MONASH University

MONASH BUSINESS SCHOOL

ETC3580: Advanced Statistical Modelling

Week 10: Nonparametric inference

Outline

1 General kernel form of linear smoothers

2 Inference for linear smoothers

3 Derivative estimation

4 Multidimensional smoothers

5 Penalized regression splines

General kernel form of linear smoothers

Linear smoother

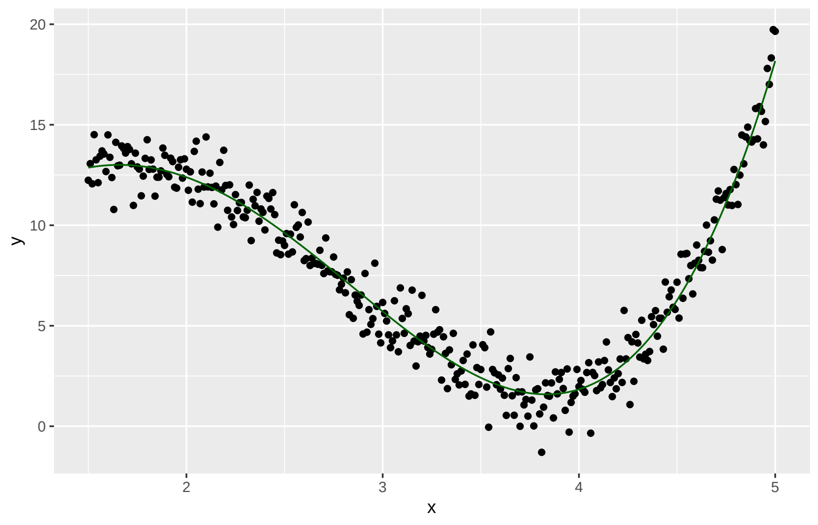
$$\hat{f}(x) = \sum_{j=1}^{n} w_j(x) y_j$$

- Nadaraya-Watson smoothing:

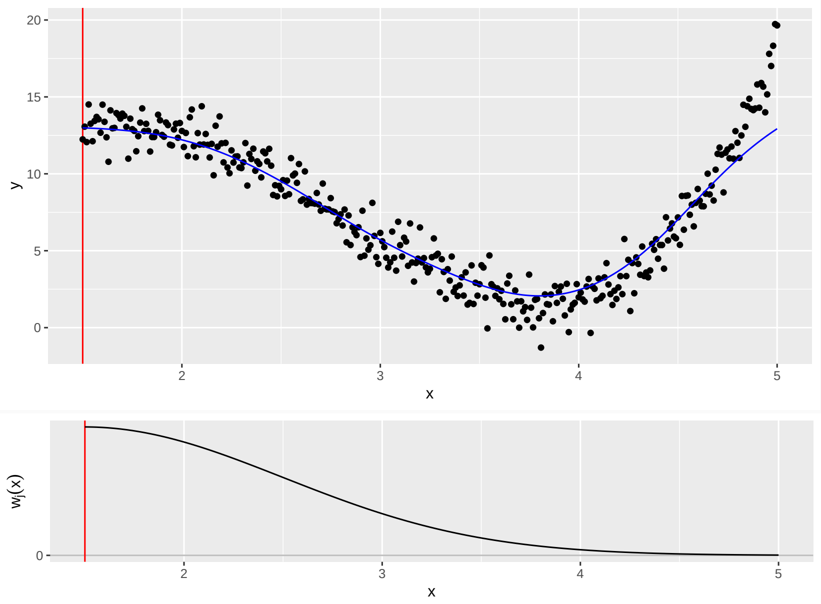
$$w_j(x) = \frac{K\left(\frac{x - x_j}{h}\right)}{\sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right)}$$

- Almost all smoothing methods can be written in this form for different functions $w_j(x)$

