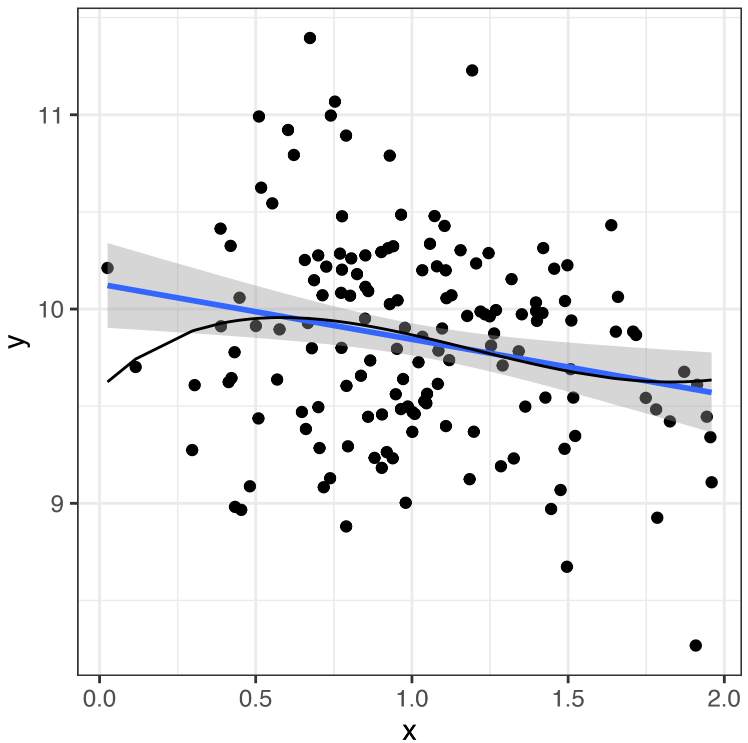
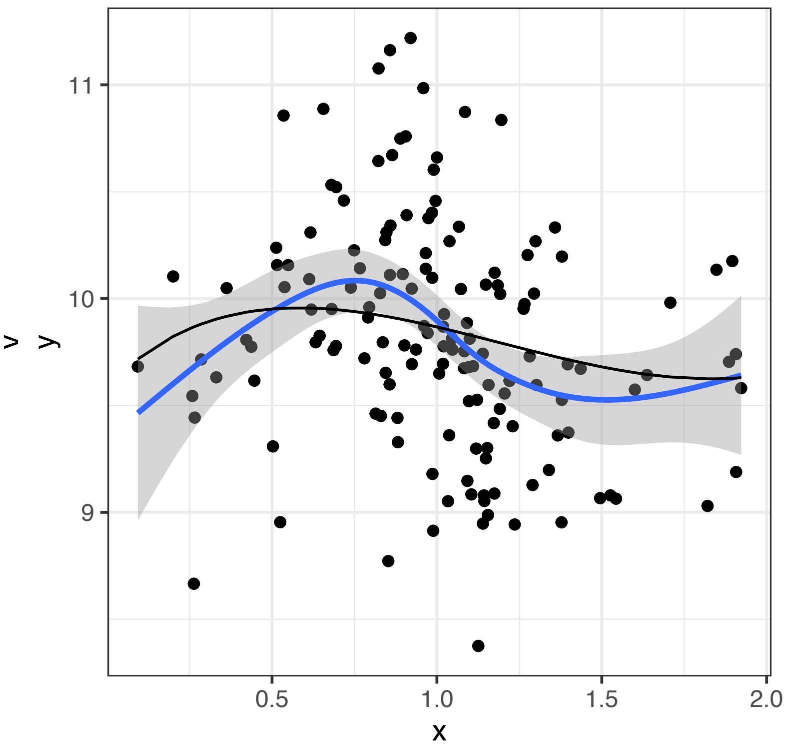
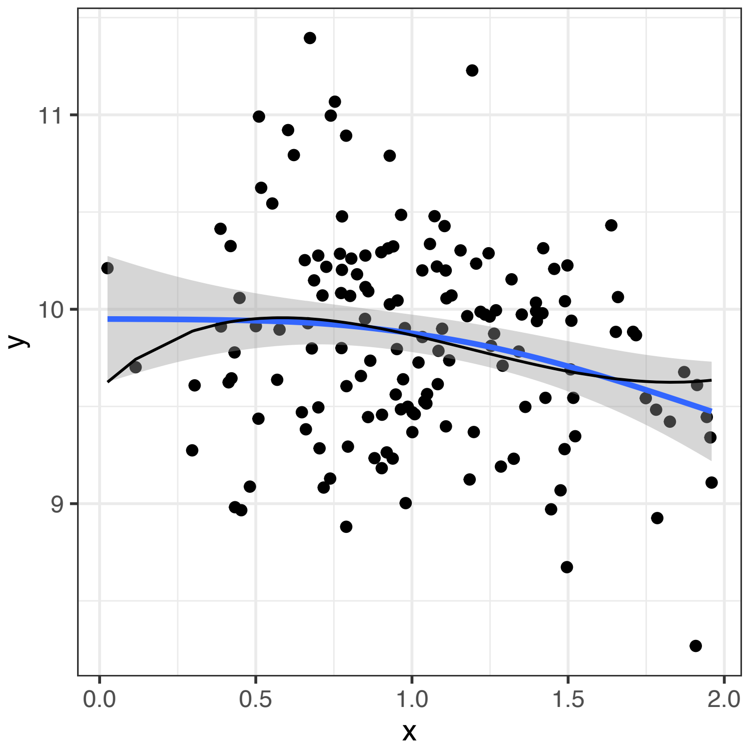




