Nonparametric regression

Data Mining - CdL CLAMSES

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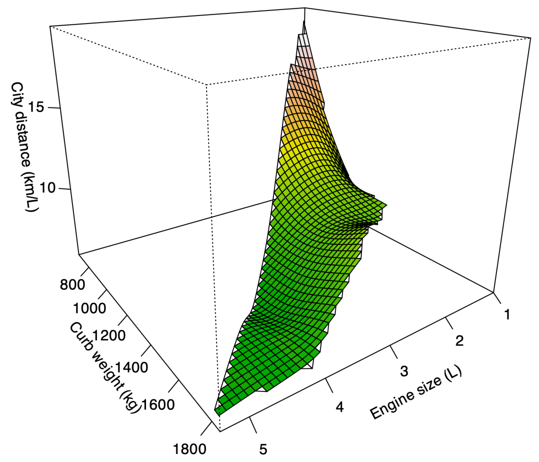


"Nonparametric regression might, like linear regression, become an object treasured both for its artistic merit as well as usefulness."

Leo Breiman

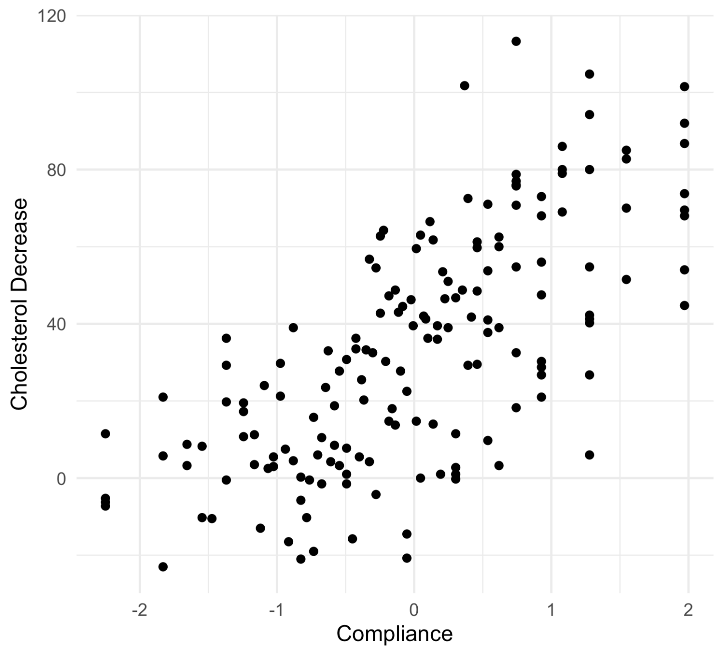
- This unit will cover the following **topics**:
  - Kernel methods and local regression;
  - Regression splines;
  - Smoothing splines.
- Let us consider again the **relationship** between a response variable Y_i and a set of covariates $\boldsymbol{x}_i$:

$$Y_i = f(\boldsymbol{x}_i) + \epsilon_i,$$

  where ϵ_i are **iid** with $\mathbb{E}(\epsilon_i) = 0$ and $\text{var}(\epsilon_i) = \sigma^2$.
- We do not believe $f(\boldsymbol{x})$ is a polynomial nor it belongs to some parametric family of functions.
- Can we fit a **nonparametric** relationship that does **not** make strong **assumptions** on $f(\boldsymbol{x})$? Let us review some old datasets...

Motivating applications

The cholesterol data



- In this first example, a drug called "cholestyramine" is administered to $n = 164$ men.
- We observe the pair (x_i, y_i) for each man.
- The response y_i is the **decrease in cholesterol level** over the experiment.
- The covariate x_i is a measure of **compliance**.
- We assume, as before, that the data are generated according to

$$Y_i = f(x_i) + \epsilon_i, \quad i = 1, \dots, n.$$

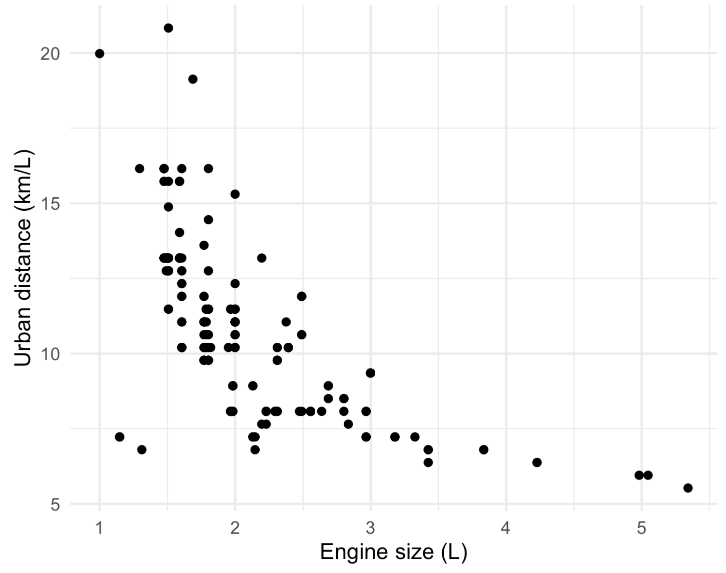
- In Unit B we fit a **polynomial** with degree 3 on this data, although there was some **uncertainty**.

The auto dataset

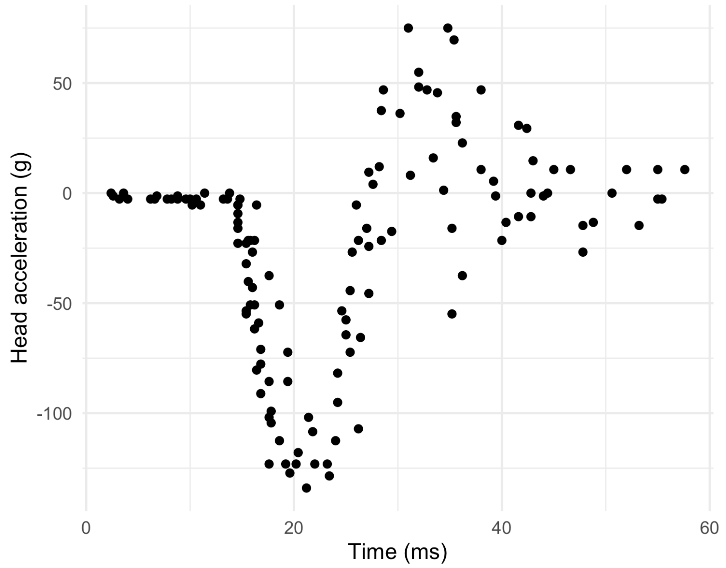
- In Unit A we considered the `auto` dataset.
- We wanted to model the relationship between `city.distance` (y) and `engine.size` (x).
- The chosen model involved a **non-linear** function

$$Y_i = f(x_i) + \epsilon_i, \qquad i = 1, \dots, n,$$

  where $f(x)$ was "manually" selected.
- There are **no** reasons to believe that $f(x) = \alpha x^\beta$ or that $f(x)$ belongs to any other **parametric** family.
- We would like the data to "speak for themselves."



The mcycle dataset



- Data consist of variables y **accelerometer** (`accel`) readings, taken through time x (`times`).
- The $n = 133$ observations were measured during a simulated **motor-cycle crash** experiment, for testing the **efficacy** of **crash helmets**.
- Some characteristics of the data:
  - The time points are **not regularly spaced** and sometimes there are **multiple observations**;
  - The observations are subject to **error**;
  - The errors ϵ_i are probably heteroscedastic, but let us ignore this now.
- It is of interest to discern the **general shape** of the underlying acceleration curve.

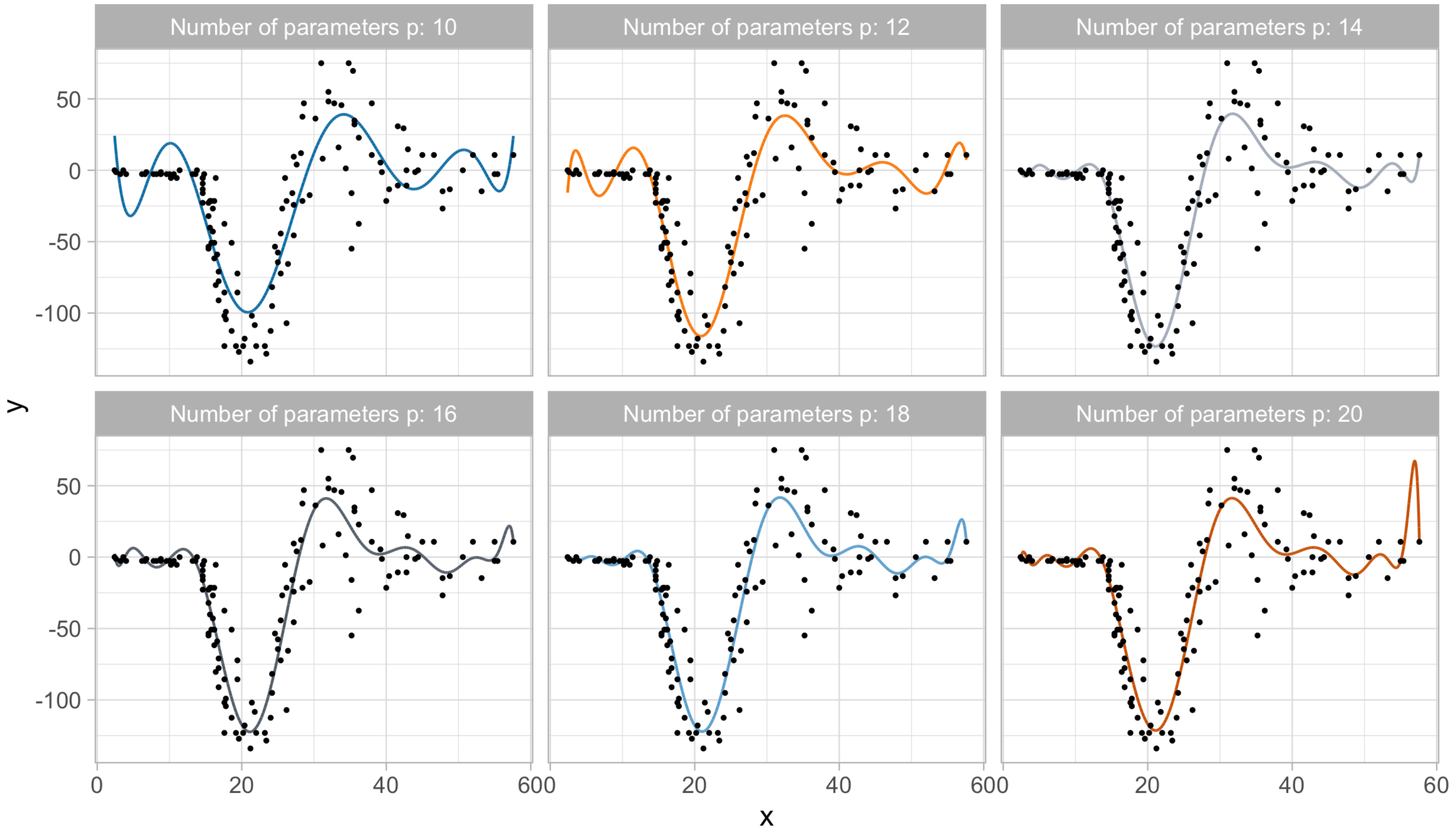
Old friends: polynomials

- In the `mcycle` dataset, it is **not** obvious which **parametric** function we should consider, therefore this route is not an option.

- In **theory** **polynomials** can **approximate** a large class of functions, as a consequence of Taylor's expansion theorem.
- In the statistical **practice**, however, polynomial regression is not very well suited for modeling complex relationships.

- When performing flexible regression, we expect the prediction at x_i to depend on observations close to x_i. However, polynomials are **not local**.
- Instead, in polynomial regression points that are far away from x_i have a big impact on $\hat{f}(x_i)$. This produces **spurious oscillations** at the boundaries and **unstable** estimates.
- This is known as Runge's phenomenon in numerical analysis.

Old friends: polynomials (`mcycle` data)



Local regression

The regression function

- The only assumption we are making in this Unit is the following **additive** structure

$$Y_i = f(x_i) + \epsilon_i, \qquad i = 1, \dots, n,$$

where ϵ_i are **iid** with $\mathbb{E}(\epsilon_i) = 0$ and $\mathrm{var}(\epsilon_i) = \sigma^2$. This structure can be relaxed even further.

- Let $\tilde{Y}_i$ be a new data point. In Unit B we showed that under the **quadratic loss**

$$\mathbb{E}\left[\{\tilde{Y}_i - \hat{f}(x_i)\}^2\right],$$

the best prediction $\hat{f}(x_i)$, i.e. the one minimizing the loss, coincides with

$$\hat{f}(x_i) = \mathbb{E}(\tilde{Y}_i) = f(x_i),$$

which is the **conditional expectation** of Y_i given the value x_i, called **regression function**.