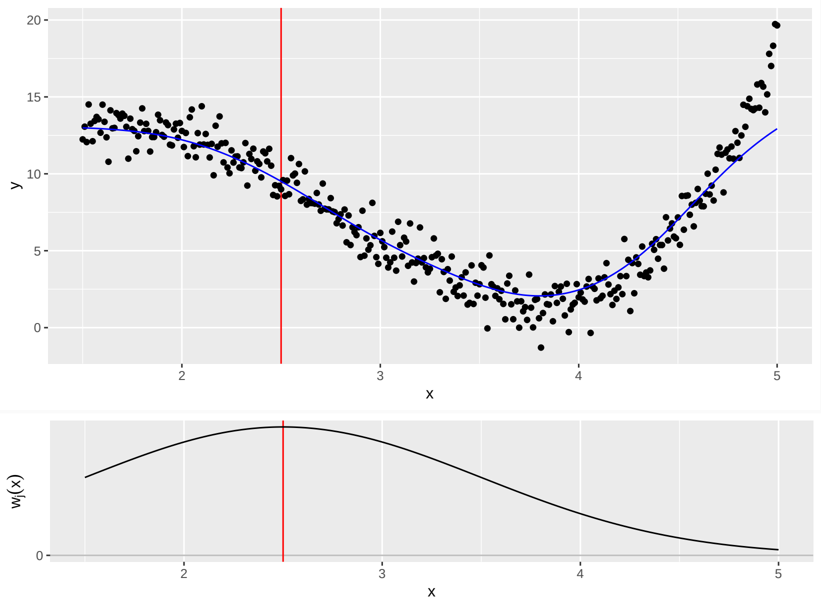
Example



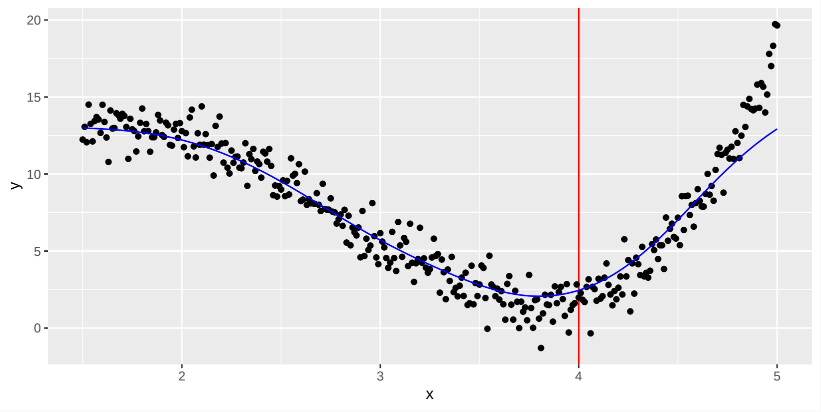
Kernel estimator

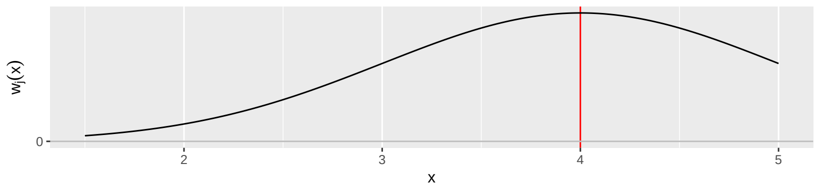


Kernel estimator

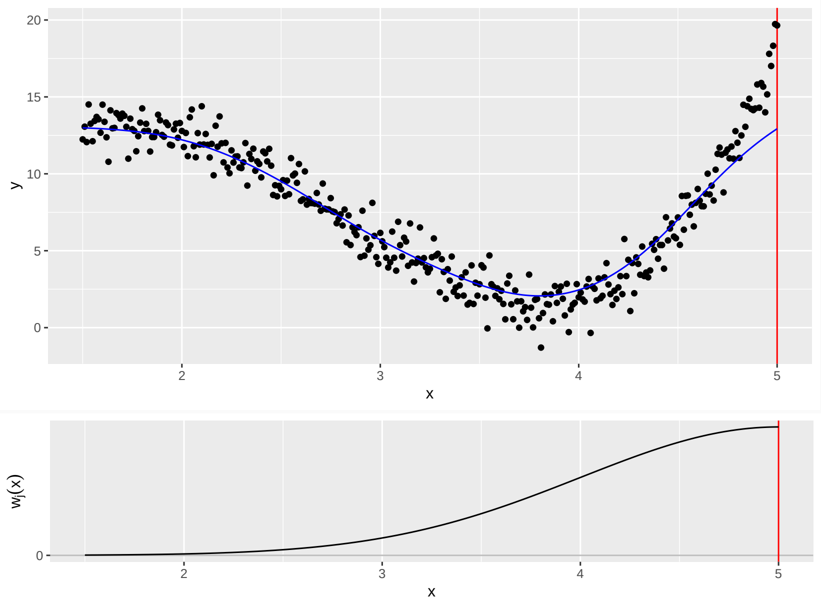


Kernel estimator





Kernel estimator



Local polynomial estimator

Assume

$$f(u) = a_0 + a_1(u - x) + \cdots + a_p(u - x)^p.$$

Then the coefficients, $\hat{a}_i$, are the values of a_i which minimise

$$\text{WLS}(x) = \sum_{j=1}^{n} w_j(x)\Big(y_j - a_0 - a_1(x_j - x) - \cdots - a_p(x_j - x)^p\Big)^2$$

and $\hat{f}(x) = \hat{a}_0$. In matrix notation we can write

$$\text{WLS}(x) = (\boldsymbol{Y} - X\boldsymbol{a})' W(x)(\boldsymbol{Y} - X\boldsymbol{a})$$

where $[X]_{ji} = (x_j - x)^i$ and $W(x)$ is the diagonal matrix with elements $w_j(x)$.

Local polynomial estimator

The minimizer of this function is

$$\hat{\boldsymbol{a}} = (X'W(x)X)^{-1}X'W(x)\boldsymbol{Y}.$$

Therefore,

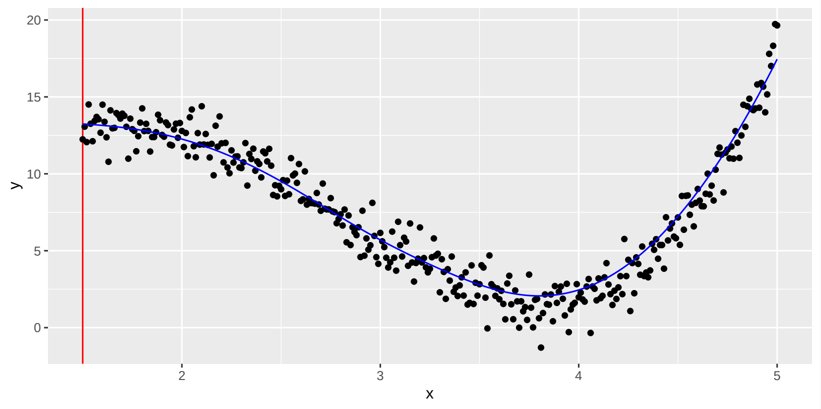
$$\hat{f}(x) = [1, 0, \dots, 0](X'W(x)X)^{-1}X'W(x)\boldsymbol{Y} = \sum_{j=1}^{n} \ell_j(x)y_j$$

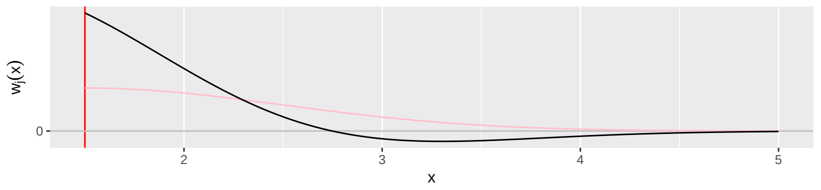
where

$$\ell_j(x) = [1, 0, \dots, 0](X'W(x)X)^{-1}[1, (x_j - x), \dots, (x_j - x)^p]w_j(x)$$