Linear smoother (=linear regression)

Inferring the trend





Generalized Additive Model smoother (=GAM regression)

Taking on nonlinearity: major ideas

- Use a **basis expansion:** a set of functions $\{h_i\}$ each of which differently transforms your original predictor X
- Learn the $Y \sim X$ as a linear comb. of the basis functions

$$f(x) = \sum_i \beta_i h_i(x) \qquad\qquad y \sim \text{Exp}(f(x))$$

Some exponential-family function (one that you could use in a generalized linear model)

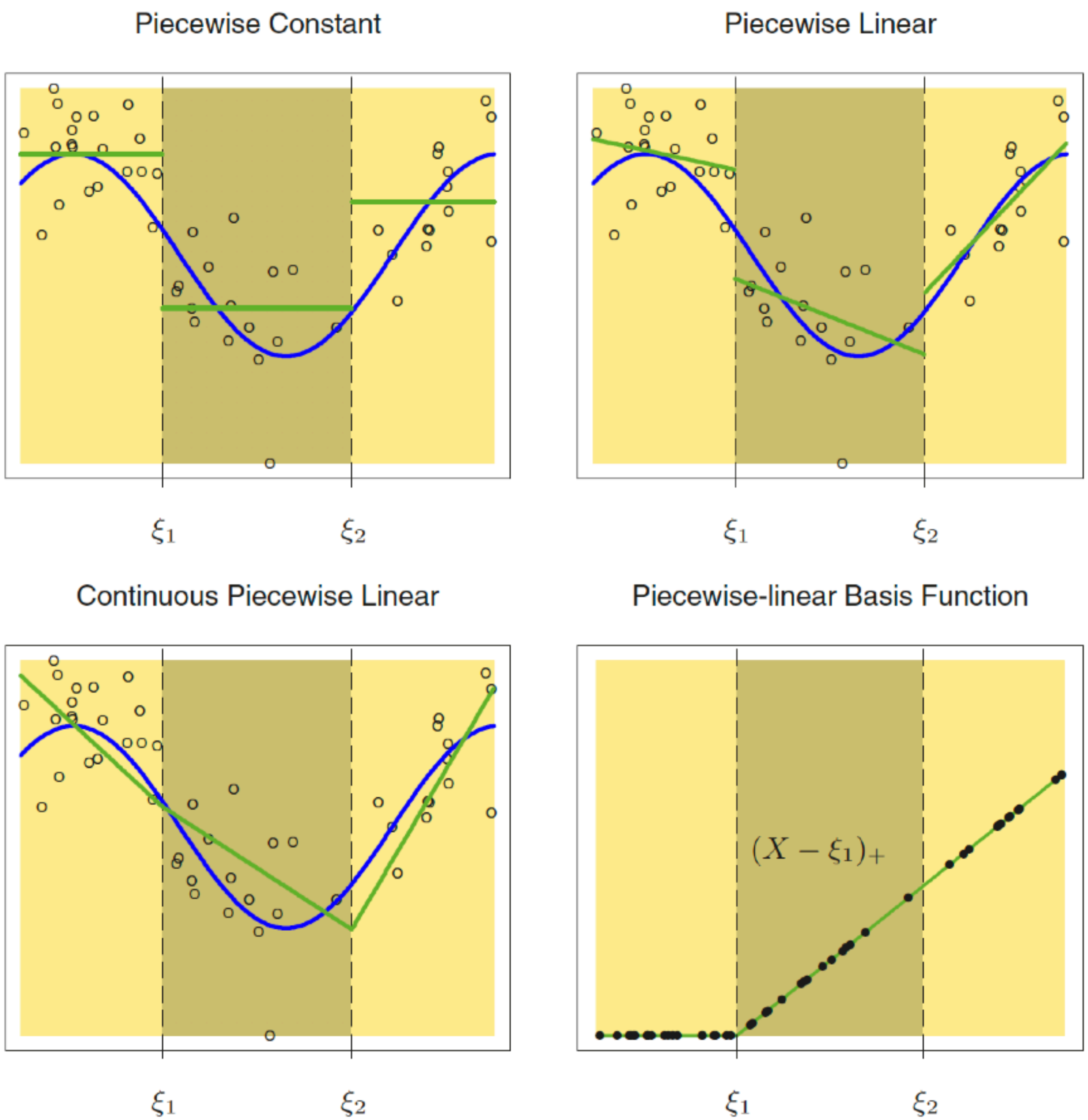
- Use **regularization** and **held-out accuracy evaluation** to guard against overfitting

