CEE 697M: Probabilistic Machine Learning

M2 Linear Methods: Splines, GAMs and GLMs

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Outline

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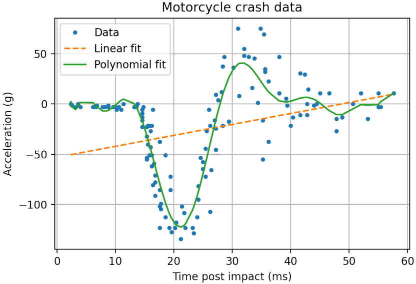

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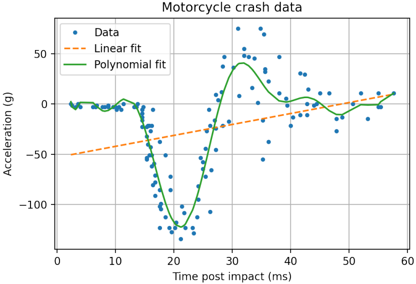

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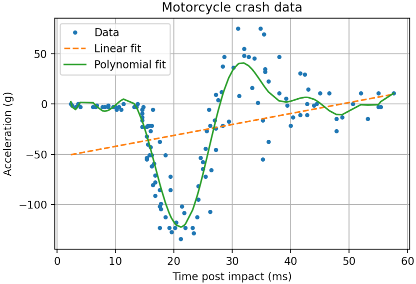

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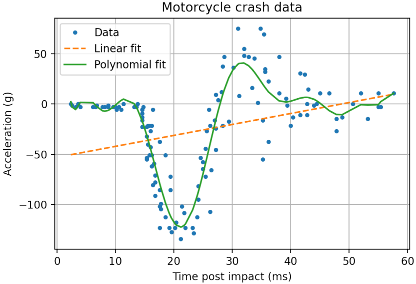

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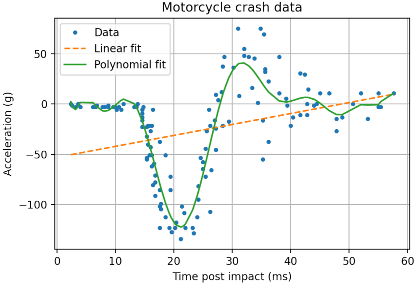

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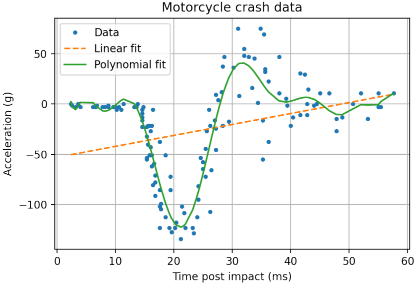

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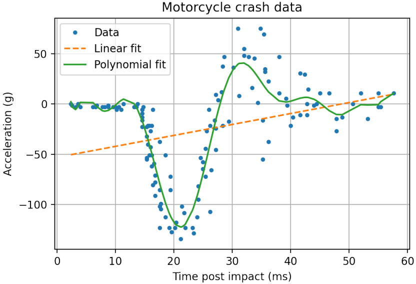

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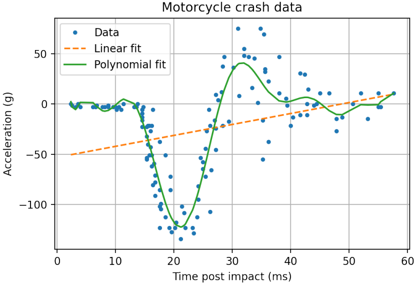

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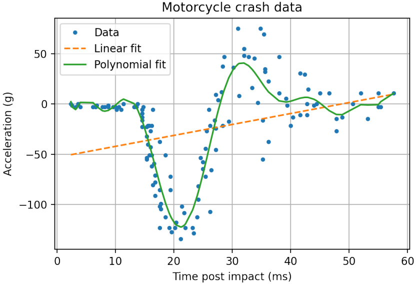

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  - local regression: allow overlap

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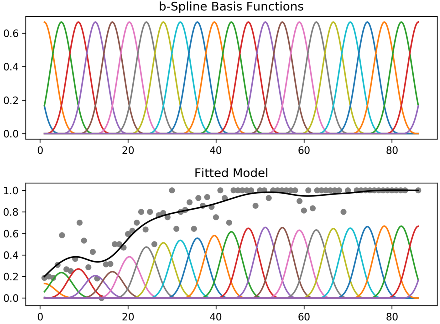

Source: `https://pygam.readthedocs.io/en/latest/notebooks/tour_of_pygam.html`

Splines

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$$f(X) = \sum_p w_p b_p(x) \tag{1}$$

Generally, the **order M (regression) spline** is given by the **truncated power basis**:

$$\begin{aligned} b_p(x) &= x^m, \quad m = 0, \ldots, M &(2)\\ b_{M+k}(x) &= (X - \xi_k)_+^M, k = 1, \ldots, K &(3) \end{aligned}$$

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In most cases, M is taken as 0 (piecewise-constant), 1 (piecewise-linear) or 3 (cubic spline).