- The regression function $f(x_i) = \mathbb{E}(\tilde{Y}_i)$ is the **optimal prediction** even in presence of **heteroschedastic** data or when the above **additive** decomposition does **not hold**.

Local estimates of the prediction

- We do not know $f(x)$, but the previous formulas suggest that we could consider an **arithmetic average** of the data points.
- Hence, a **prediction** for a generic value x could be obtained as follows:

$$\hat{f}(x) = \frac{1}{n_x} \sum_{i: x_i = x} y_i, \qquad n_x = \sum_{i=1}^{n} I(x_i = x).$$

- This idea, unfortunately, **does not work** in most practical cases.
- Indeed, in a typical dataset it is very unlikely that there exist multiple observations **exactly equal** to x among the points (x_i, y_i).
- Even if there were values such that $x_i = x$, the **sample size** n_x would be so **small** (e.g. $n_x = 1$) that the variance of $\hat{f}(x)$ would be extremely high, making this estimator useless.
- However, this "local average" idea seems **intuitively appealing**. Can we "fix" it?

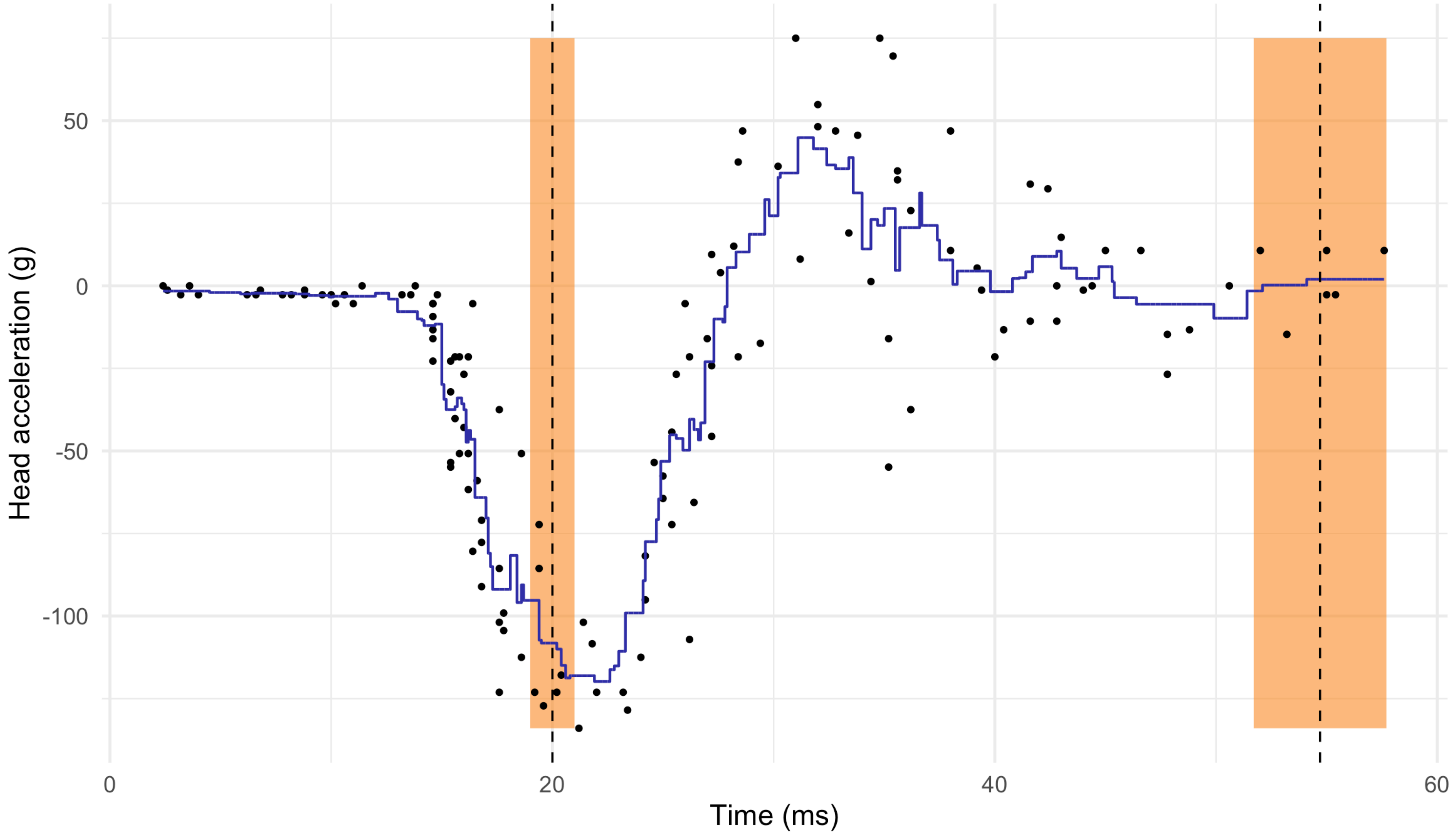
K-nearest neighbours

- Instead of considering the values exactly equal to x, we could identify the pairs (x_i, y_i) that are **close** to (i.e. in a **neighbour** of) x.
- A natural measure of proximity between x and the data points x_i is the **Euclidean distance** $|x_i - x|$, but in principle any other metric could be used.
- We consider an average of the k **values** y_i whose x_i are **nearest** to x, that is:

$$\hat{f}(x) = \frac{1}{|\mathcal{N}_x|} \sum_{i \in \mathcal{N}_x} y_i,$$

  where $\mathcal{N}_x$ is indeed the set of k points nearest to x in Euclidean distance.
- This method is called **k-nearest neighbours** (KNN).

K-nearest neighbours ($k = 6$)



Comments and limitations about the KNN method

- The number of neighbours k influences how "**local**" is the estimate.
- When k is low, the KNN estimator $\hat{f}(x)$ has **high variance**. The extreme case $k = 1$ corresponds to an "average" of a single data point.
- When k is high, the KNN estimator $\hat{f}(x)$ is not local and it has **high bias**. The extreme case $k = n$ produces a constant, i.e., the average of all the observations.
- Thus, there is a **bias-variance trade-off** in the choice of k, which should be selected, e.g., via **cross-validation**.
- The k-nearest neighbors produce a **sensible result**, but the method **can be improved**.
- The **blue curve** is bumpy, because $\hat{f}(x)$ is **discontinuous** in x.
- Indeed, as we move x from left to right, the k-nearest neighborhood remains constant until a new point x_i to the right of x is included, and one to the left is excluded.
- This discontinuity is **ugly** and **unnecessary**. We are looking instead for a **smooth** prediction.

Nadaraya-Watson estimator

- The **Nadaraya-Watson** estimator addresses the aforementioned issues of the KNN method. It is a **weighted average**

$$\hat{f}(x) = \frac{1}{\sum_{i'=1}^{n} w_{i'}(x)} \sum_{i=1}^{n} w_i(x) y_i = \sum_{i=1}^{n} s_i(x) y_i,$$

  where $s_i(x) = w_i(x) / \sum_{i'=1}^{n} w_{i'}(x)$ are the **normalized weights**.

- The values $w_i(x) \geq 0$ are chosen so that the points x_i **close** to x are **weighted more**.

- A convenient way of selecting these weights is through **kernel functions**:

$$w_i(x) = \frac{1}{h} w\left(\frac{x_i - x}{h}\right), \qquad i = 1, \dots, n,$$

  where $w(\cdot)$ is a **density** function, **symmetric** around the origin, called kernel in this context.

- The value $h > 0$ is a **scale factor**, sometimes called **bandwidth** or **smoothing parameter**.

Nadaraya-Watson estimator: comments

- The fitted function $\hat{f}(x)$ is **continuous** and is obtained by computing several weighted averages, one for each value of x.
- A popular kernel is the **Gaussian kernel**, that is:

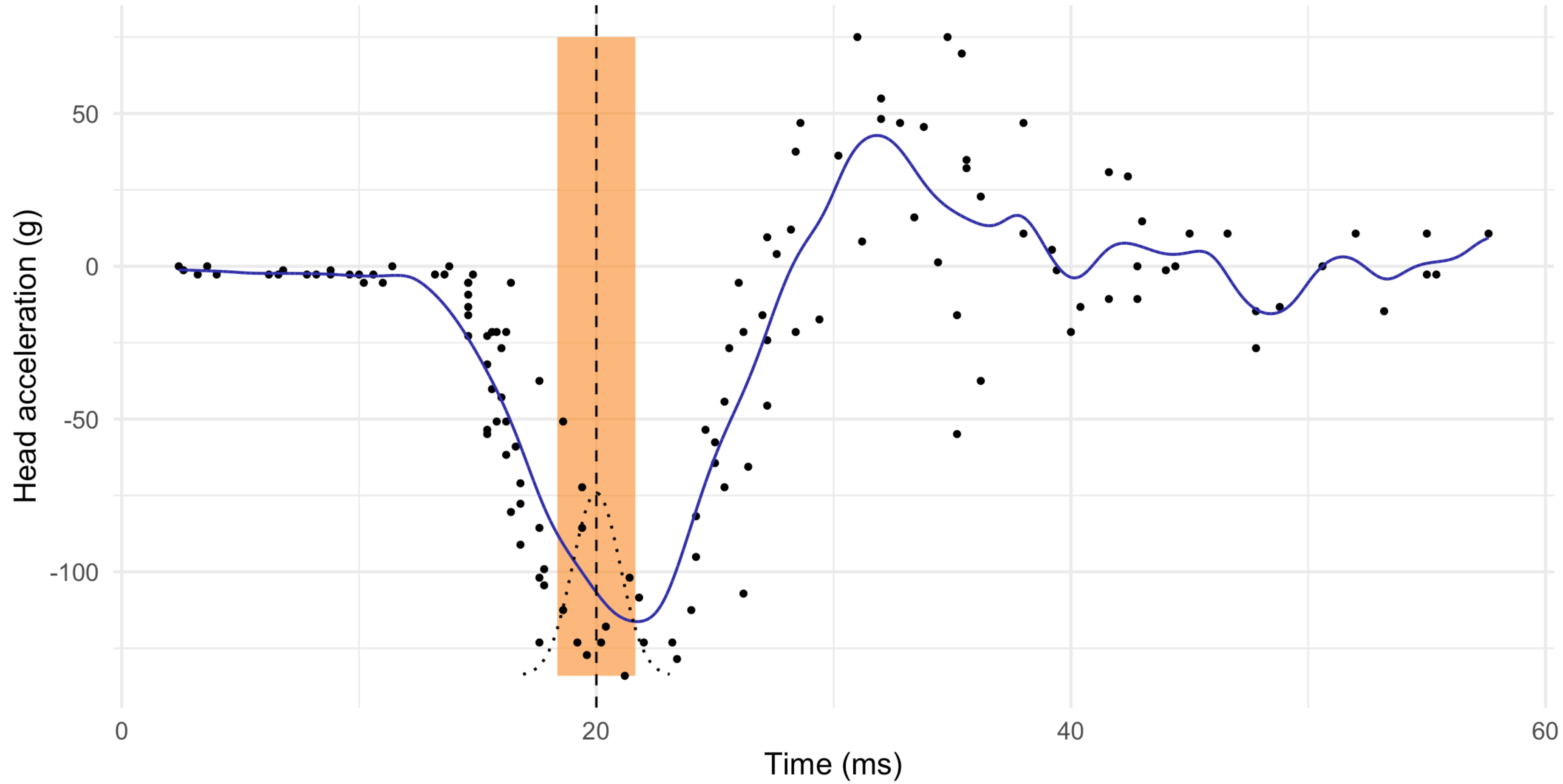
$$w_i(x) = \frac{1}{h}\phi\left(\frac{x_i - x}{h}\right), \qquad i = 1, \dots, n,$$

  therefore h^2 represents the **variance**. We will discuss alternative choices later on.

- The most important factor, however, is not the functional form of $w(\cdot)$, but rather the **smoothing parameter** h, which is a complexity parameter.
- Indeed, h defines the "**smoothing window**" on the x-axis, i.e. the relevant data points that are considered for $\hat{f}(x)$.
- As with any complexity parameter, h should be chosen via cross-validation or related ideas.