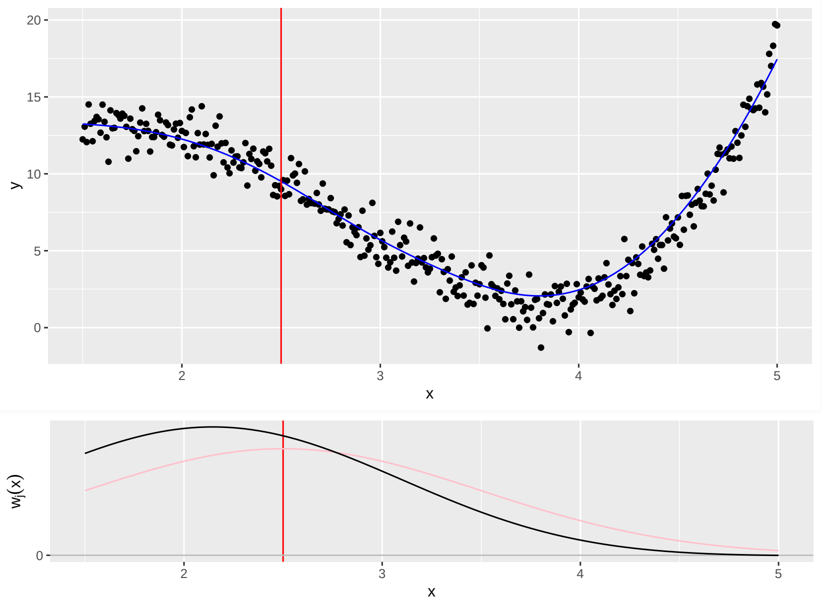
So a local polynomial is equivalent to a kernel smoother but with an unusual weight function. We call the weights $\ell_j(x)$ the *effective kernel* at x. If $p = 0$, then $\ell_j(x) = w_j(x)$.