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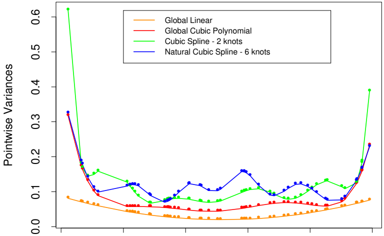

Figure: Pointwise variance curves for 4 different models. $x \sim \mathcal{U}(0,1)$; error assumed constant

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In this form, it can be easily seen that $\hat{\boldsymbol{w}}$ can be found via least squares.

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$$\Omega_{k',k} = \int S''_{k'}(t) S''_k(t) dt \tag{15}$$

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This is simply a generalized ridge regression!

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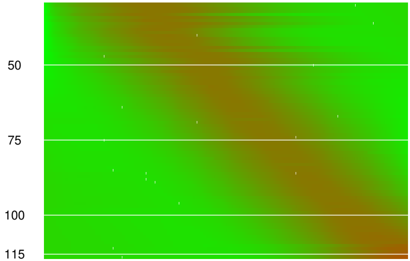

Figure: Visualization of a smoother matrix. Reddish hues indicate higher values.

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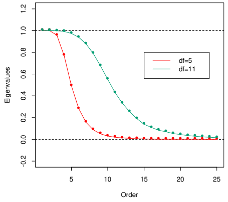

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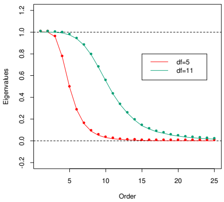

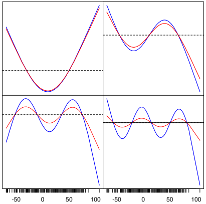

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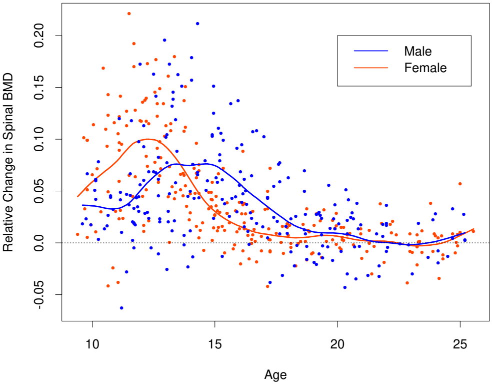

Figure: Estimating a smoothing spline for bone mineral density for male and female adolescents. $df_\lambda \approx 12$. The fitted splines shows that changes in BMD occur earlier in females than males.

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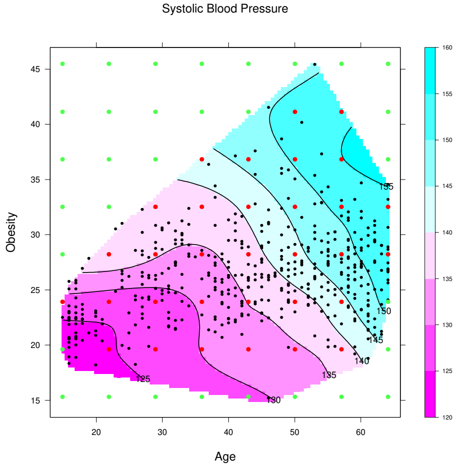

Figure: Estimating systolic blood pressure (response) as a function of obesity and age. Knots used are shown in red.