Nadaraya-Watson (Gaussian kernel)

Smoothing $h = 1$ | Smoothing $h = 0.3$ | Smoothing $h = 2$ | Smoothing $h = 4$



Local linear regression I

- **Local linear regression** is a refinement of the Nadaraya-Watson estimator that has typically **lower bias**, especially at the **boundaries**, without noticeable increases in variance.
- If $f(x)$ is differentiable, then it can be **approximated** with a linear function tangent in x_0:

$$f(x) = \underbrace{f(x_0)}_{\beta_1} + \underbrace{f'(x_0)}_{\beta_2}(x - x_0) + \text{rest}.$$

- Hence, instead of computing a **local average** ($\beta_2 = 0$), we consider a **local linear model**. In other words, for every x we seek the coefficients solving:

$$\hat{\beta}(x) = \left(\hat{\beta}_1(x), \hat{\beta}_2(x)\right) = \arg\min_{(\beta_1,\beta_2)} \sum_{i=1}^n w_i(x)\left\{y_i - \beta_1 - \beta_2(x_i - x)\right\}^2.$$

- Once the parameter $\hat{\beta}_1(x)$ and $\hat{\beta}_2(x)$ are obtained, the local **linear regression estimator** is

$$\hat{f}(x) = \hat{\beta}_1(x) + \hat{\beta}_2(x)(x - x) = \hat{\beta}_1(x).$$

Local linear regression II

- The local linear regression, as we have seen in Unit A, has an **explicit solution**:

$$\hat{\beta}(x) = (\boldsymbol{X}_x^T \boldsymbol{W}_x \boldsymbol{X}_x)^{-1} \boldsymbol{X}_x^T \boldsymbol{W}_x \boldsymbol{y},$$

where the rows of $\boldsymbol{X}_x$ are $\boldsymbol{x}_{i,x} = (1, x_i - x)$ and $\boldsymbol{W}_x = \text{diag}\{w_1(x), \dots, w_n(x)\}$.

- In practice, we do **not** need to solve this **linear algebra** problem. An even more explicit and **non-iterative** solution can be found (see Exercises).

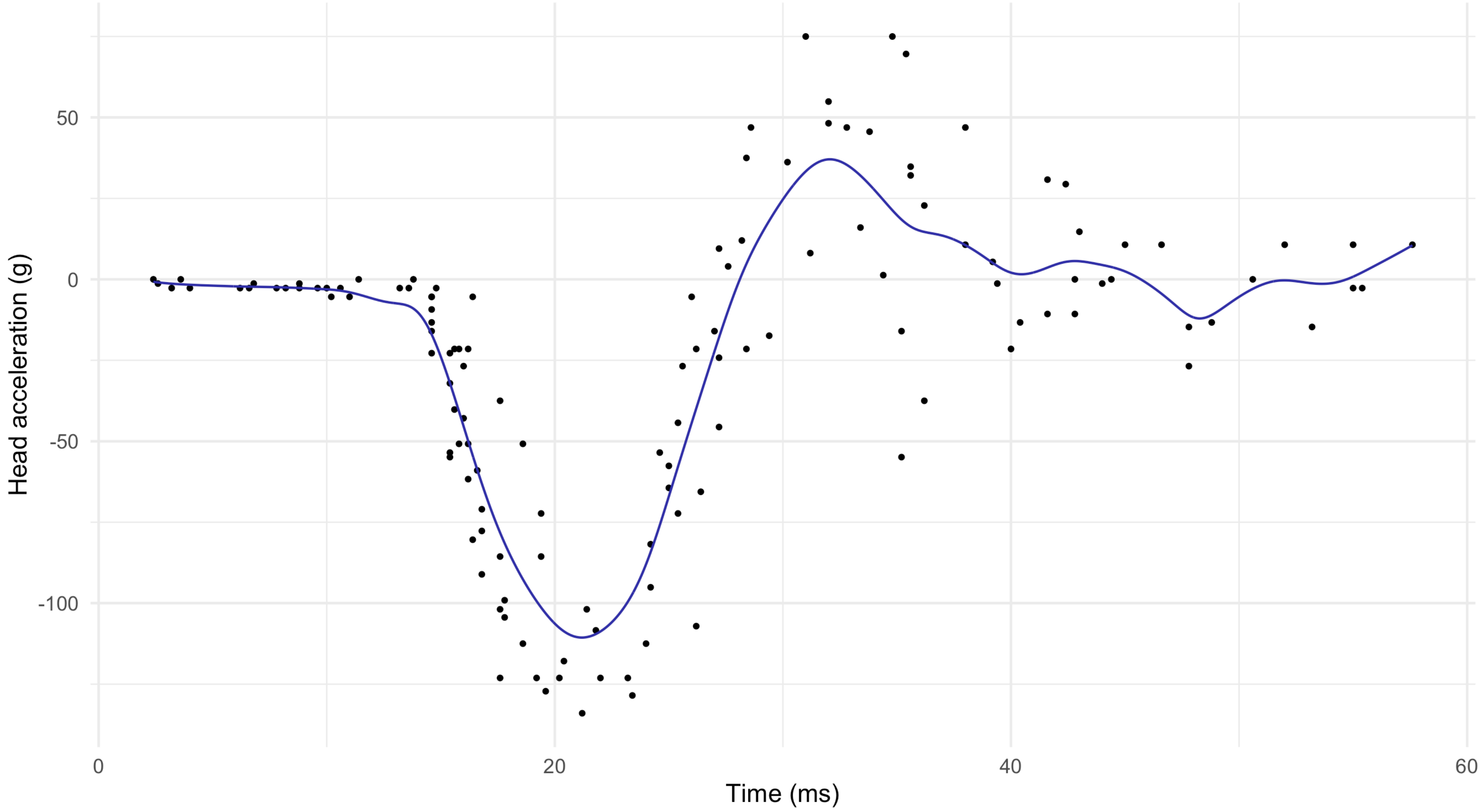
Theorem (Local linear smoothing)

The local linear regression smoother, evaluated in x, admits an **explicit expression**:

$$\hat{f}(x) = \frac{1}{n}\sum_{i=1}^{n} \frac{w_i(x)\{a_2(x) - (x_i - x)a_1(x)\}}{a_2(x)a_0(x) - a_1(x)^2} y_i = \sum_{i=1}^{n} s_i(x) y_i,$$

where $a_j(x) = n^{-1}\sum_{i=1}^{n} w_i(x)(x_i - x)^j$, for $j = 0, 1, 2$.

Local linear regression ($h = 1.46$, Gaussian kernel)



Linear smoothers I

- The Nadaraya-Watson estimator and local linear regression are special instances of **linear smoothers**, which are estimators having the following form:

$$\hat{f}(x) = \sum_{i=1}^n s_i(x) y_i.$$

- We will study other members of this class, such as regression and smoothing splines.
- Polynomial regression, ridge regression, **Gaussian processes** and **moving averages** are also linear smoothers.

- The **mean** (and hence the bias), and the **variance** of a linear smoother can be easily obtained:

$$\mathbb{E}\{\hat{f}(x)\} = \sum_{i=1}^n s_i(x) f(x_i), \qquad \text{var}\{\hat{f}(x)\} = \sigma^2 \sum_{i=1}^n s_i(x)^2.$$

Linear smoothers II

- In linear smoothers, we can express the predicted values $\hat{\boldsymbol{y}}$ using **matrix notation**

$$\hat{\boldsymbol{y}} = \sum_{i=1}^n \tilde{\boldsymbol{s}}_i y_i = \boldsymbol{S}\boldsymbol{y}, \qquad \tilde{\boldsymbol{s}}_i = (s_i(x_1), \dots, s_i(x_n))^T,$$

  where $\boldsymbol{S} = (\tilde{\boldsymbol{s}}_1, \dots, \tilde{\boldsymbol{s}}_n)$ is the so-called $n \times n$ **smoothing** matrix.

- Each row of the smoothing matrix $\boldsymbol{s}_i$ is called **equivalent kernel** for estimating $\hat{f}(x_i)$; in the Nadaraya Watson estimator $\boldsymbol{s}_i$ is indeed a normalized kernel.

- The weights of all the smoothers we will use are such that $\sum_{i=1}^n s_i(x) = 1$ for all x.
- Hence, the smoother **preserves constant curves**, namely if all $y_i = c$, then $\hat{f}(x) = c$.

On the choice of the kernel

- As mentioned before, the choice of the kernel is **not crucial**. Some alternatives are:

Kernel	$w(x)$	**Support**
Gaussian	$\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$	$\mathbb{R}$
Rectangular	$\frac{1}{2}$	$(-1, 1)$
Epanechnikov	$\frac{3}{4}(1 - x^2)$	$(-1, 1)$
Bi-quadratic	$\frac{15}{16}(1 - x^2)^2$	$(-1, 1)$
Tri-cubic	$\frac{70}{81}(1 - \lvert x\rvert^3)^3$	$(-1, 1)$

- Some **asymptotic** considerations lead to the choice of the "**optimal**" Epanechnikov kernel.
- **Bounded** kernels have **computational** advantages, because one needs to compute averages of a limited number of data points.
- On the other hand, bounded kernels may lead to **discontinuous derivatives** of $\hat{f}(x)$ that could be unappealing in certain contexts.

Bias-variance tradeoff

Theorem (Fan and Gijbels, 1996, Theorem 3.1)

Let (X_i, Y_i) be iid random vectors with $g(x)$ denoting the **marginal density** of X_i. The conditional law is such that $Y_i = f(X_i) + \epsilon_i$, with ϵ_i iid and $\mathbb{E}(\epsilon_i) = 0$, $\text{var}(\epsilon_i) = \sigma^2$.

Moreover, suppose $g(x) > 0$ and that $g(\cdot)$ and $f''(\cdot)$ are continuous in a neighborhood of x. Then, as $h \to 0$ and $nh \to \infty$ we have that for the **local linear regression** $\hat{f}(x)$ the **bias** is

$$\mathbb{E}\{\hat{f}(x) - f(x)\} \approx \frac{h^2}{2}\sigma_w^2 f''(x),$$

where $\sigma_w^2 = \int z^2 w(z)\mathrm{d}z$. In addition, the **variance** is

$$\text{var}\{\hat{f}(x)\} \approx \frac{\sigma^2}{nh}\frac{\alpha_w}{g(x)},$$

where $\alpha_w = \int w^2(z)\mathrm{d}z$.

Bias-variance tradeoff II

- The previous theorem shows that **bias** is of **order** h^2 and the **variance** is of **order** $(1/nh)$.
- Once again, there is a trade-off because we would like $h \to 0$ but, at the same time, we need to keep the variance under control.
- We can select h so that the **asymptotic mean squared error** is **minimal**. This leads to the following optimal choice for the bandwidth:

$$h_{\text{opt}}(x) = \left(\frac{1}{n}\frac{\sigma^2 \alpha_w}{\sigma_w^4 f''(x)^2 g(x)}\right)^{1/5}.$$

- Unfortunately, $h_{\text{opt}}(x)$ is of **little practical utility**, as it involves the **unknown** terms $f''(x)$, $g(x)$ and σ^2. However, it highlights two important facts:
- The bandwidth h should decrease at the rate $n^{-1/5}$, i.e. **quite slowly**.
- If we plug-in $h_{\text{opt}}(x)$ into the bias/variance formulas, we get that the mean squared error tends to 0 at the rate $n^{-4/5}$, which is much **slower** than the **parametric** case n^{-1}.

Bias reduction of local linear regression

- Compared to the Nadaraya-Watson estimator, local linear regression corrects the **first-order** term of the **bias**, without affecting the variance sensibly.
- Indeed, it can be shown that the **asymptotic variance** of Nadaraya-Watson and local linear regression is the **same**, but the **asymptotic bias** is **different**.
- To get an intuition of this, consider the following Taylor expansion for $\mathbb{E}\{\hat{f}(x)\}$ around x, and for the local linear regression case:

$$\begin{aligned}\mathbb{E}\{\hat{f}(x)\} &= \sum_{i=1}^{n} s_i(x) f(x_i) \\ &= f(x)\underbrace{\sum_{i=1}^{n} s_i(x)}_{=1} + f'(x)\underbrace{\sum_{i=1}^{n}(x_i - x)s_i(x)}_{=0} + \frac{f''(x)}{2}\sum_{i=1}^{n}(x_i - x)^2 s_i(x) + \text{rest}.\end{aligned}$$

- It can be shown with some algebra that the first-order term simplifies $(= 0)$ in the local linear regression case, but it doesn't for the Nadaraya-Watson, therefore **reducing the bias**.

Choice of the bandwidth I

- In practice, we need to choose the bandwidth by other means. A first solution is based on **information criteria** such as the C_p or the AIC/BIC.
- However, as before, their usage requires a suitable notion of **effective degrees of freedom**.

Effective degrees of freedom for linear smoothers

Let $\hat{f}(x) = \sum_{i=1}^n s_i(x) y_i$ be a linear smoother. Then the effective degrees of freedom are

$$\text{df}_{\text{sm}} = \frac{1}{\sigma^2}\sum_{i=1}^n \text{cov}(Y_i, \hat{f}(x_i)) = \frac{1}{\sigma^2}\text{tr}\{\text{cov}(\boldsymbol{Y}, \boldsymbol{S}\boldsymbol{Y})\} = \frac{\sigma^2}{\sigma^2}\text{tr}(\boldsymbol{S}) = \text{tr}(\boldsymbol{S}).$$

- Some authors proposed to use $\text{tr}(\boldsymbol{S}\boldsymbol{S}^T)$ or $\text{tr}(2\boldsymbol{S} - \boldsymbol{S}\boldsymbol{S}^T)$, but the connection with the **optimism** and the definition of effective degrees of freedom is less clear.