Local linear estimator

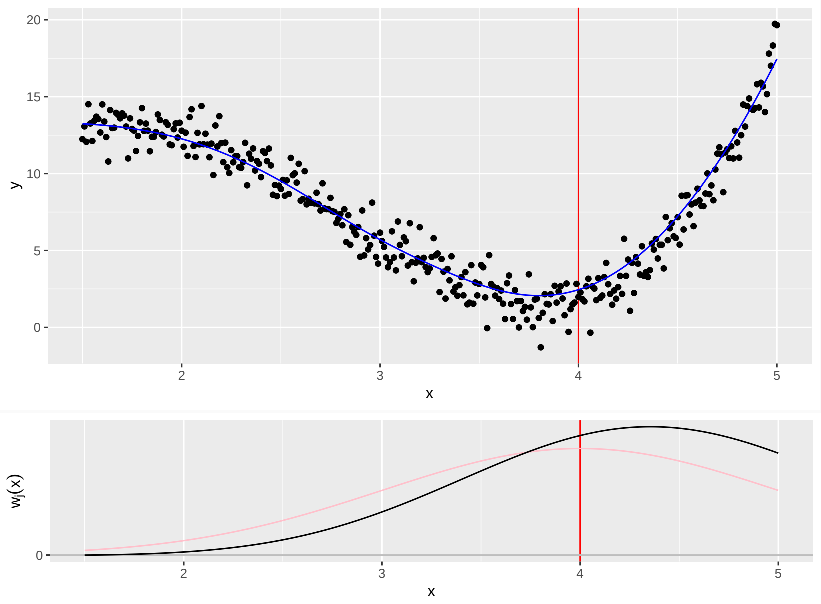




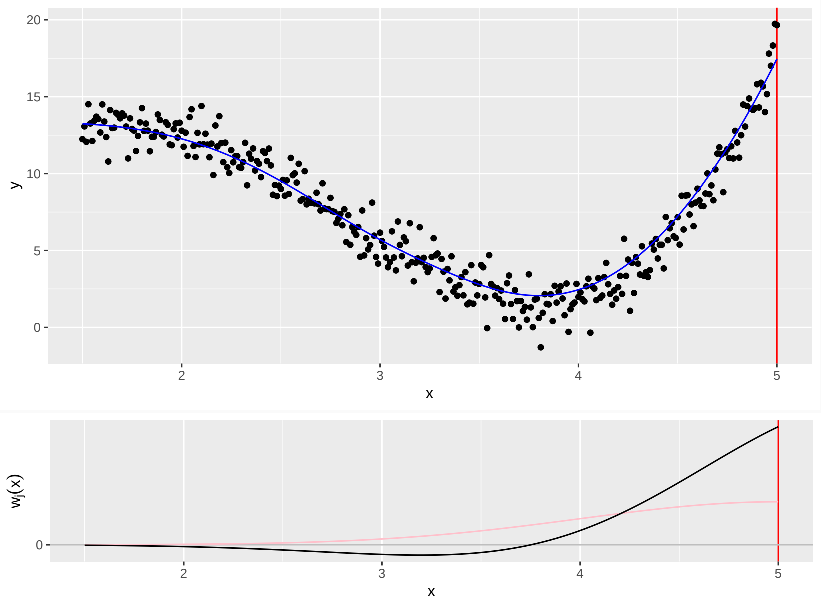
Local linear estimator



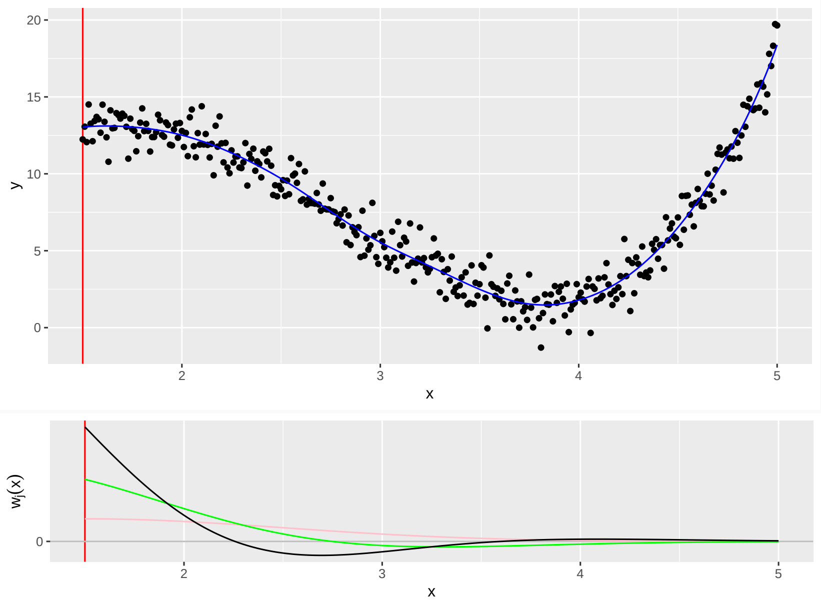
Local linear estimator



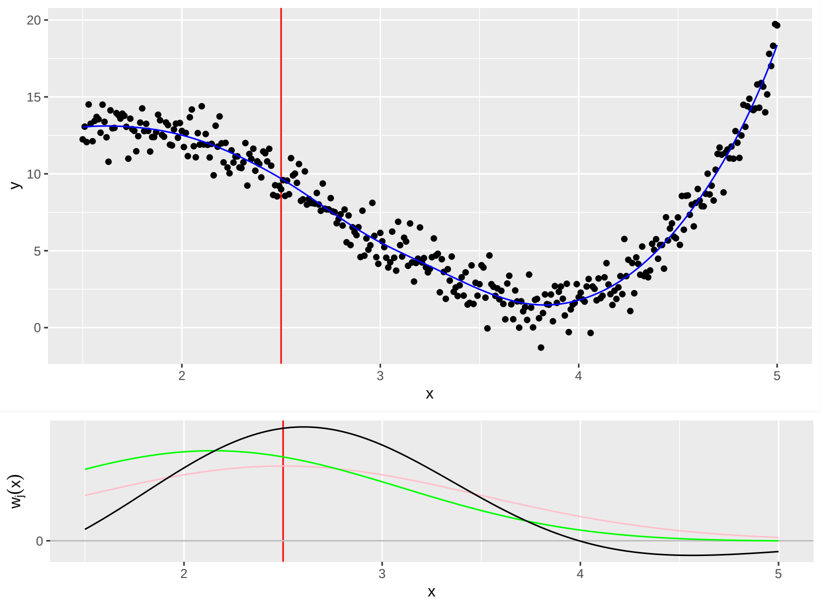
Local linear estimator



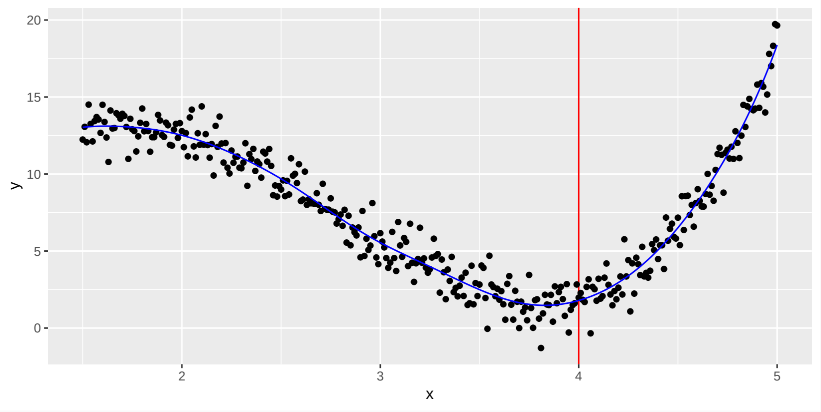
Local quadratic smoother

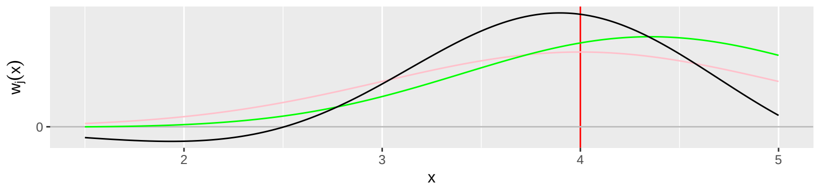


Local quadratic smoother

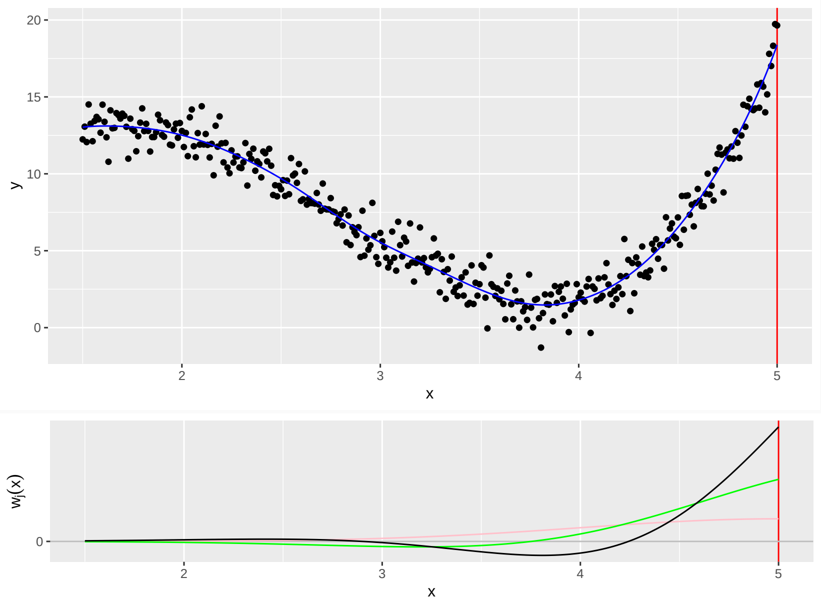