Generalized additive models

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Note: $\boldsymbol{S}_d$ is the natural cubic spline smoother matrix

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where $\boldsymbol{N}_d$ is the matrix of the natural cubic spline basis functions for feature j

Example: fitting a GAM to predict wages

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Three predictors: 2 continuous, 1 factor

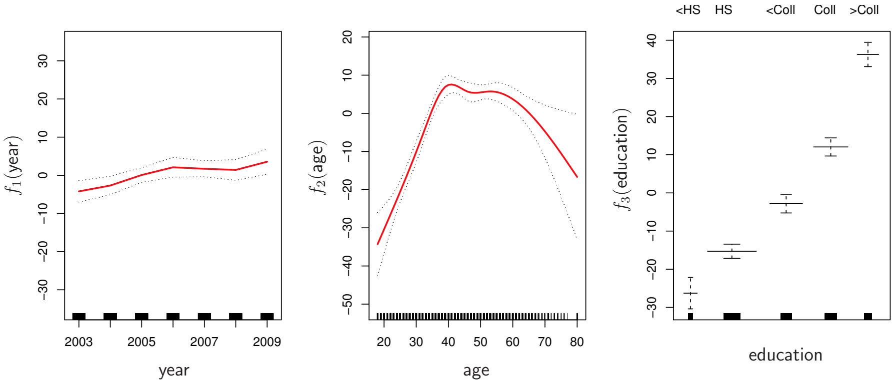

Figure: GAM estimate for Wage on year, age and education.

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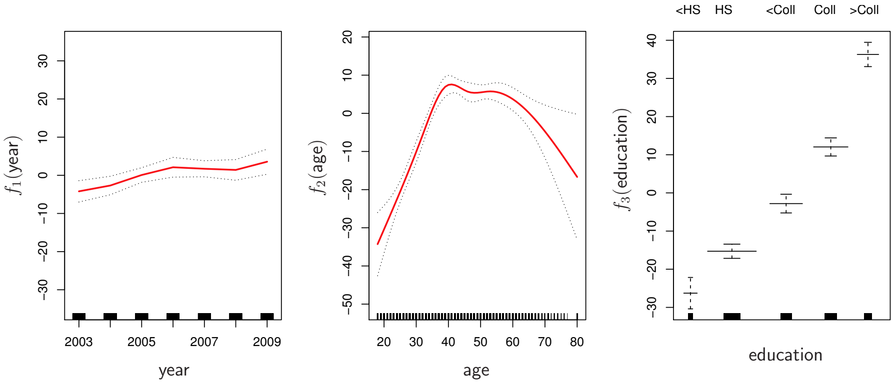

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Model estimation

The additive logistic regression model can also be solved via backfitting using iteratively reweighted least squares for the model estimation in the second step (Newton-Raphson for maximum likelihood)[a]

[a]See ESL page 300 for a description of this algorithm.

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Piecewise-linear basis functions (2 knots); no continuity:

$$\begin{pmatrix} h_{0,0}(x) = 1_{|x \leq \xi_1|} & h_{1,0}(x) = 1_{|\xi_1 \leq x \leq \xi_2|} & h_{2,0}(x) = 1_{|x \geq \xi_2|} \\ h_{0,1}(x) = 1_{|x \leq \xi_1|}x & h_{1,1}(x) = 1_{|\xi_1 \leq x \leq \xi_2|}x & h_{2,1}(x) = 1_{|x \geq \xi_2|}x \end{pmatrix} \tag{36}$$

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- Only 4 basis functions are then needed

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- Introduce roughness penalty:

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  where $\boldsymbol{S}_\lambda$ is the **shrinking smoother**.

Reading

- **PMLI** 11.5
- **ESL** 5.2-5

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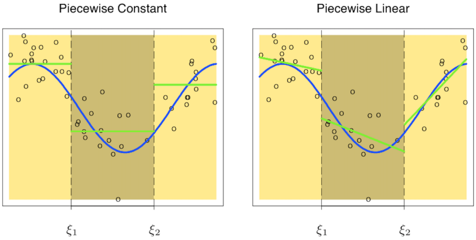

(Left) Piecewise constant function (green) fitted to a simulated dataset whose true function is shown in blue. Basis functions:

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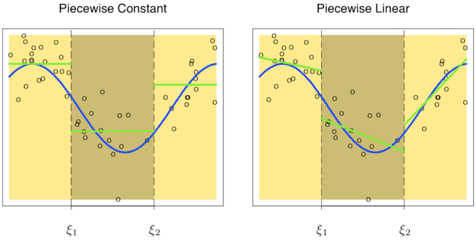

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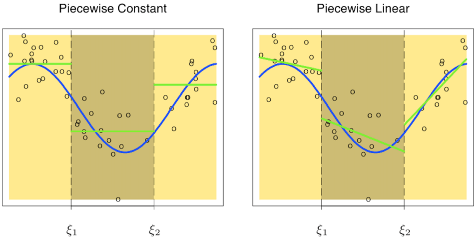