Choice of the bandwidth II

- Cross-validation is another option for selecting the bandwidth h. For **most linear smoothers** there is a brilliant **computational shortcut** for the leave-one-out case.

- Any reasonable linear smoother is constant preserving, that is $\sum_{j=1}^n s_j(x) = 1$ for all x. Moreover, for most linear smoothers the following property holds:

$$\hat{y}_{-i} = \frac{1}{1 - s_i(x_i)} \sum_{j \neq i} s_j(x_i) y_j .$$

- In other words, the **leave-one-out predictions** can be obtained by **excluding** the ith observation and **re-normalizing** the weights.

- A linear smoother is called **projective** if it has the above property.
- **All** the **linear smoothers** presented in this unit (Nadaraya-Watson, local linear regression, regression an smoothing splines) are projective (see Exercises).

Choice of the bandwidth III

Theorem (LOO-CV for linear smoothers)

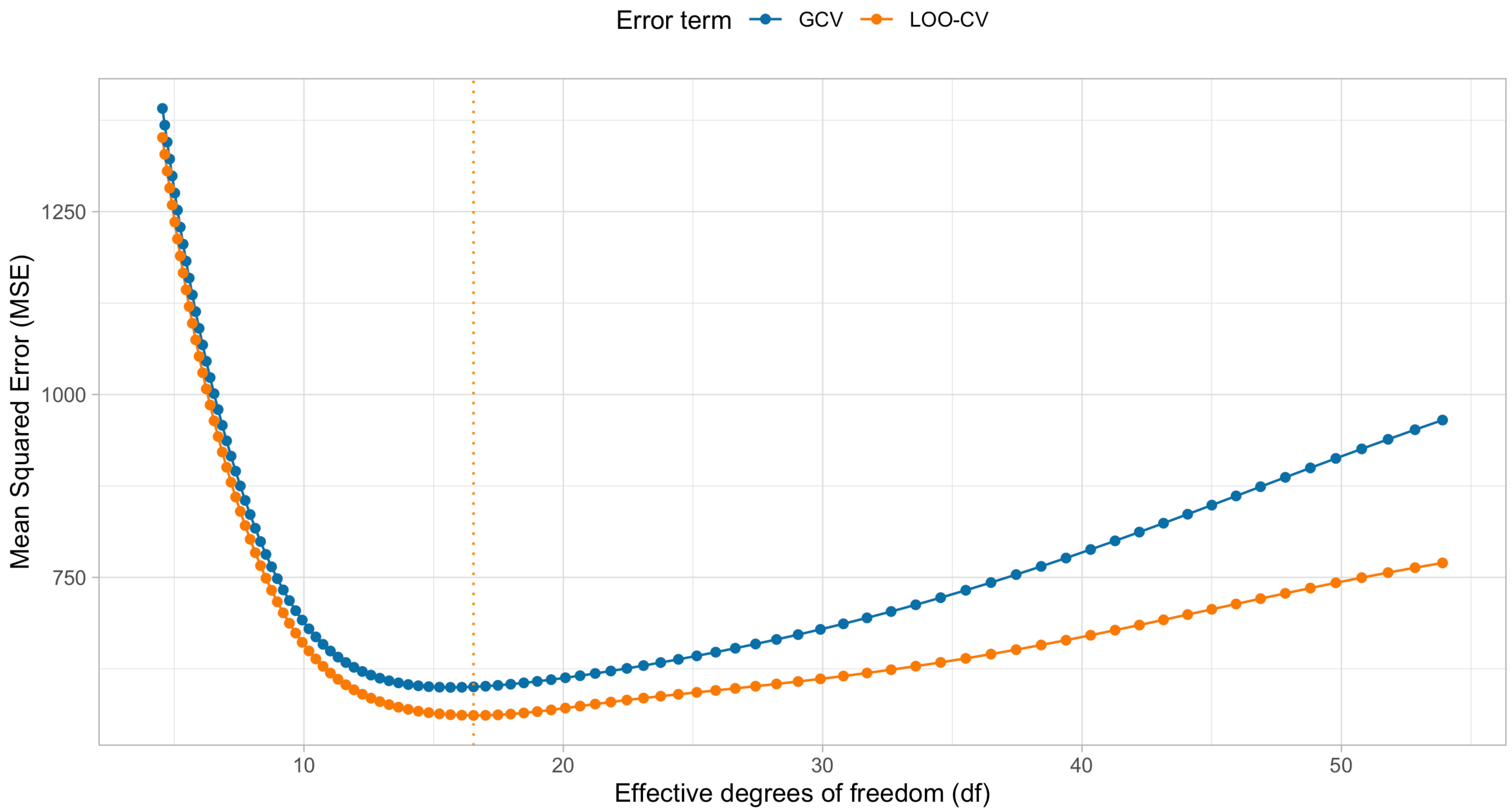
Let $\hat{y}_{-i} = \hat{f}_{-i}(x_i)$ be the leave-one-out predictions of a **projective linear smoother** and let $\hat{\boldsymbol{y}} = \boldsymbol{S}\boldsymbol{y}$ be the predictions of the full model. Then:

$$y_i - \hat{y}_{-i} = \frac{y_i - \hat{y}_i}{1 - [\boldsymbol{S}]_{ii}}, \qquad i = 1, \dots, n.$$

Therefore, the leave-one-out mean squared error is

$$\widehat{\mathrm{Err}} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - [\boldsymbol{S}]_{ii}}\right)^2.$$

Choice of the bandwidth IV



Loess

- Sometimes it is convenient to choose h **adaptively**, i.e. specifying a variable bandwidth $h(x)$ that depends on the local density of the data.
- Indeed, recall that the asymptotic variance depends on the sampling design of the x_is

$$\mathrm{var}\{\hat{f}(x)\} \approx \frac{\sigma^2}{nh}\frac{\alpha_w}{g(x)}.$$

- The `loess` (Cleveland, 1979) considers a **fixed percentage** of data points (assuming a bounded kernel is used), which automatically induces a **variable bandwidth**, as in KNN.
- Moreover, the `loess` algorithm combines the **variable bandwidth** with some **robust estimation** ideas, so that outliers less influence the resulting estimate.
- `loess` is a short-hand for "**l**ocally **w**eighted **e**stimated **s**catterplot **s**moothing".

Local likelihoods

- The concept of local regression and varying coefficients is extremely **broad**.
- In principle, any **parametric** model can be made **local** as long as it accommodates **weights**.
- Let us consider a **logistic regression** with a single predictor. For every value x we seek

$$\hat{\beta}(x) = \arg\max_{(\beta_1,\beta_2)} \sum_{i=1}^{n} w_i(x) \left[y_i(\beta_1 + \beta_2 x_i) - \log\{1 + \exp(\beta_1 + \beta_2 x_i)\} \right],$$

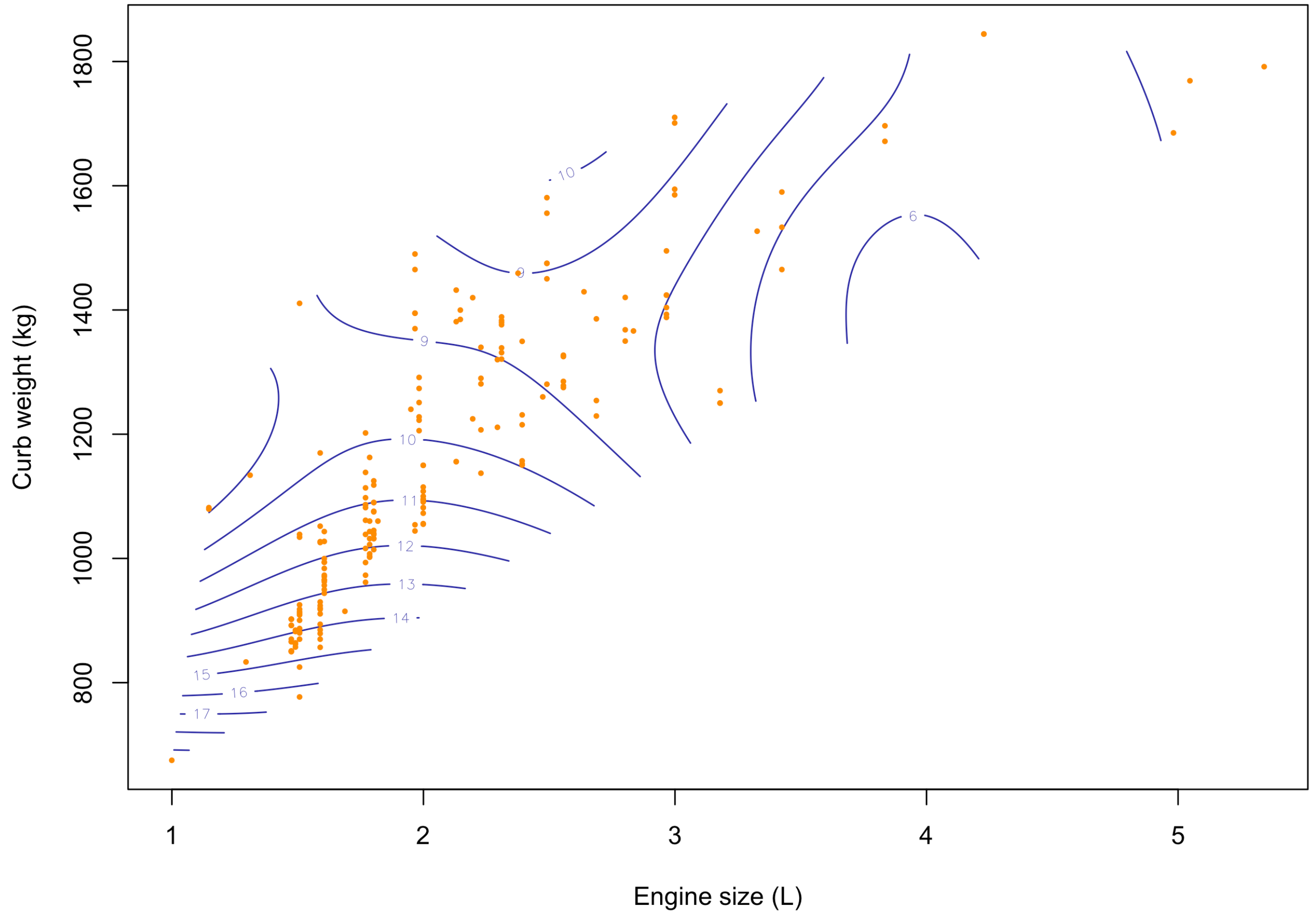
  whose solution can be found using iteratively re-weighted least squares.

- The **computations** and the **theory** are not as straightforward and limpid as in the regression case, but they do hold in an **approximate** sense.
- Once again, the conceptual scheme is: (i) perform a **quadratic approximation** of the log-likelihood; (ii) proceed as in the **regression** case.

The bivariate case

- Local linear regression can be applied when **two** or **more covariates**, say p, are used. Let us begin with two covariates so that
$$y_i = f(x_{i1}, x_{i2}) + \epsilon_i.$$
- To estimate f on a specific point $\boldsymbol{x} = (x_1, x_2)^T$, a **natural extension** of local linear regression takes the form
$$\hat{\beta}(\boldsymbol{x}) = \arg \min_{(\beta_1,\beta_2,\beta_3)} \sum_{i=1}^{n} w_i(\boldsymbol{x}) \left\{y_i - \beta_1 - \beta_2(x_{i1} - x_1) - \beta_3(x_{i2} - x_2)\right\}^2 .$$
- A common way of choosing the **weights** $w_i(\boldsymbol{x})$ is to set
$$w_i(\boldsymbol{x}) = \frac{1}{h_1 h_2} w\left(\frac{x_{i1} - x_1}{h_1}\right) w\left(\frac{x_{i2} - x_2}{h_2}\right).$$
- Clearly, this now involves the choice of **two** different **smoothing parameters**.

The bivariate case $(h_1 = 0.5, h_2 = 150)$



Pros and cons of kernel nonparametric regression

Pros

- Local linear regression is a **nonparametric** estimator for unknown functions $f(x)$ which makes very **few assumptions** on its form.
- The procedure is simple and **computationally efficient**.
- The smoothing parameter h can be easily handled, since $\hat{f}(x)$ a linear smoother.

Cons

- There is a price to pay for not making assumptions: estimation is **less efficient** in terms of mean squared error compared to parametric models (when they are correctly specified!).
- This is a drawback of all nonparametric estimators, not just local linear regression.

Regression splines

Basis expansions

- The idea of polynomial regression can be **generalized** and **improved**. The main idea is to augment or replace the input x with additional variables (**basis expansion**).