Local quadratic smoother





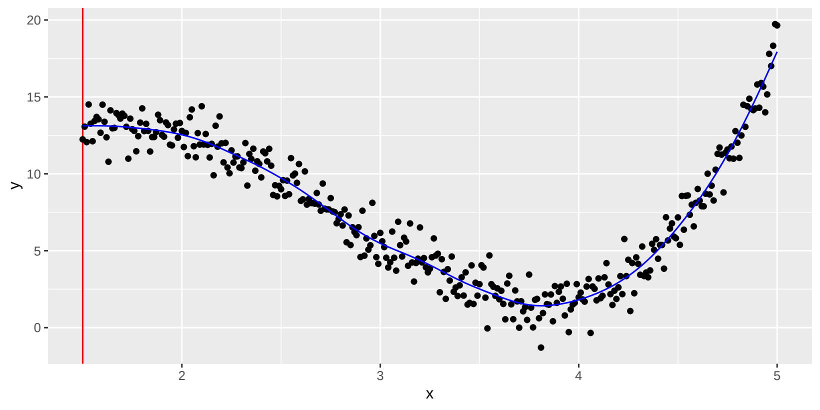
Local quadratic smoother

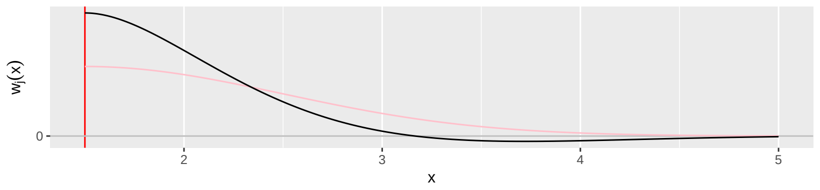


Smoothing spline

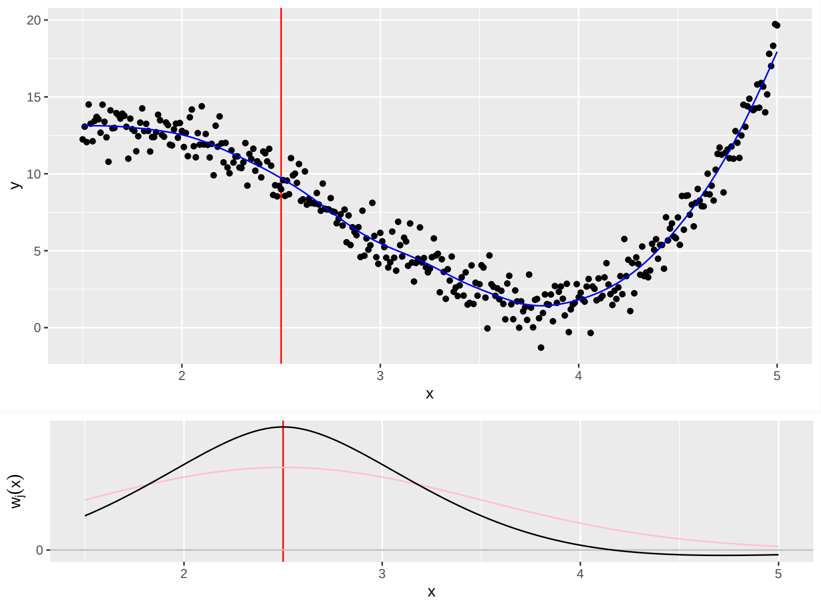
- A cubic smoothing spline can also be written as a kernel smoother with kernel function asymptotically equal to
$$K_s(u) = \frac{1}{2}\exp\left(-\frac{|u|}{h\sqrt{2}}\right)\sin\left(\frac{|u|}{h\sqrt{2}}+\frac{\pi}{4}\right).$$