Example basis expansions for *piecewise* fits

$$h_1 = I(X < \xi_1)$$

$$h_2 = I(\xi_1 < X \leq \xi_2)$$

$$h_3 = I(\xi_2 < X \leq \xi_3)$$



(From Hastie et al., 2009)

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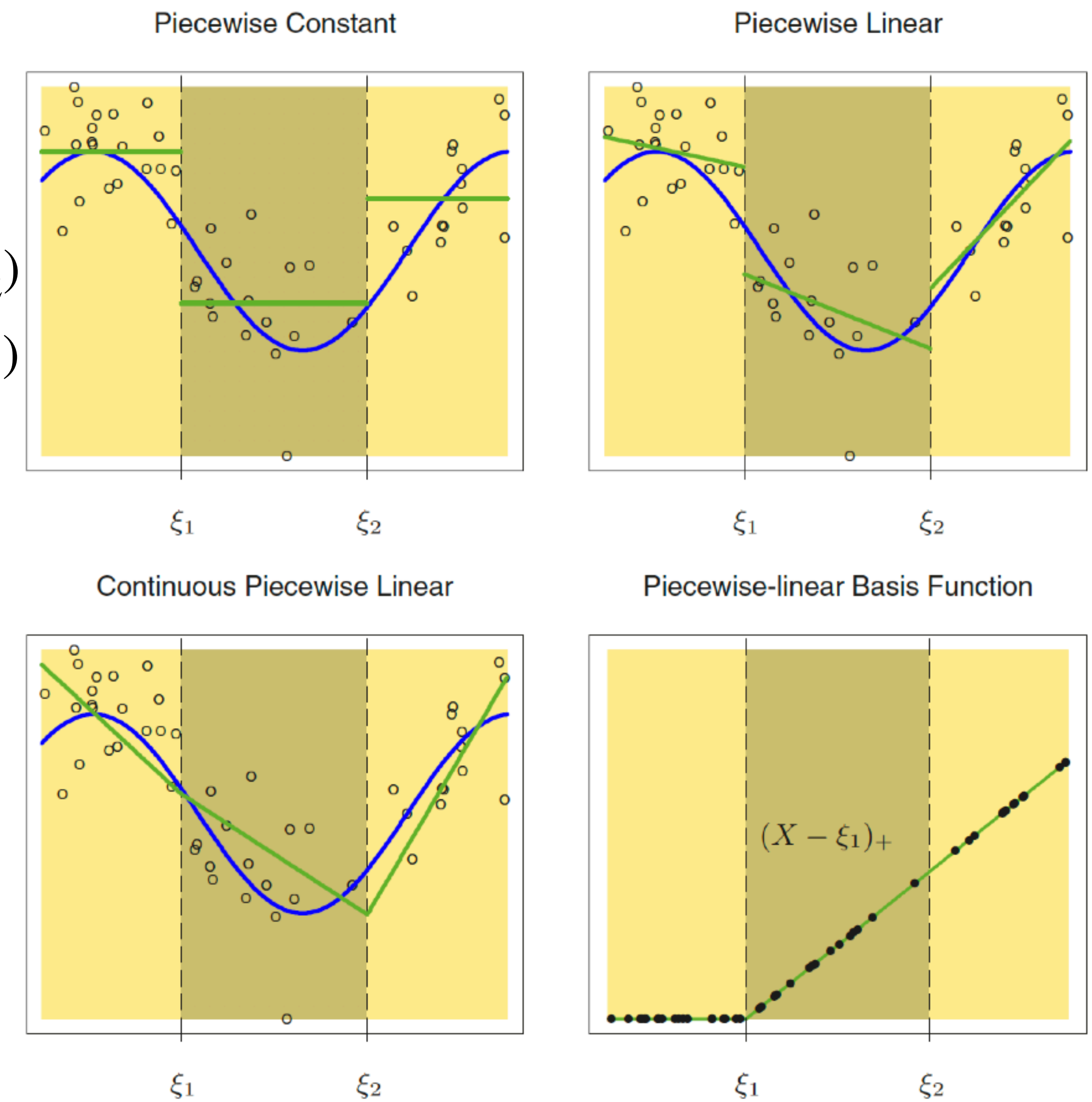

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$$h_4 = h_1(X)X$$
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$$h_6 = h_3(X)X$$