- Let $h_1(x), \dots, h_p(x)$ be **pre-specified** functions $h_j(x) : \mathbb{R} \to \mathbb{R}$ that transform the original predictor x in some **non-linear** fashion. Then, we let

$$f(x;\beta) = \sum_{j=1}^{p} h_j(x)\beta_j,$$

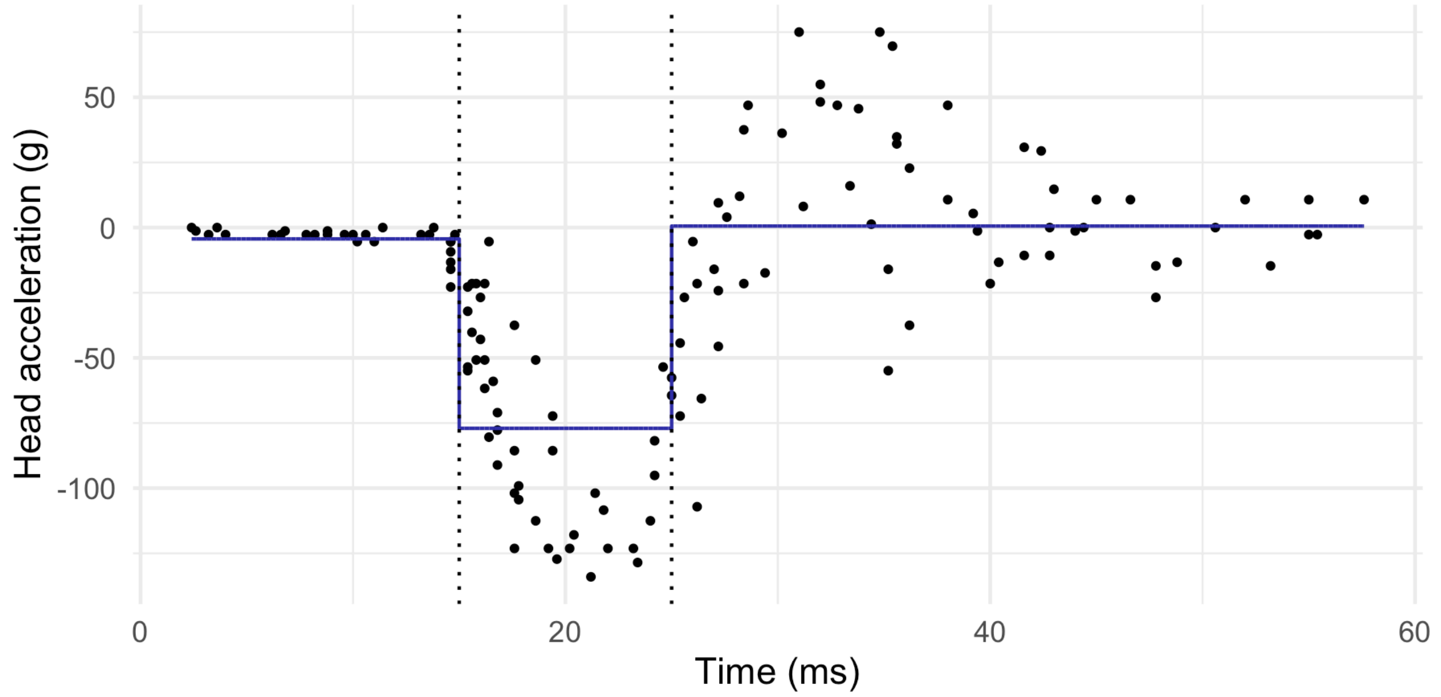
  where $\beta = (\beta_1, \dots, \beta_p)^T$ is a vector of **unknown coefficients**.

- **Polynomials** are a specific instance of basis expansion, in which

$$h_1(x) = 1, \quad h_2(x) = x, \quad h_3(x) = x^2, \quad \dots \quad h_p(x) = x^{p-1}.$$

- The main advantage of this approach is its **linearity** in the **parameters**, because it means that **ordinary least squares** can be used for the estimation of β.

Piecewise regression I



- A **piecewise constant** regression model is another instance of basis expansions, in which we consider step functions, say $p = 3$

$$h_1(x) = I(x < \xi_1), \quad h_2(x) = I(\xi_1 \le x < \xi_2), \quad h_3(x) = I(x \ge \xi_2),$$

where $\xi = (\xi_1, \xi_2)$ are pre-specified cutpoints, called **knots**. Here $\xi = (15, 25)$.

Piecewise regression II

- The previous choice of knots is **not working** very well. The model is not flexible enough.

- To improve the fit, we could consider **piecewise polynomial** functions rather than constant. For example, a piecewise **quadratic** function with $p = 30$ is

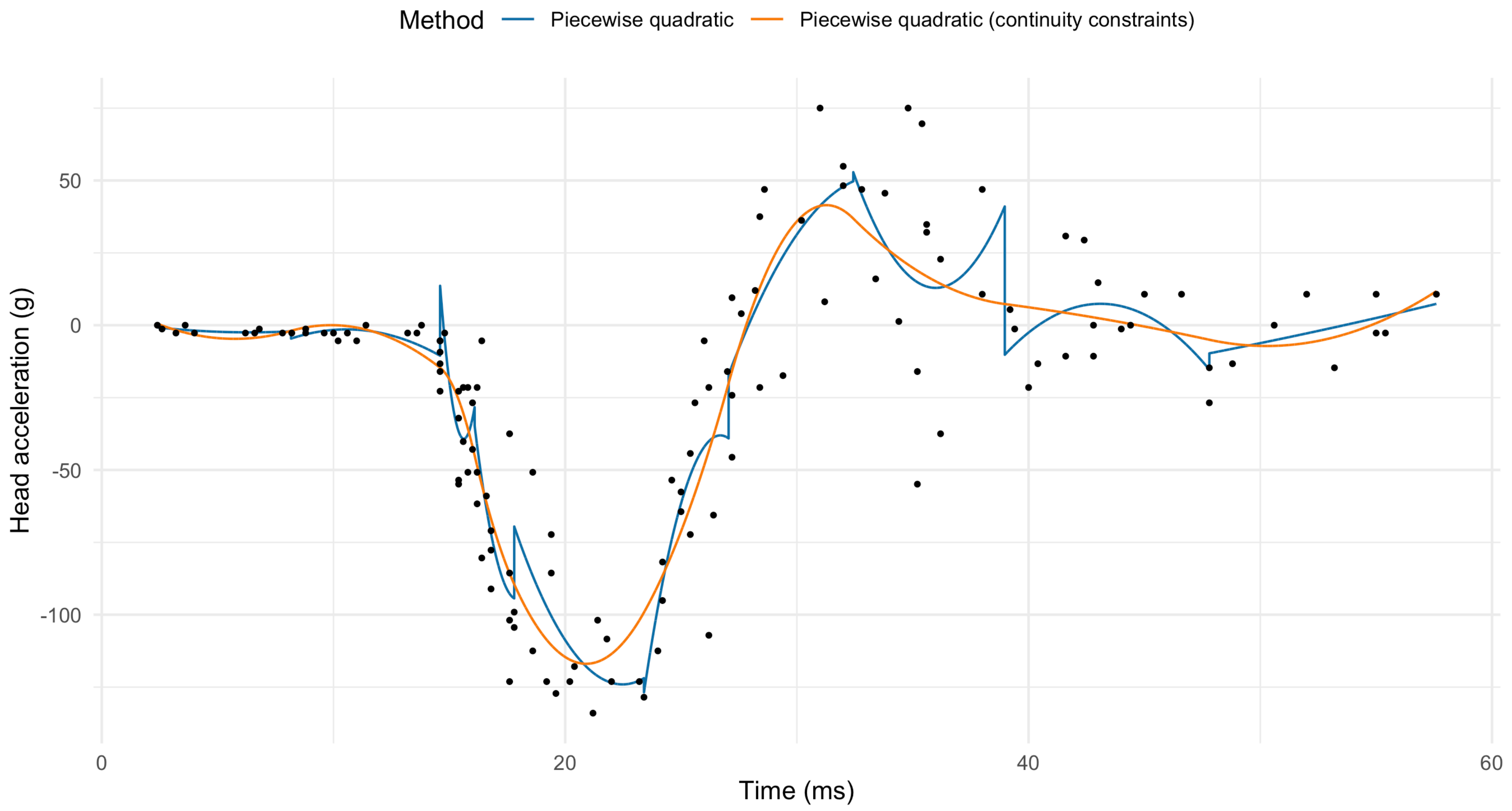
$$\begin{aligned}
h_1(x) &= I(x < \xi_1), & h_2(x) &= x\, I(x < \xi_1), & h_3(x) &= x^2\, I(x < \xi_1),\\
h_4(x) &= I(\xi_1 \le x < \xi_2), & h_5(x) &= x\, I(\xi_1 \le x < \xi_2), & h_6(x) &= x^2\, I(\xi_1 \le x < \xi_2),\\
&\vdots & &\vdots & &\vdots\\
h_{28}(x) &= I(x \ge \xi_9), & h_{29}(x) &= x\, I(x \ge \xi_9), & h_{30}(x) &= x^2\, I(x \ge \xi_9).
\end{aligned}$$

- The piecewise quadratic $f(x;\beta) = \sum_{j=1}^{30} h_j(x)\beta_j$ is **not continuous** e.g. at the knot ξ_1:

$$\beta_1 + \beta_2\xi_1 + \beta_3\xi_1^2 \neq \beta_4 + \beta_5\xi_1 + \beta_6\xi_1^2.$$

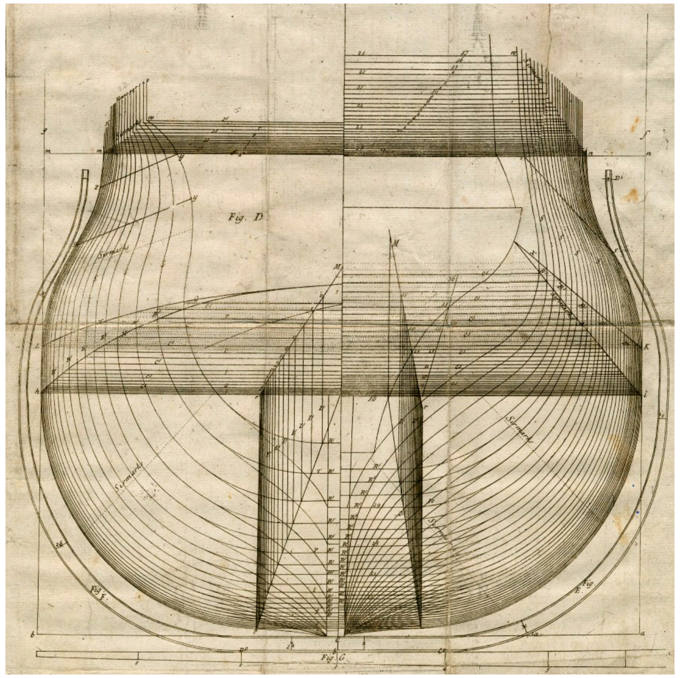
  To achieve **smoothness**, it would be appealing to add some **continuity constraints**.

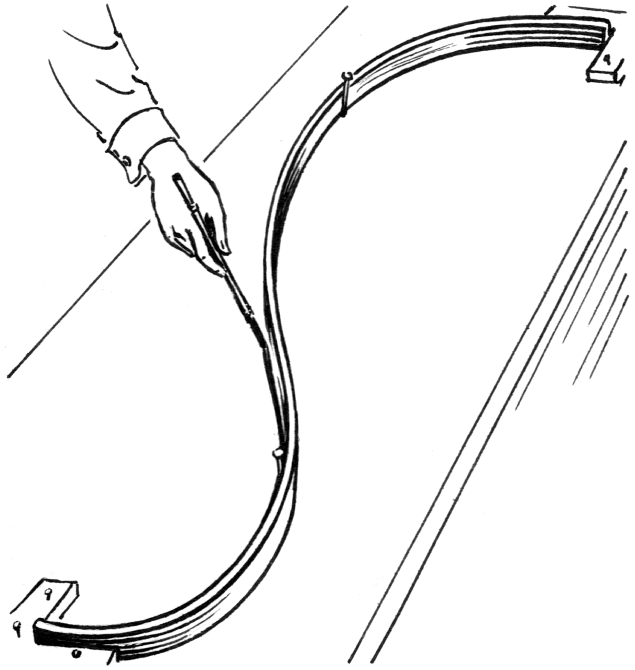
Piecewise polynomial functions



Splines I

- Splines are **piecewise polynomial functions** with **smoothness** and **continuity** constraints.
- Originally developed for **ship-building** to **draw a smooth curve** through a set of points.
- The solution was to place metal weights (called **knots**) at the control points, and bend a thin metal or wooden beam (called a **spline**) through the weights.





Splines II

Definition (Spline of degree d)

Let $\xi_1 < \cdots < \xi_k$ be a set of ordered points called **knots** belonging to the interval (a, b).

A **spline** $f(x; \beta) : (a, b) \to \mathbb{R}$ of degree d is a piecewise polynomial function of degree d that has continuous derivatives up to order $d - 1$.