Smoothing spline

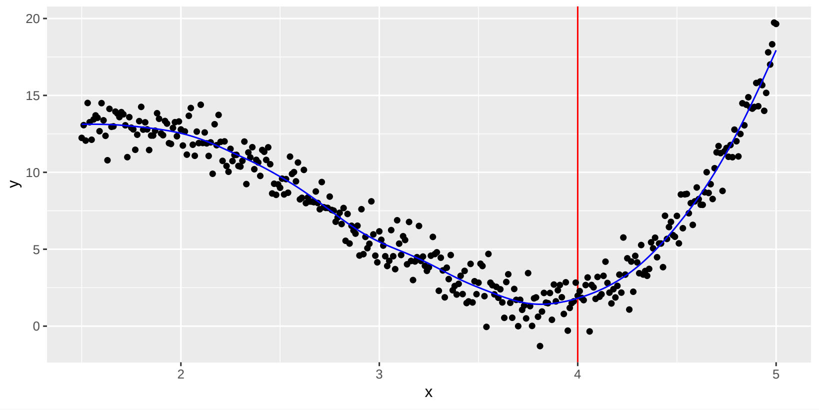


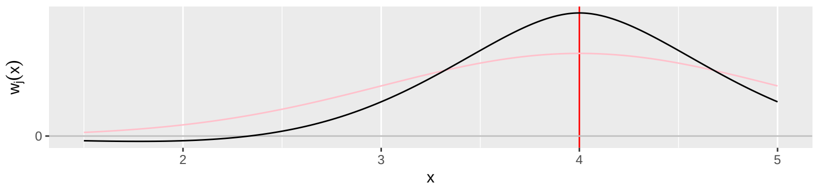


Smoothing spline

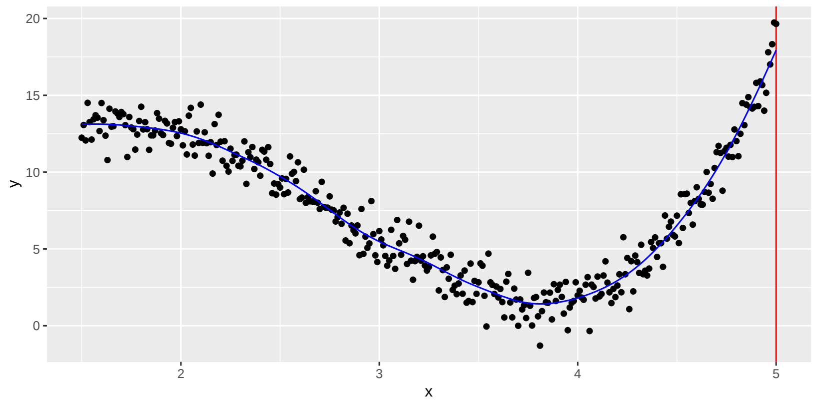


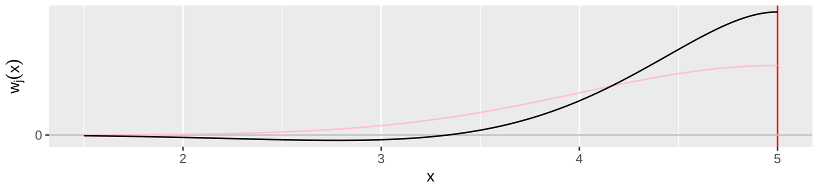
Smoothing spline





Smoothing spline





Regression splines

Regression splines are linear models, and so fitted values can be written as

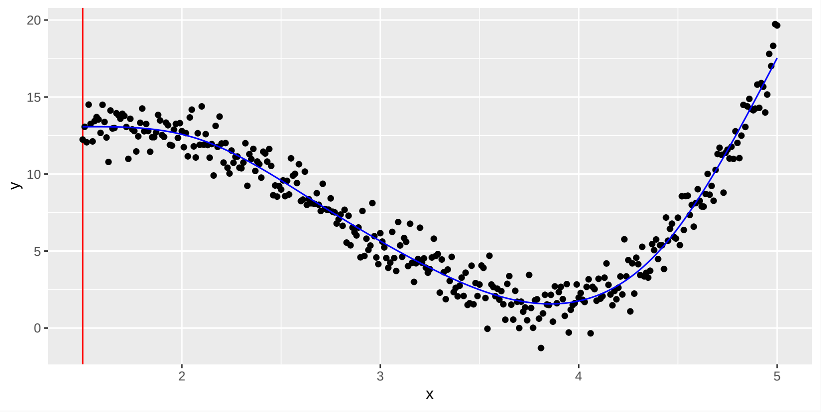
Therefore,

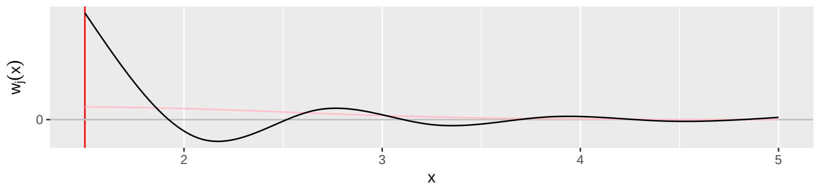
$$\hat{f}(x) = \boldsymbol{x}^{*\prime}(X'X)^{-1}X'\boldsymbol{Y} = \sum_{j=1}^{n} \ell_j(x) y_j$$

where

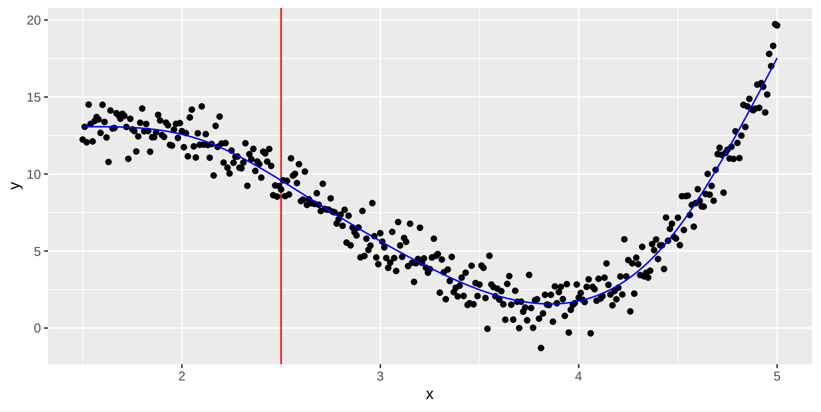
$$\ell_j(x) = \boldsymbol{x}^{*\prime}(X'X)^{-1}\boldsymbol{x}^{*\prime}$$