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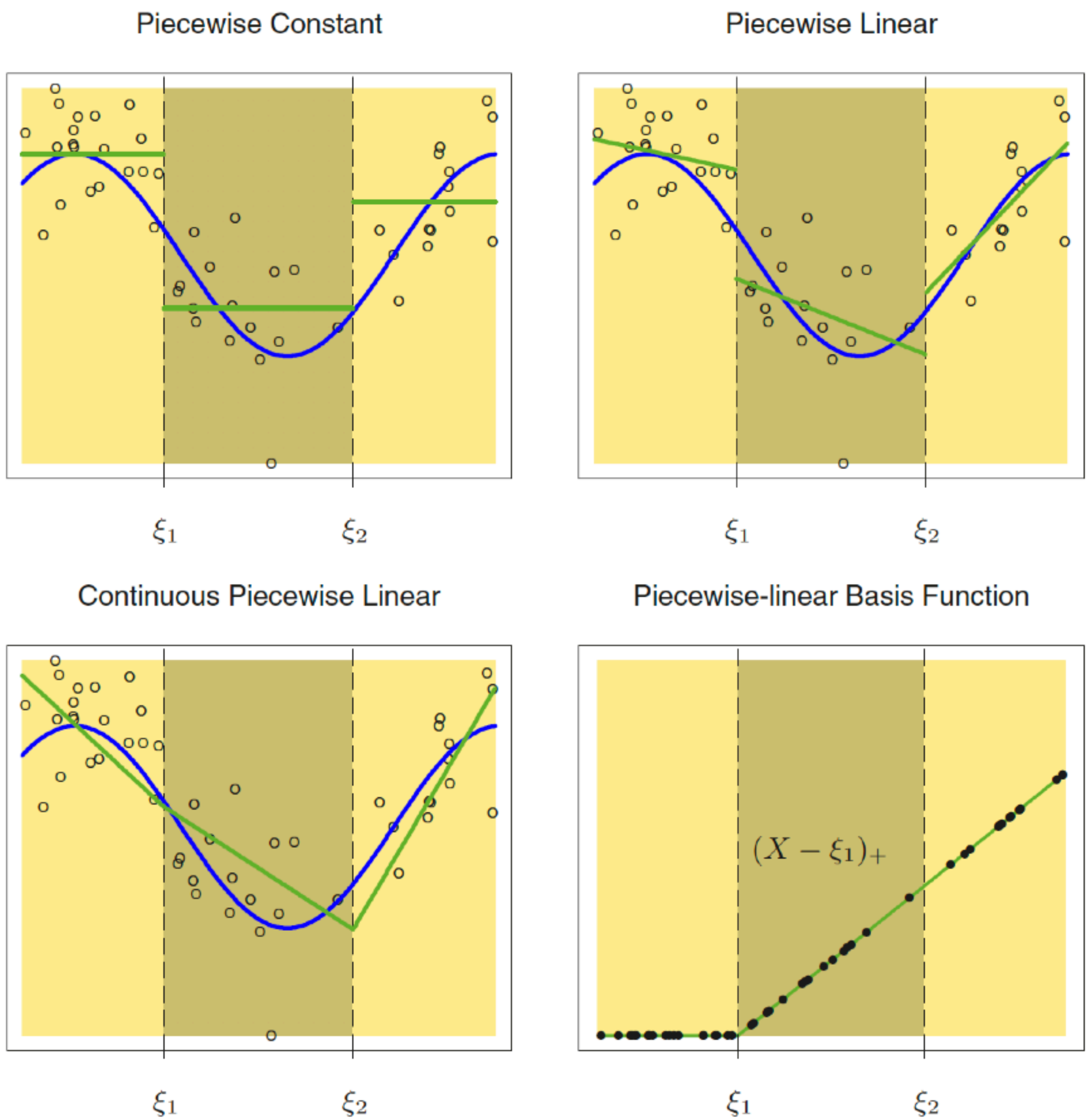