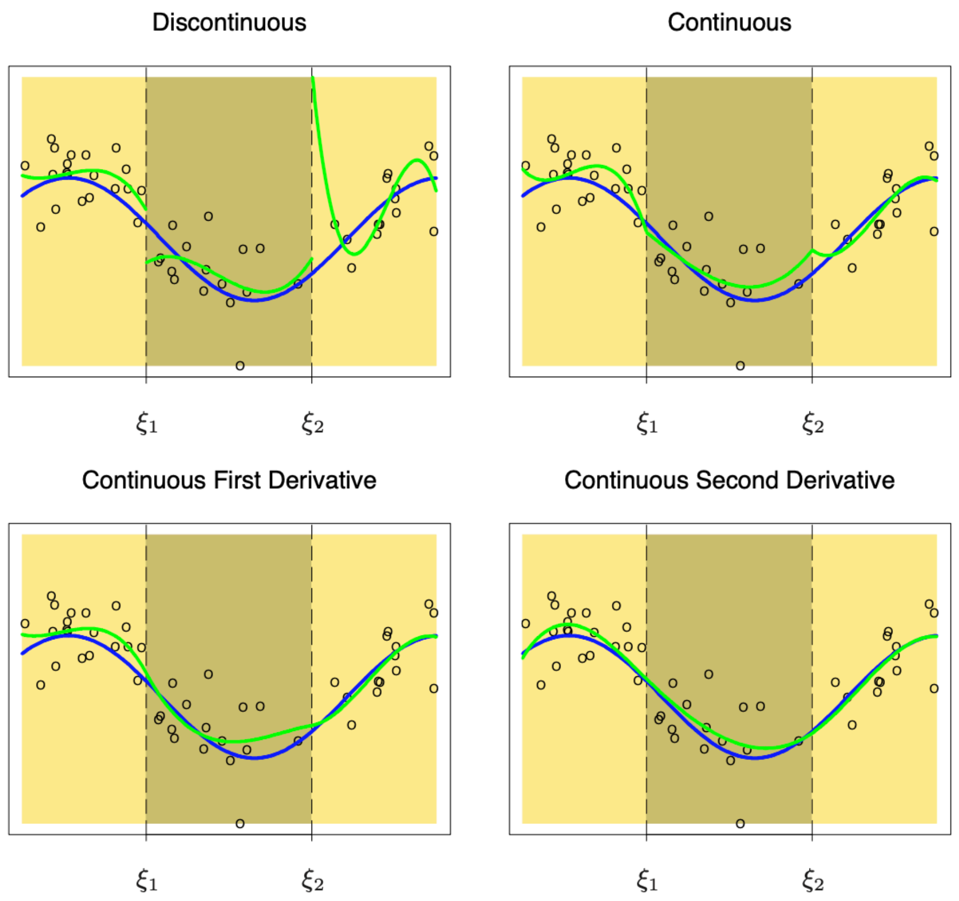
- **Cubic splines** $(d = 3)$ are the most common spline used in practice.

Definition (Cubic spline, $d = 3$)

Letting $\xi_1 < \cdots < \xi_k$ denote a set of ordered knots, a **cubic spline** $f(x; \beta)$ is a piecewise cubic polynomial that has **continuous first** and **second derivatives**.

Splines III

- Figure 5.2 of **HTF (2011)**, in which are shown piecewise **cubic polynomials** with **increasing regularity**. The bottom-right plot (green line) depicts a **cubic spline**.



Splines IV

- To **recap**: a spline of degree d is a piecewise polynomial $f(x;\beta)$ of order d such that

$$f(\xi_j^+) = f(\xi_j^-), \dots, f^{(d-1)}(\xi_j^+) = f^{(d-1)}(\xi_j^-), \qquad j = 1, \dots, k,$$

  where ξ_j^+ and ξ_j^- denote the left and the right limits.

- The degree d controls the amount of smoothness:
  - $d = 0$ is a **piecewise constant** function;
  - $d = 1$ is a **polygonal line** (continuous, but with discontinuous first derivative).
- Higher values of d increase the smoothness, but the spline behaves more and more like a global polynomial. In practice, one rarely goes beyond $d = 3$.

- The current definition of spline is quite **abstract** and **non-operative**. How do we fit a regression model whose $f(x;\beta)$ is a spline?

Truncated power basis

Theorem (Truncated power basis)

Let $\xi_1 < \cdots < \xi_k$ be a set of ordered points called **knots** belonging to (a, b). Let

$$h_j(x) = x^{j-1}, \qquad j = 1, \ldots, d+1,$$

and

$$h_{j+d+1}(x) = (x - \xi_j)_+^d, \qquad j = 1, \ldots, k.$$

Then, the functions $\{h_1, \ldots, h_{k+d+1}\}$ form a basis for the set of splines of degree d at these knots, called the **truncated power basis**.

Thus, any **dth degree spline** $f(x, \beta)$ with these knots can be written as a basis expansion

$$f(x; \beta) = \sum_{j=1}^{k+d+1} h_j(x)\beta_j.$$

Regression splines

- The truncated power basis is a **constructive** way of defining splines. Moreover, it clarifies that splines are **linear in the parameters**.

- Let $\boldsymbol{B}$ be a $n \times p$ design matrix whose elements are obtained from the basis functions:

$$[\boldsymbol{B}]_{ij} = h_j(x_i), \qquad j = 1, \dots, p; \quad i = 1, \dots, n.$$

- Let $f(x; \beta) = \sum_{j=1}^p h_j(x)\beta_j$. Then, the **ordinary least squares** for β are obtained as usual:

$$\hat{\beta} = (\boldsymbol{B}^T\boldsymbol{B})^{-1}\boldsymbol{B}^T\boldsymbol{y} \implies \hat{f}(x) = \sum_{j=1}^p h_j(x)\hat{\beta}_j = \sum_{i=1}^n s_i(x)y_i.$$

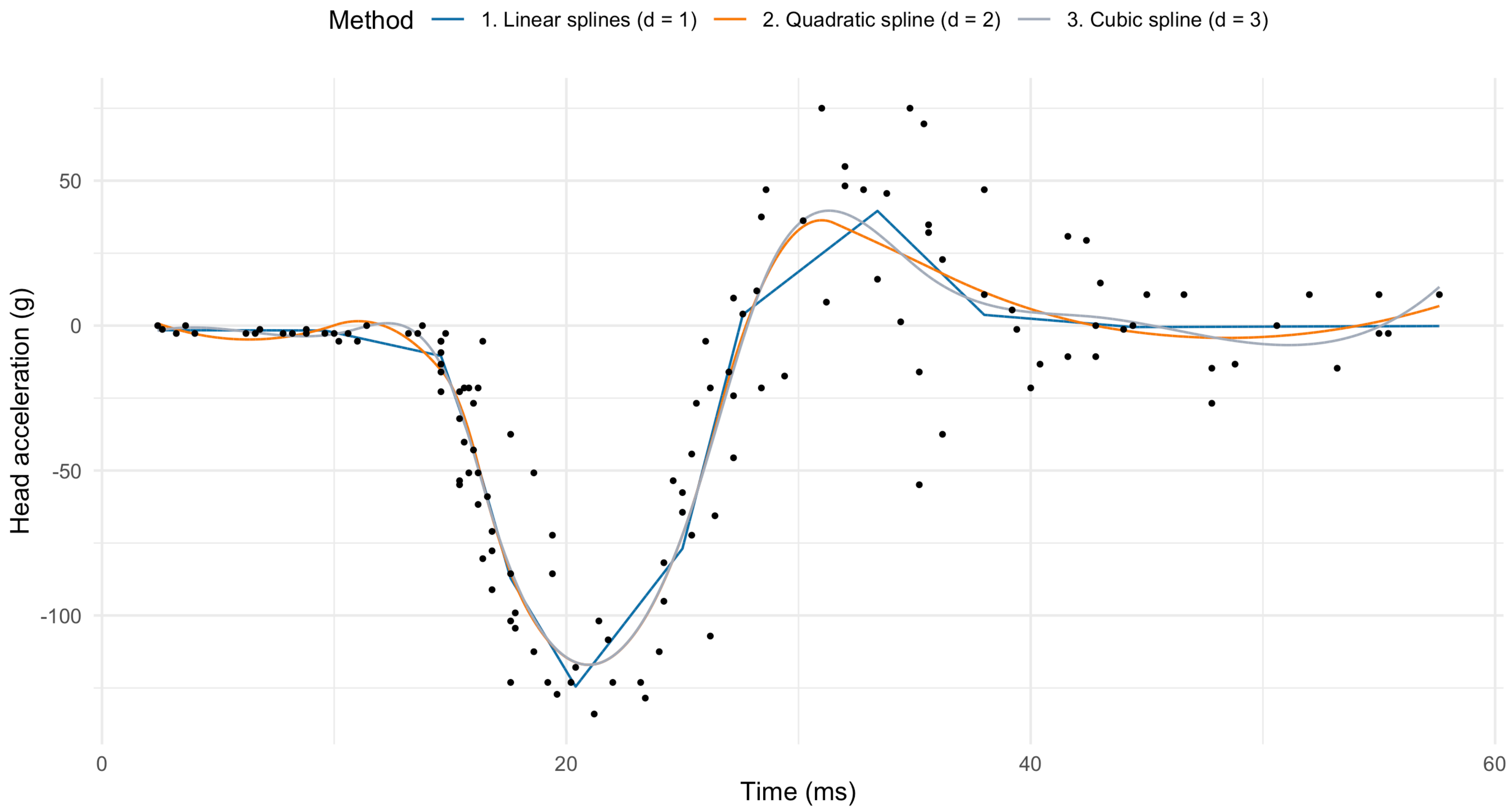
- Hence, **regression splines** are another instance of **linear smoother** (actually, of **linear model**). The smoothing matrix in this case is $\boldsymbol{S} = \boldsymbol{B}(\boldsymbol{B}^T\boldsymbol{B})^{-1}\boldsymbol{B}^T$, so that $\mathrm{tr}(\boldsymbol{S}) = p$.

- Regression splines are generating "new" covariates. Hence, their extension to GLMs, particularly to **logistic regression**, is straightforward.

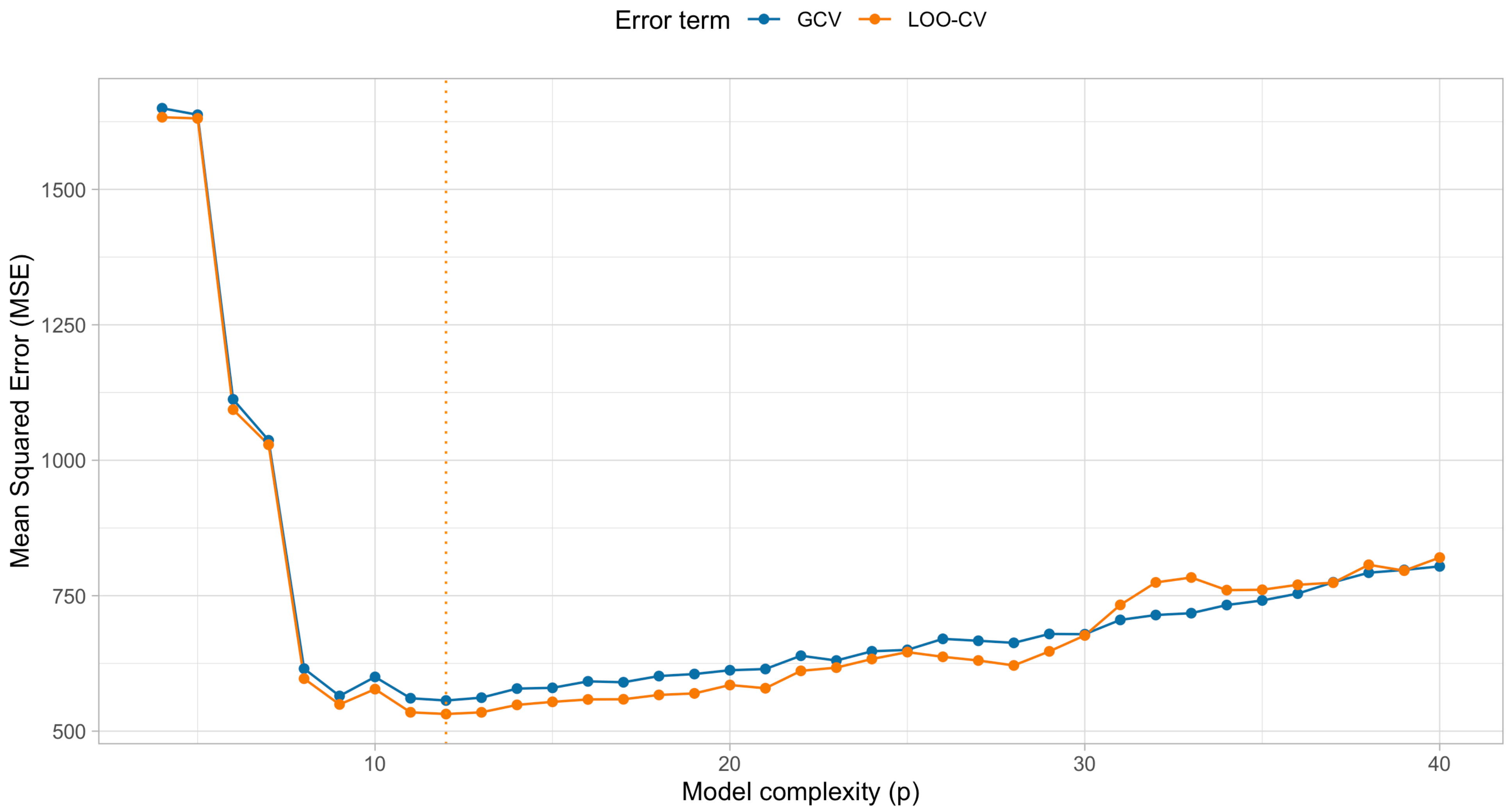
On the choice of the knots

- The knots' placement and their number k are **complexity parameters**, which should be chosen via cross-validation or other tools.
- In principle, the **position of the knots** could be manually selected to get the best fit. However, this results in an **incredible optimization problem**.
- In practice, the knots are typically selected in two ways:
  1. Knots are **equally spaced** on a grid of values ranging from $\min(x)$ to $\max(x)$;
  2. Knots are placed on **quantiles** (`bs` default), to get **variable bandwidth**.
- The **degree** d influences the **number of knots** we can place for a fixed number of degrees of freedom p. For example:
  - In linear splines $(d = 1)$, with $p = 12$ we can place $k = p - d - 1 = 10$ knots;
  - In quadratic splines $(d = 2)$, with $p = 12$ we can place $k = 9$ knots;
  - In cubic splines $(d = 3)$, with $p = 12$ we can place $k = 8$ knots.