Regression splines

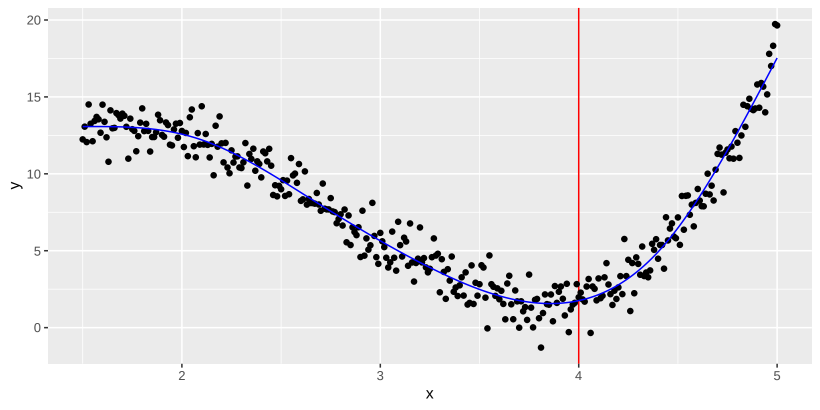




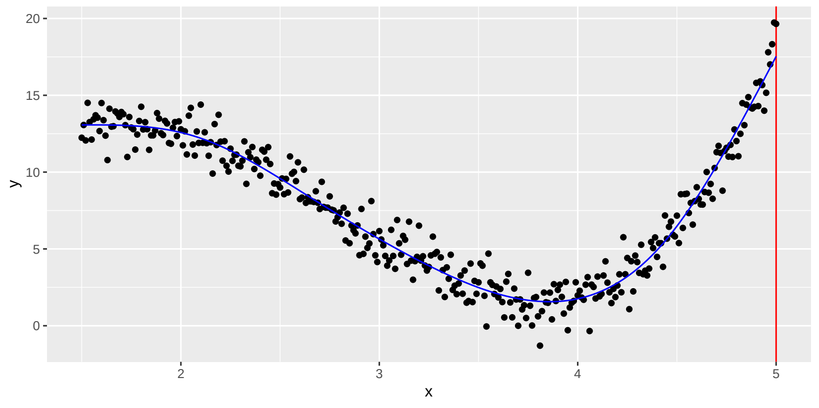
Regression splines

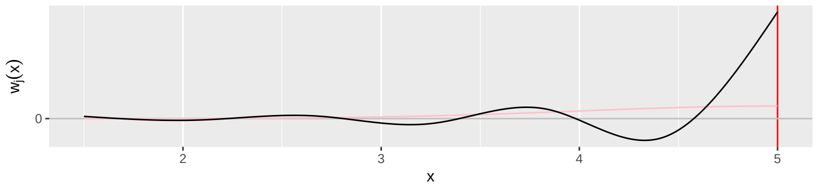


Regression splines



Regression splines





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2 Inference for linear smoothers

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Inference for linear smoothers

All of the methods we have looked at can be written in the form

$$\hat{f}(x) = \sum_{j=1}^{n} w_j(x) y_j.$$

Thus they are linear in the observations. The set of weights, $w_j(x)$, is known as the equivalent kernel at x. Let $\hat{\boldsymbol{f}} = [\hat{f}(x_1), \hat{f}(x_2), \dots, \hat{f}(x_n)]'$. Then

$$\hat{\boldsymbol{f}} = \boldsymbol{S}\boldsymbol{y}$$

where $\boldsymbol{S} = [w_j(x_i)]$ is an $n \times n$ matrix that we call a *smoother matrix*.

Inference for linear smoothers

- The rows of $\boldsymbol{S}$ are the equivalent kernels for producing fits at each of the observed values $x_1, \ldots, x_n$.
- Any reasonable smoother should preserve a constant function so that $\boldsymbol{S}\mathbf{1} = \mathbf{1}$ where $\mathbf{1}$ is a vector of ones. This implies that the sum of the weights in each row is one.
- The matrix $\boldsymbol{S}$ is analogous to the hat matrix $\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'$ in a standard linear model.

Degrees of freedom

Want: Approximate df for our linear smoothers.

- high df for very wiggly smoothers
- low df for very smooth smoothers.
- Least squares regression: $\boldsymbol{S} = \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'$.

$$
\begin{aligned}
\gamma = \text{df} &= \text{\# linearly independent predictors in model} \\
&= \text{rank}(\boldsymbol{S}) \\
&= \text{tr}(\boldsymbol{S}) \\
&= \text{tr}(\boldsymbol{S}\boldsymbol{S}') \\
&= \text{tr}(2\boldsymbol{S} - \boldsymbol{S}\boldsymbol{S}').
\end{aligned}
$$

Any of these could be used for df of general linear smoother.

Estimating the variance

- Linear regression: error has $n - \gamma$ df.
- Hence define df of error for a linear smoother as $n - \gamma$ where $\gamma = \text{tr}(\boldsymbol{S})$.
- Assuming zero bias for smoother, an unbiased estimator of σ^2 is given by

$$\hat{\sigma}^2 = \frac{1}{n - \gamma} \sum_{j=1}^{n} (y_j - \hat{f}(x_j))^2.$$

Confidence intervals

$\text{Cov}(\hat{\boldsymbol{f}}) = \boldsymbol{S}\boldsymbol{S}'\sigma^2$

Assuming negligible bias, approximate 95% CI for $\boldsymbol{f}$ are:

$$\hat{\boldsymbol{f}} \pm 1.96\hat{\sigma}\sqrt{\text{diag}(\boldsymbol{S}\boldsymbol{S}')}.$$

- Pointwise intervals. (i.e,. 95% CI for each value of x.)
- On average, true value of $f(x)$ lies outside these intervals 5% of the time.

Approximate F tests

Approximate F tests using the approximate df.

To compare two smooths:

$$\hat{\boldsymbol{f}}_1 = \boldsymbol{S}_1\boldsymbol{y} \qquad (\text{df} = \gamma_1)$$
$$\hat{\boldsymbol{f}}_2 = \boldsymbol{S}_2\boldsymbol{y} \qquad (\text{df} = \gamma_2).$$

$\gamma_i = \text{df} = \text{tr}(2\boldsymbol{S}_i - \boldsymbol{S}_i\boldsymbol{S}_i')$ for each of the models $i = 1, 2$.

Let RSS_1 and RSS_2 be residual sum of squares for each smoother.

$$\frac{(\text{RSS}_1 - \text{RSS}_2)/(\gamma_2 - \gamma_1)}{\text{RSS}_2/(n - \gamma_2)} \sim F_{\gamma_2-\gamma_1, n-\gamma_2}.$$

- Implemented by `anova` in R

Applications

Test for linearity

Let $\hat{f}_1$ represent a linear regression and we wish to test if the linearity is real by fitting a nonparametric nonlinear smooth curve $\hat{f}_2$.