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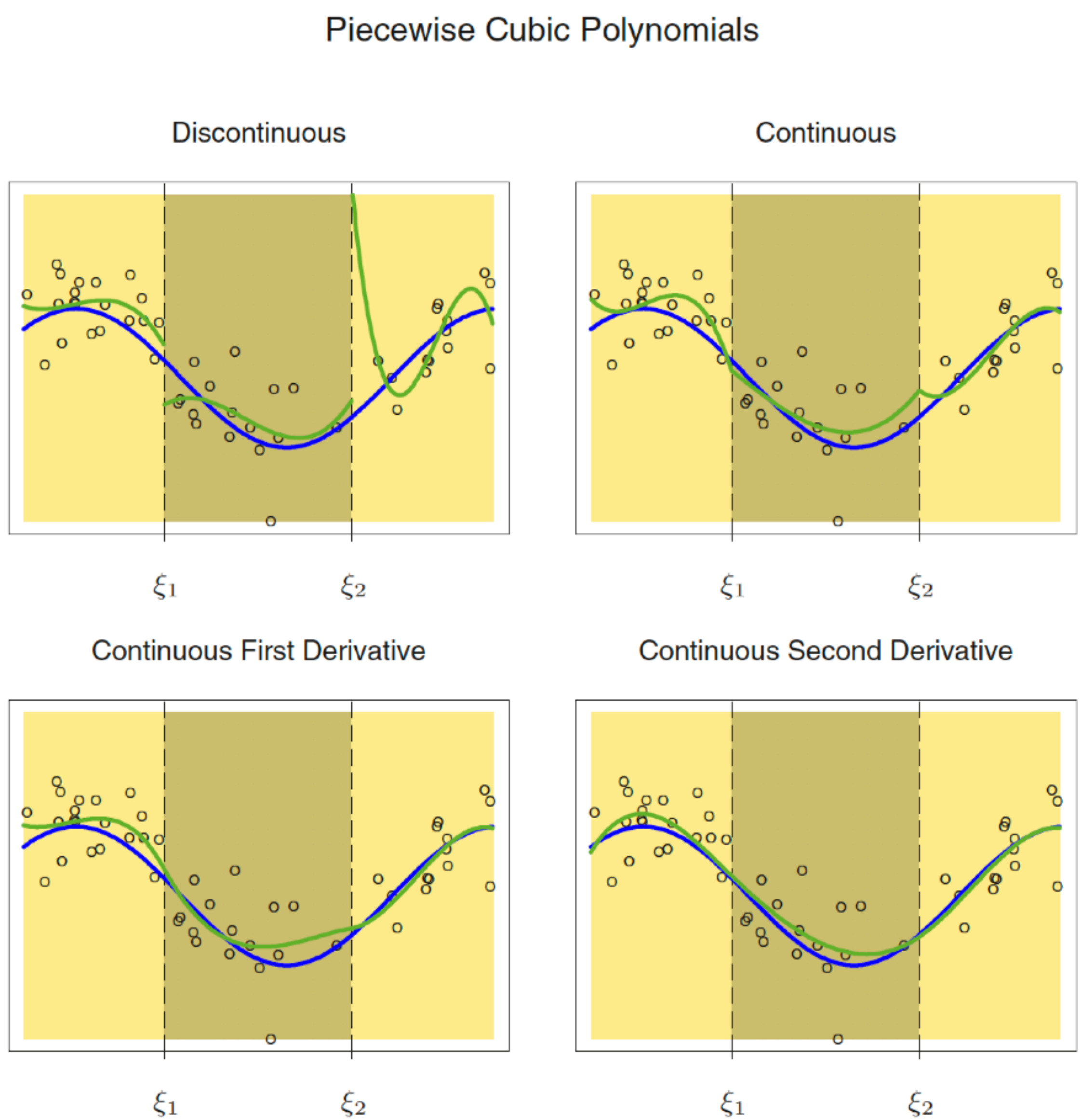
$$h_6 = h_3(X)X$$