Regression splines ($p = 12$)



On the choice of p (cubic splines)



Natural cubic splines I

- Polynomials fit **beyond** the **boundary knots** ξ_1 and ξ_k tends to be **erratic**. Prediction and extrapolations can be dangerous.

Definition (Natural cubic spline)

A **natural cubic spline** $f(x;\beta)$ is a cubic spline which is **linear** beyond the boundary knots ξ_1 and ξ_k, which means $f''(\xi_1) = f''(\xi_k) = 0$.

- Natural cubic splines enforce 4 **additional constraints**; these degrees of freedom can be used more efficiently to place more internal knots.

Proposition

A set of $n \geq 2$ **distinct** points (x_i, y_i) can be **interpolated** using a natural cubic spline with the data points $x_1 < \cdots < x_n$ as knots. The interpolating natural cubic spline is **unique**.

Natural cubic splines II

- In practice, the **truncated power basis** can be easily **modified**, to get the following basis

$$N_1(x) = 1, \quad N_2(x) = x,$$
$$N_{j+2}(x) = \frac{(x-\xi_j)_+^3 - (x-\xi_k)_+^3}{\xi_k - \xi_j} - \frac{(x-\xi_{k-1})_+^3 - (x-\xi_k)_+^3}{\xi_k - \xi_{k-1}}, \quad j = 1, \dots, k-2.$$

- This formula is a **scaled version** of the truncated power basis for any $x \le \xi_{k-1}$, namely

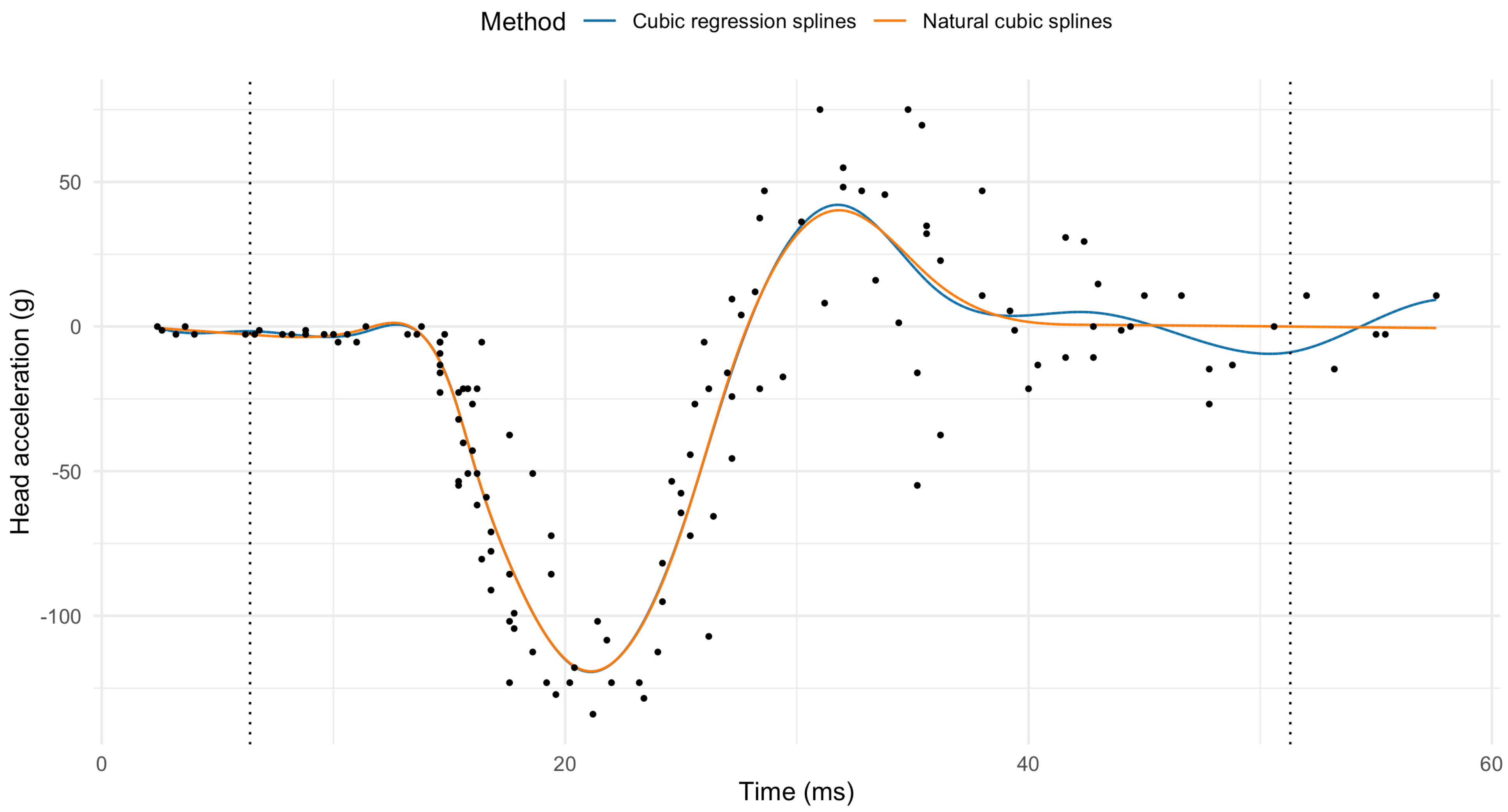
$$N_{j+2}(x) = \frac{(x-\xi_j)_+^3}{\xi_k - \xi_j}, \qquad x \le \xi_{k-1}, \quad j = 1, \dots, k-2.$$

  The formula becomes more complicated when $x > \xi_{k-1}$ and the constraint is enforced.

- Hence, in **natural cubic splines** $k = p$ and the function can be express as follows

$$f(x;\beta) = \sum_{j=1}^{k} N_j(x)\beta_j.$$

Natural cubic splines ($k = 12$)



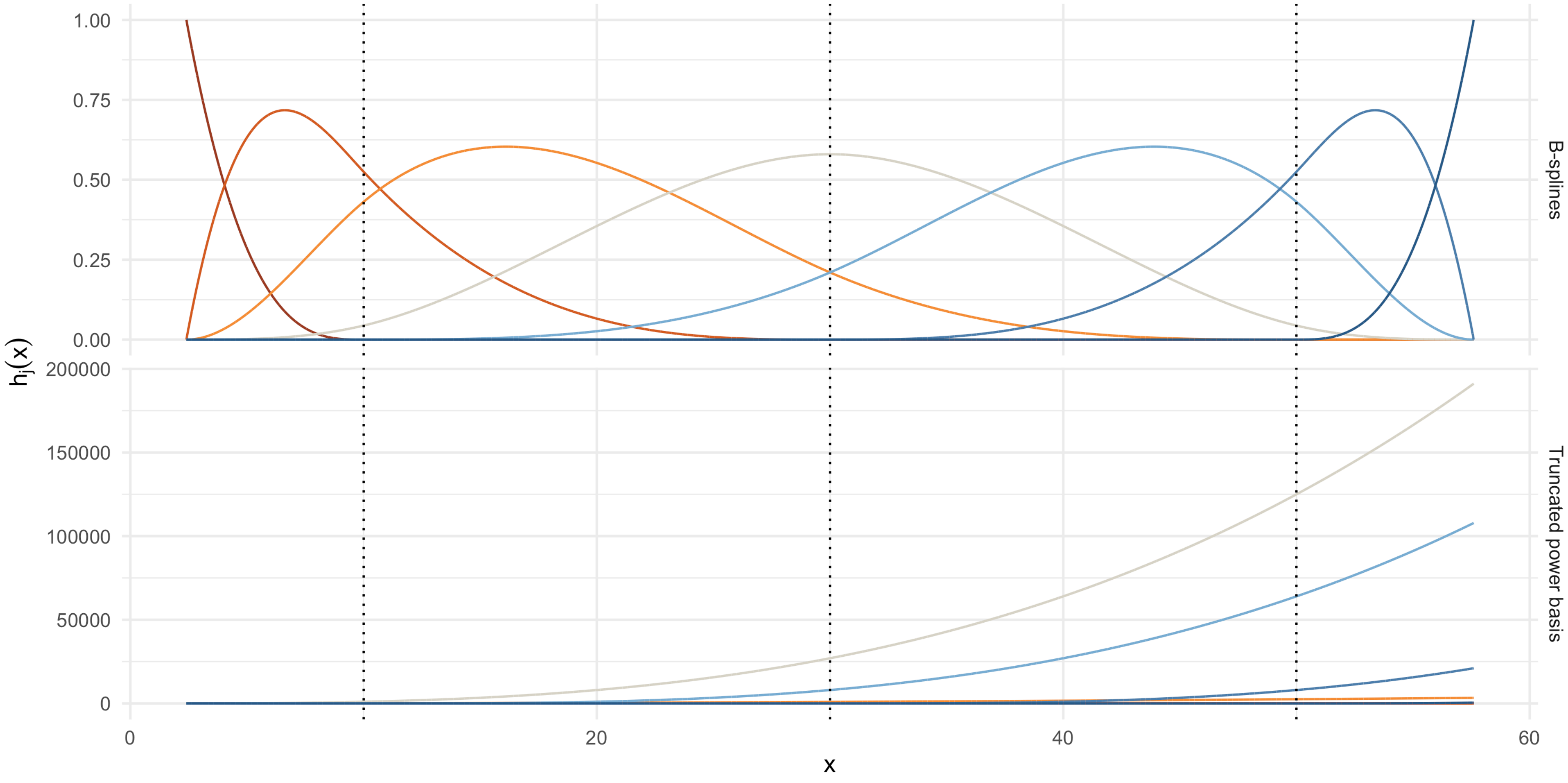
Computations: B-splines I

- Despite their conceptual simplicity, the truncated power basis and its "natural" modification are **not** used in **practice**, due to **ill-conditioning**.
- Indeed, the condition number of $\boldsymbol{B}^T\boldsymbol{B}$ using a truncated power basis is very large, leading to **numerical inaccuracies**.
- For this reason, more **computationally convenient** bases are preferred. This means we will consider an **equivalent** set of functions $\mathcal{B}_1(x), \dots, \mathcal{B}_p(x)$ such that

$$\mathcal{B}_j(x) = \sum_{\ell=1}^{p} \gamma_{\ell j} h_\ell(x), \qquad j = 1, \dots, p,$$

  for some set of weights $\gamma_{\ell j}$ that makes this transformation **one-to-one**.
- Since we are performing a linear transformation, if ordinary least squares are used, this **does not change** the fit.
- A particularly convenient basis are **B-splines**, which are **local** and **numerically stable**. They admit a direct construction; i.e., we do not need to compute the coefficients $\gamma_{\ell j}$.

Computations: B-splines II



☠️ - Details of B-splines I

- Define $\xi = (\xi_1, \dots, \xi_k)$ and consider an **augmented** sequence of ordered **knots**

$$\tau = (\tau_1, \dots, \tau_{k+2d+2}) = (\underbrace{\xi_{-d}, \dots, \xi_0}_{\text{auxiliary knots}}, \ \xi, \ \underbrace{\xi_{k+1}, \dots, \xi_{k+d+1}}_{\text{auxiliary knots}}).$$

  The most common choice is $\xi_{-d} = \dots = \xi_0 = a$ and $\xi_{k+1} = \dots = \xi_{k+d+1} = b$.