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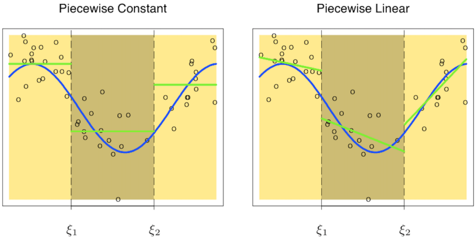

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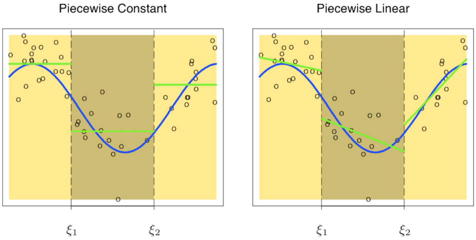

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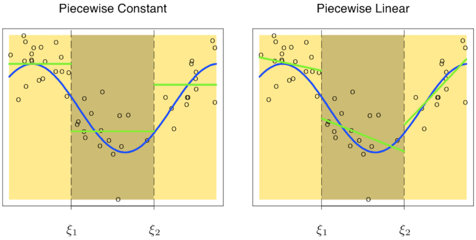

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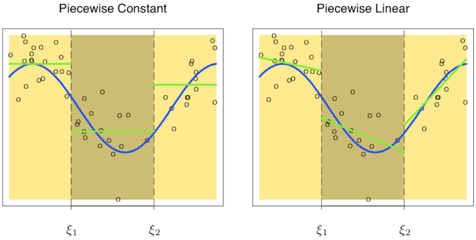

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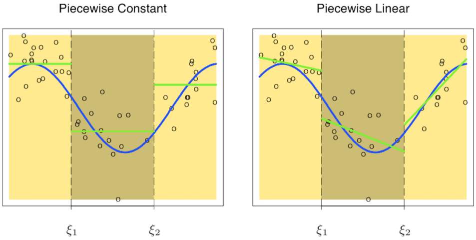

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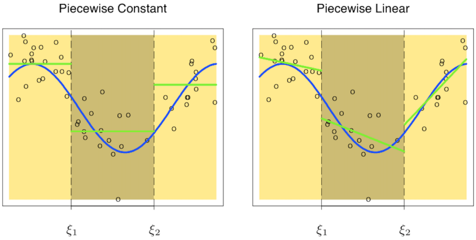

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(Right) Piecewise linear function (green) fitted to simulated dataset whose true function is shown in blue: Basis functions:

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Piecewise-linear basis functions (cont.)

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- When entering a new region, the added linear component alters the slope

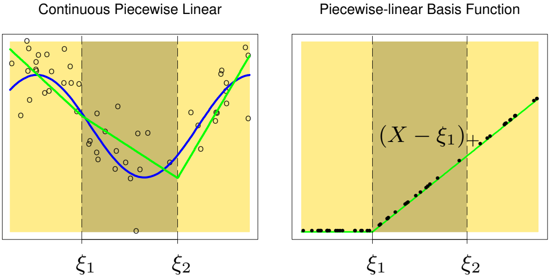

Figure: (Left): Piecewise-linear fit with continuity (but not smoothness) at the knots. $f(X) = w_0 + w_1 X + w_2(X - \xi_1)_+ + w_3(X - \xi_2)_+$.
(Right): Piecewise-linear fit with continuity at ξ_1. $f(X) = w_2(X - \xi_1)_+$

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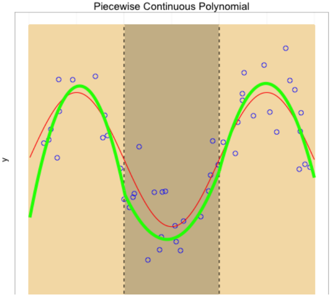

Figure: Piecewise-quadratic fit: $f(X) = w_0 + w_1 X + w_2 X^2 + w_3 (X-\xi_1)_+^2 + w_4 (X-\xi_2)_+^2$

Piecewise polynomials (cont.)

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Commonly used GLM models and their components

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Multinomial logit/logistic	Categorical	Multinomial logit: $g(\mu_{ic}) = \ln\left(\frac{\mu_{ic}}{\mu_{iC}}\right)$
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Its job is to "link" the response to the systematic component via a suitable transformation that results in a linear function of the w's.

Further reading on GLMs

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- German Rodriguez's lecture notes on GLMs: `https://data.princeton.edu/wws509/notes/`
- Penn State: `https://online.stat.psu.edu/stat504/lesson/6/6.1` (Including more on logistic and multinomial logistic)