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

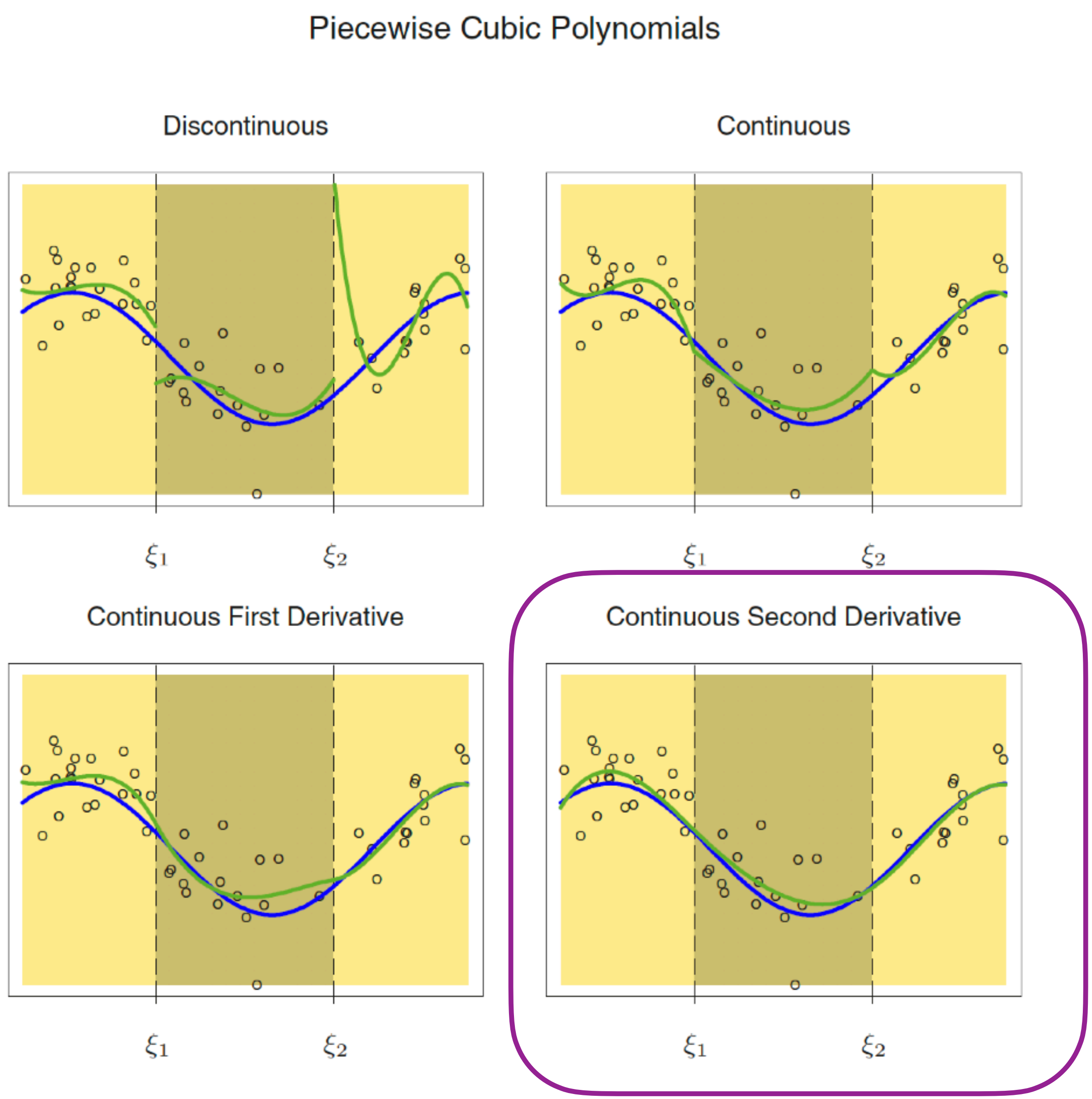
(From Hastie et al., 2009)