- **Step 1**. For $j = 1, \dots, k + 2d + 1$, obtain the B-spline of degree $m = 0$ as follows:

$$\mathcal{B}_{j,0}(x) = I_{[\tau_j, \tau_{j+1})}(x),$$

  where by convention we say that $\mathcal{B}_{j,0}(x) = 0$ if the knots are equal $\tau_j = \tau_{j+1}$.

- **Step 2 (recursion)**. The B-spline of **degree** $m \le d$ are obtained **recursively**, so that

$$\mathcal{B}_{j,m}(x) = \frac{x - \tau_j}{\tau_{j+m} - \tau_j}\mathcal{B}_{j,m-1}(x) + \frac{\tau_{j+m+1} - x}{\tau_{j+m+1} - \tau_{j+1}}\mathcal{B}_{j+1,m-1}(x),$$

  for $j = 1, \dots, k + 2d + 1 - m$ and for $m = 1, \dots, d$.

☠️ - Details of B-splines II

- The **intercept** term is **implicitly included** in a B-spline basis, in fact

$$\sum_{j=1}^{k+d+1} \mathcal{B}_{j,d}(x) = 1, \qquad x \in (a,b).$$

- B-splines τ have **local support**, which means that for $j = 1, \dots, k + 2d + 1 - m$ we have

$$\begin{aligned} \mathcal{B}_{j,d}(x) &= 0, \qquad x \notin (\tau_j, \tau_{j+d+1}), \\ \mathcal{B}_{j,d}(x) &> 0, \qquad x \in (\tau_j, \tau_{j+d+1}). \end{aligned}$$

  This implies that the support of cubic B-splines is at most 4 knots.

- The presence of **structural zeros** implies that, when computing ordinary least squares, extremely efficient Cholesky factorization for **banded matrices** can be exploited.
- The B-spline basis can be modified to produce a **natural cubic spline**, by numerically enforcing the linearity constraint. This is implemented in the `ns` **R** function.

Pros and cons of regression splines

Pros

- Regression splines is a **semi-parametric** estimator for unknown functions $f(x)$.
- They are essentially a **linear model** with smart covariates that account for non-linearity. Hence, the procedure is simple and **computationally efficient** (thanks to B-splines).
- The smoothing parameter k is discrete and can be easily handled, being directly associated with the number of degrees of freedom.
- They are trivial to extend to generalized linear models.

Cons

- Knot placement based on quantiles or other automatic choices could be inefficient.
- Manual placement of the knots is out of question because it is an almost impossible optimization problem.

Smoothing splines

Smoothing splines I

- Let us consider the following penalized least squares criterion

$$\mathscr{L}(f;\lambda) = \sum_{i=1}^{n}\{y_i - f(x_i)\}^2 + \underbrace{\lambda\int_a^b \{f''(t)\}^2 \mathrm{d}t}_{\text{roughness penalty}},$$

  where (a, b) is an interval containing the data points and $\lambda > 0$ is a **smoothing parameter**.

- We consider as our estimator the **minimizer** of the above loss, that is

$$\hat{f}(x) = \arg\min_{f \in \mathcal{F}} \mathscr{L}(f;\lambda),$$

  where $\mathcal{F}$ is a sufficiently regular **functional space** (Sobolev space).

- The **roughness penalty** quantifies the "wiggliness" of the curve. There are two extremes:
  - When $\lambda = 0$ there is no penalization: any solution **interpolates** the points (x_i, y_i);
  - When $\lambda = \infty$ then necessarily $f''(x) = 0$, i.e. the solution is a **linear model**.

Smoothing splines II

Theorem (Green and Silverman, 1994)

Let $n_0 \leq n$ be the **distinct** points among $x_1, \dots, x_n$, with $x_i \in (a, b)$. Suppose $n_0 \geq 3$.

Then, for any $\lambda > 0$ the minimizer of $\mathscr{L}(f; \lambda)$ is **unique** and is a **natural cubic spline** with n_0 knots at the distinct points.

- The Green and Silverman theorem is remarkably **elegant** and **powerful**.
- Since the solution is a **natural cubic spline**, we can write it as follows:

$$f(x; \beta) = \sum_{j=1}^{n_0} N_j(x)\beta_j,$$

  whose coefficients β still **needs** to be **determined**.

- In smoothing splines, we do **not** need to **choose the knots**: every distinct observation is a knot. The model is not overparametrized because the **complexity** is controlled by λ.

Smoothing splines III

- Since $f(x;\beta)$ is a **natural cubic spline**, the penalized least squares criterion becomes

$$\mathscr{L}(\beta;\lambda) = \sum_{i=1}^{n}\{y_i - f(x_i;\beta)\}^2 + \lambda\beta^T\boldsymbol{\Omega}\beta, \qquad [\boldsymbol{\Omega}]_{jk} = \int_a^b N_j''(t)N_k''(t)\mathrm{d}t,$$

  whose **minimization** over β is much easier, because it becomes **finite-dimensional**.

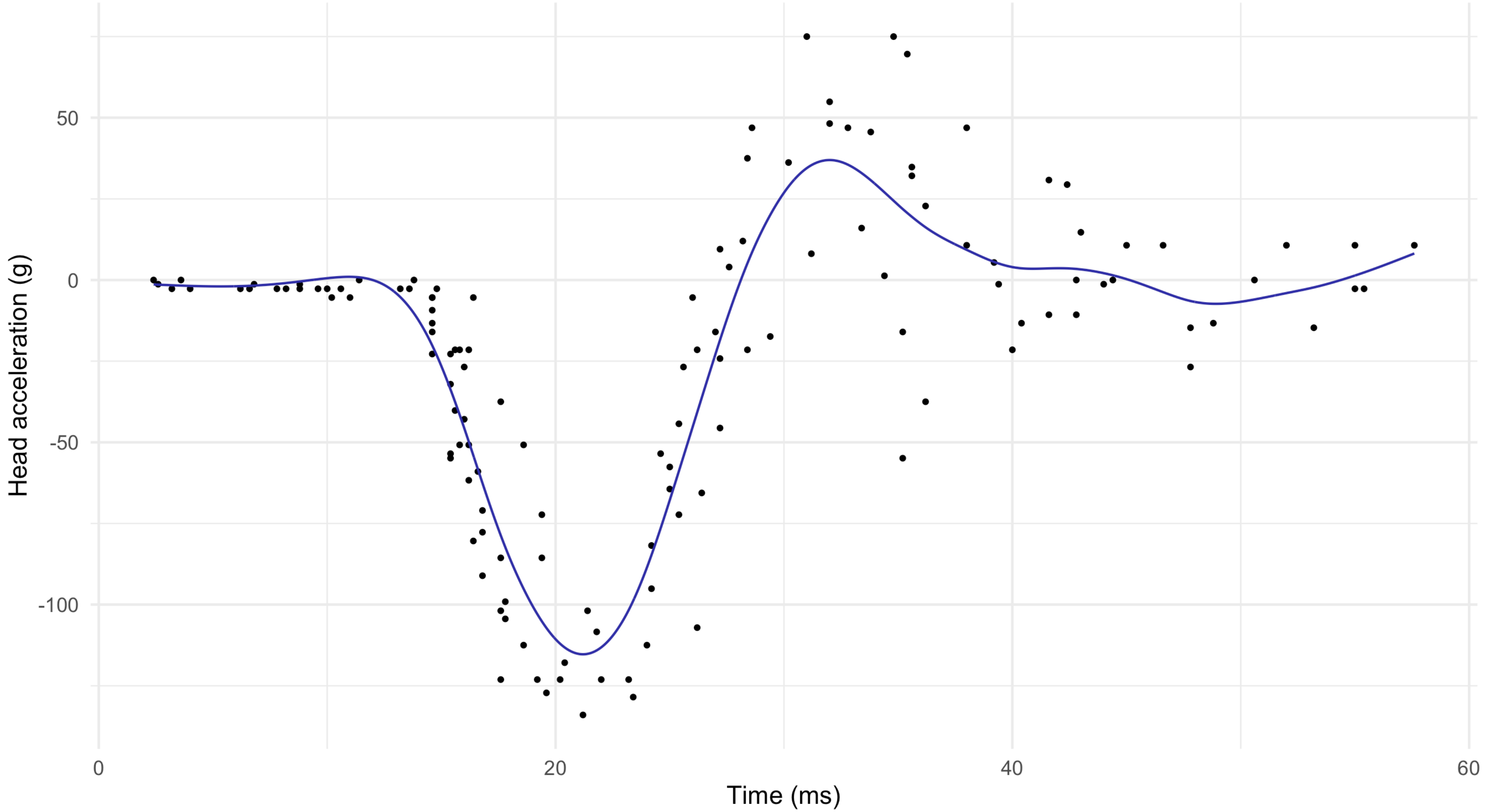
- The minimization of $\mathscr{L}(\beta;\lambda)$ is reminiscent of **ridge regression**, and in fact the solution is

$$\hat{\beta} = (\boldsymbol{N}^T\boldsymbol{N} + \lambda\boldsymbol{\Omega})^{-1}\boldsymbol{N}^T\boldsymbol{y}, \qquad [\boldsymbol{N}]_{ij} = N_j(x_i).$$

  which leads to a **linear smoother**, with $\boldsymbol{S} = \boldsymbol{N}(\boldsymbol{N}^T\boldsymbol{N} + \lambda\boldsymbol{\Omega})^{-1}\boldsymbol{N}^T$.

- The above formula is not used in practice directly. The `smooth.spline` **R** implementation relies on B-splines to make computations **fast** and **stable**.
- Alternatively, the so-called Reinsch (1967) algorithm has computational complexity $\sim n$.

Smoothing splines ($\text{df}_{\text{sm}} = 12.26$)



The equivalent kernel

- As already mentioned, smoothing splines are **linear smoothers**, which means that

$$\hat{f}(x) = \sum_{i=1}^{n} s_i(x) y_i.$$

- Provided x is not too near the edge of the interval (a, b), and λ is not too big or too small, we obtain the following **approximation** for the **equivalent kernel**

$$s_i(x) \approx \frac{1}{g(x)} \frac{1}{h(x)} w\left(\frac{x - x_i}{h(x)}\right).$$

- The **kernel function** $w(t)$, which is not a density, and the **local bandwidth** equal to

$$w(t) = \frac{1}{2} \exp\left(-\frac{|t|}{\sqrt{2}}\right) \sin\left(\frac{|t|}{\sqrt{2}} + \frac{\pi}{4}\right), \qquad h(x) = \lambda^{1/4}\{n g(x)\}^{-1/4}.$$

- Smoothing splines **automatically** incorporate a **local bandwidth** decreasing with n.

Multi-dimensional splines

- There are several ways of extending regression and smoothing splines to the multivariate case. An example are **tensor splines**, based on the cross-multiplication of basis functions.

- Another instance are the **thin-plate splines**, in which the 2d **roughness** penalty becomes

$$\int_{\mathbb{R}^2} \left\{ \left(\frac{\partial^2 f(x_1, x_2)}{\partial x_1^2}\right)^2 + 2\left(\frac{\partial^2 f(x_1, x_2)}{\partial x_1 \partial x_2}\right)^2 + \left(\frac{\partial^2 f(x_1, x_2)}{\partial x_2^2}\right)^2 \right\} \mathrm{d}x_1 \mathrm{d}x_2.$$

  The minimization of the above loss has a simple **finite-dimensional** solution.

- We do not discuss any further multi-dimensional splines because, when the **dimension is large**, they are affected by the so-called **curse of dimensionality**; see Unit E.

- Nonetheless, the 2d case is extremely useful in **spatial statistics**, in which x_1 and x_2 represent longitude and latitude.

- There will be a strong connection between the **smoothers** we have seen in this unit and the so-called **kriging equations**.

Further properties of smoothing splines

- Extension of smoothing splines to **generalized linear models** is possible by adding the "roughness" penalty to the log-likelihood function.

- Smoothing splines have a Bayesian interpretation, being an instance of **Gaussian process**.
- From a theoretical perspective, there exists (Chapter 5.8 of **HTF, 2011**) an elegant theory based on **reproducing kernel Hilbert spaces**, that **unifies**:
  - Gaussian processes;
  - Smoothing splines;
  - Support vector machine.

Pro-tip (a joke?)

"If you want to derive an estimator that performs well in practice, define a Bayesian model, derive the posterior mean, call this a frequentist estimator, and hide all evidence you ever considered a Bayesian approach." Credits to Eric B. Laber

Pros and cons of smoothing splines

Pros

- Smoothing splines is a **nonparametric** estimator for unknown functions $f(x)$.
- They are a **linear smoother** with variable bandwidth.
- Compared to regression splines, they do not require the choice of the knots.
- Simple and efficient algorithms for computing 1d smoothing splines exist, such as `smooth.spline` available in **R**.

Cons

- Efficient implementations require a profound knowledge of linear algebra, B-spline basis, etc.
- Hence, the "manual" incorporation (i.e., the coding) of smoothing splines into bigger, non-standard models is not straightforward.

References

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