Example basis expansions for *piecewise* fits



(From Hastie et al., 2009)

Example basis expansions for *piecewise* fits



Popular modeling choice

(From Hastie et al., 2009)

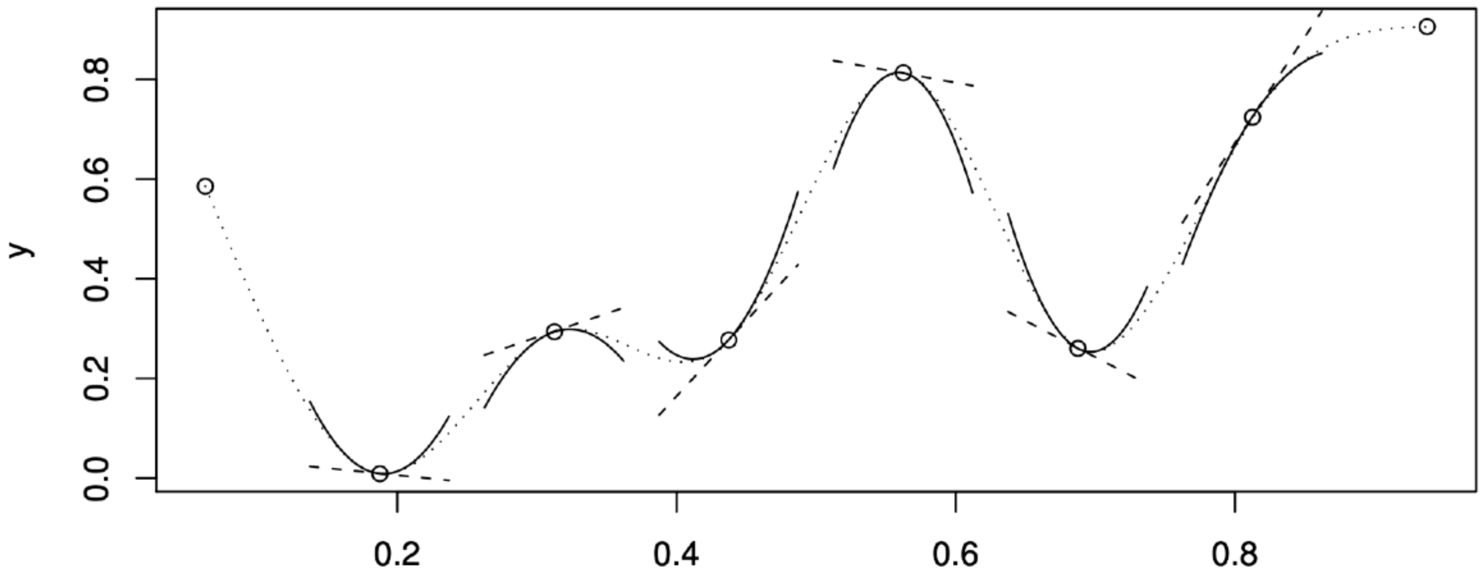
Natural, or restricted, cubic splines

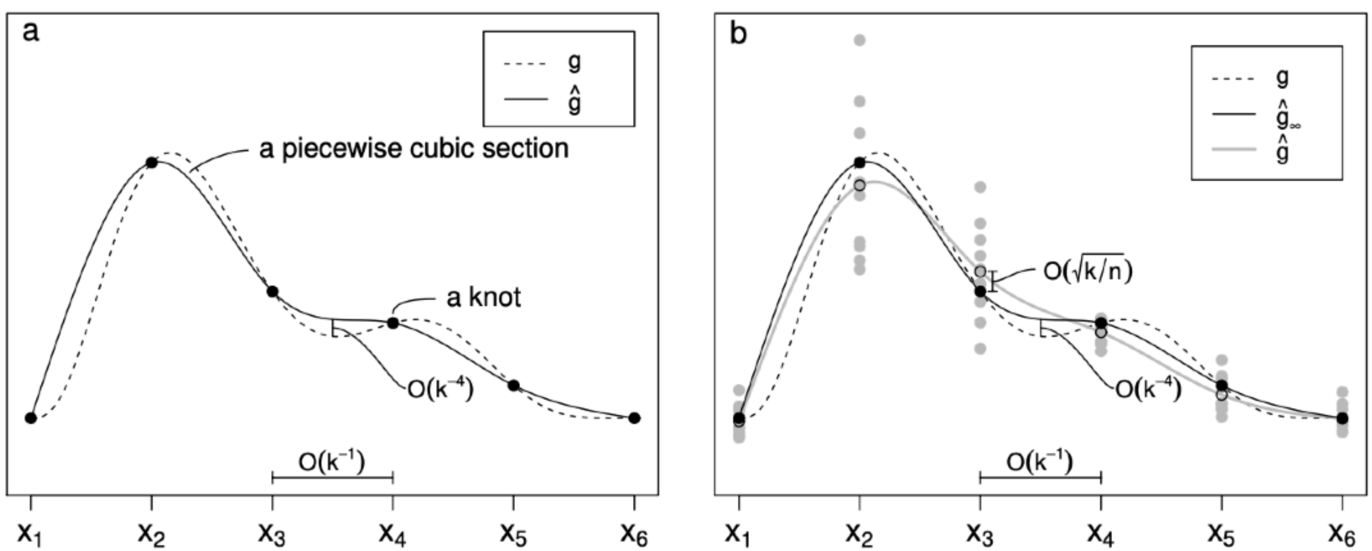
- Intuitively: a piecewise cubic function whose 0th, 1st, and second derivatives are continuous at all the **knots**
- Technically, for n knots:

$$
\begin{aligned}
h_1(X) &= 1 \\
h_2(X) &= X \\
h_3(X) &= X^2 \\
h_4(X) &= X^3 \\
h_i(X) &= (x - \xi_i)_+^3, \text{ for } i = 5, \ldots, n+4
\end{aligned}
$$

- Powerful framework, but leaves open:
  - How many knots to use
  - Where to put the knots

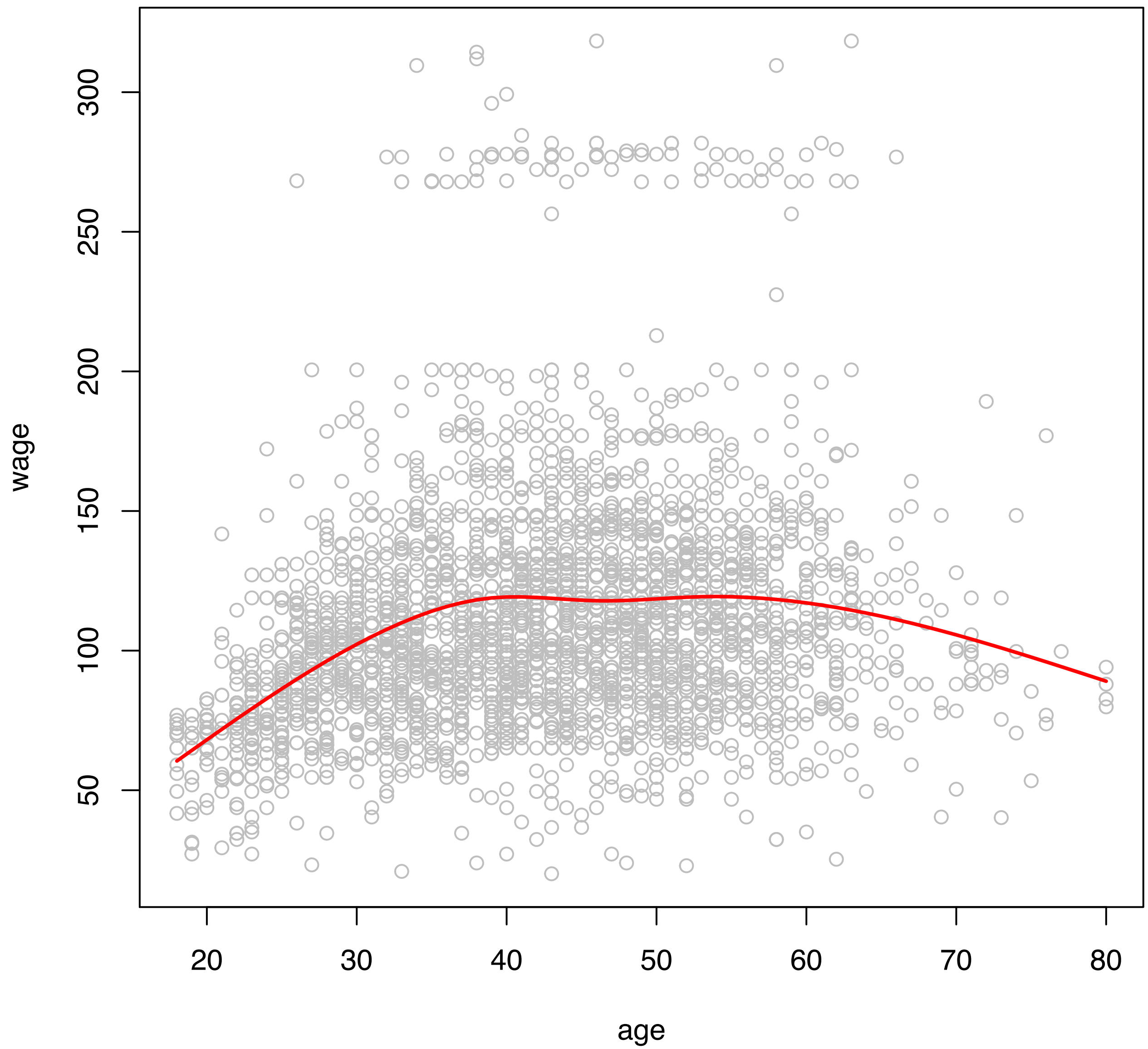
Natural cubic splines, visualized





(Wood, 2017, Chapter 5)

Example of fitted natural splines (5 d.f.)



(From James et al., 2013)

From smooths to GAMs

- A **generalized additive model** (GAM) involving 2 predictors X and V for response Y looks like this:

$$y_i = \mathbf{A}_i\theta + f_1(x_i) + f_2(v_i) + f_3(x_i, v_i) + \epsilon_i$$

  where each $f_i()$ is a **smooth function** of its arguments
- This is a highly general and expressive formalism, and cannot be fitted via maximum likelihood (why?)
- So in practice, GAMs are fitted by:
  - choosing a **penalization** or **regularization** component for the objective function;
  - choosing a set of **basis functions** by which to represent each smooth function;
  - Searching for a fit that optimizes the objective function

(Wood 2017, Chapter 7)

Penalization & cross-validation

$$\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \underbrace{\lambda_1 \boldsymbol{\beta}^\mathsf{T} \mathbf{S}_1 \boldsymbol{\beta}} + \underbrace{\lambda_2 \boldsymbol{\beta}^\mathsf{T} \mathbf{S}_2 \boldsymbol{\beta}}$$

Terms penalizing wiggliness for f_1 and f_2

How well data are predicted

Penalization & cross-validation

- Penalized objective:

$$\underbrace{\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2}_{\text{How well data are predicted}} + \underbrace{\lambda_1 \boldsymbol{\beta}^\mathsf{T}\mathbf{S}_1\boldsymbol{\beta} + \lambda_2 \boldsymbol{\beta}^\mathsf{T}\mathbf{S}_2\boldsymbol{\beta}}_{\text{Terms penalizing wiggliness for } f_1 \text{ and } f_2}$$

(Wood 2017, Chapter 7)

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How well data are predicted

- How to choose $\{\lambda_i\}$?

(Wood 2017, Chapter 7)

Penalization & cross-validation

- Penalized objective:

$$\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \underbrace{\lambda_1 \boldsymbol{\beta}^\mathsf{T}\mathbf{S}_1\boldsymbol{\beta} + \lambda_2 \boldsymbol{\beta}^\mathsf{T}\mathbf{S}_2\boldsymbol{\beta}}_{\text{Terms penalizing wiggliness for } f_1 \text{ and } f_2}$$

How well data are predicted

- How to choose $\{\lambda_i\}$?

- Here: **cross-validation**

(Wood 2017, Chapter 7)

Strategy for getting proficient in GAMs

- Read Jones et al. 2013 Chapter 7, and do the exercises
- Read Wood 2017, starting with Chapter 4 and Chapter 7, and do the exercises
- To build expertise read Wood 2017 Chapter 6 and also Chapter 5
- Both these books are available online via MIT Libraries
- For the rest of this class, we will build a bit of expertise via worked examples
  - Data from Boyce & Levy, 2023
  - Material from the "GAMs in R" interactive course (https://noamross.github.io/gams-in-r-course/)