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Let $\hat{\boldsymbol{f}}_1$ represent a linear regression and we wish to test if the linearity is real by fitting a nonparametric nonlinear smooth curve $\hat{\boldsymbol{f}}_2$.

Test for bias in residuals

After fitting a model, the residuals can be modelled as a function of the predictor variable. If the function is not significantly different from the zero function, there is no significant bias.

Bias and variance

The bias vector is $\boldsymbol{b} = \boldsymbol{f} - \mathrm{E}(\boldsymbol{S}\boldsymbol{y}) = \boldsymbol{f} - \boldsymbol{S}\boldsymbol{f} = (\boldsymbol{I} - \boldsymbol{S})\boldsymbol{f}$.

Then we can compute the mean square error as

$$\begin{aligned}\text{MSE} &= \frac{1}{n}\sum_{j=1}^{n}\text{Var}(\hat{f}_i) + \frac{1}{n}\sum_{j=1}^{n} b_i^2 \\ &= \frac{\text{tr}(\boldsymbol{S}\boldsymbol{S}')}{n}\sigma^2 + \frac{\boldsymbol{b}'\boldsymbol{b}}{n}\end{aligned}$$

The first term measures variance while the second measures squared bias.

- Smoothing is a bias-variance tradeoff

Cross-validation

Find h which minimises cross-validation function

$$\mathrm{CV}(h) = \frac{1}{n}\sum_{j=1}^{n}[\hat{f}_j(x_j) - y_j]^2$$

$$\hat{f}_j(x) = \frac{1}{1 - w_j(x)}\sum_{\substack{i=1\\ i\neq j}}^{n} w_i(x)y_i.$$

- residuals: $\hat{e}_j = y_j - \hat{f}(x_j)$
- LOO residuals: $\hat{e}_{(j)} = y_j - \hat{f}_j(x_j)$

Use same computational trick as for LM to avoid computing n separate smoothers.

Cross-validation

$$
\begin{aligned}
\hat{e}_{(j)} &= y_j - \hat{f}_j(x_j) \\
&= y_j - \frac{1}{1 - w_j(x_j)} \sum_{\substack{i=1 \\ i \neq j}}^{n} w_i(x_j) y_i . \\
&= y_j - \frac{1}{1 - w_j(x_j)} \left(\hat{f}(x_j) - w_j(x_j) y_j \right) \\
&= y_j \left(1 + \frac{w_j(x_j)}{1 - w_j(x_j)} \right) - \frac{1}{1 - w_j(x_j)} \hat{f}(x_j) \\
&= y_j \left(\frac{1 - w_j(x_j) + w_j(x_j)}{1 - w_j(x_j)} \right) - \frac{1}{1 - w_j(x_j)} \hat{f}(x_j) \\
&= \left(y_j - \hat{f}(x_j) \right) \frac{1}{1 - w_j(x_j)} = \frac{\hat{e}_j}{1 - w_j(x_j)}
\end{aligned}
$$

Cross-validation

$$\mathrm{CV}(h) = \frac{1}{n}\sum_{j=1}^{n} \hat{e}_{(j)}^2 = \frac{1}{n}\sum_{j=1}^{n} \hat{e}_j^2 \left(1 - w_j(x_j)\right)^{-2}$$

Cross-validation

$$\mathrm{CV}(h) = \frac{1}{n}\sum_{j=1}^{n} \hat{e}_{(j)}^2 = \frac{1}{n}\sum_{j=1}^{n} \hat{e}_j^2 \left(1 - w_j(x_j)\right)^{-2}$$

CV(h) is a **penalized mean squared error**.

Cross-validation

$$\mathrm{CV}(h) = \frac{1}{n}\sum_{j=1}^{n} \hat{e}_{(j)}^2 = \frac{1}{n}\sum_{j=1}^{n} \hat{e}_j^2 \left(1 - w_j(x_j)\right)^{-2}$$

CV(h) is a **penalized mean squared error**.

Generalization:

Find h which minimises penalized MSE:

$$G(h) = \frac{1}{n}\sum_{j=1}^{n}[\hat{f}(x_j) - y_j]^2 p(w_j(x_j))$$

where $p(u)$ is a penalty function.

CV: $p(u) = (1 - u)^{-2}$.

Penalized MSE

Examples:

Shibata's selector	$p(u) = 1 + 2u$
Generalized cross-validation	$p(u) = (1 - u)^{-2}$
Akaike's information criterion	$p(u) = \exp(2u)$
Finite prediction error	$p(u) = (1 + u)/(1 - u)$
Rice's T	$p(u) = (1 - 2u)^{-1}$

- Goal is to penalize small bandwidths.
- $w_j(x_j) \to 1$ as $h \to 0$ and $w_j(x_j) \to 0$ as $h \to \infty$.
- Different $p(u)$ almost equal for large h but penalize small h differently.

Penalized MSE

- `mgcv::gam` function uses GCV.
- If $\hat{h}$ is minimising bandwidth of $G(h)$ and $\hat{h}_0$ is MSE optimal bandwidth, then
$$\frac{\text{MSE}(\hat{h})}{\text{MSE}(\hat{h}_0)} \xrightarrow{p} 1 \qquad \text{and} \qquad \frac{\hat{h}}{\hat{h}_0} \xrightarrow{p} 1.$$

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Derivative estimation

$$\hat{f}(x) = \sum_{j=1}^{n} w_j(x) y_j \qquad \Rightarrow \qquad \hat{f}^{(k)}(x) = \sum_{j=1}^{n} w_j^{(k)}(x) y_j.$$

- if $w_j(x)$ is not smooth, then $w_j^{(k)}(x)$ will have some discontinuities.
- To obtain smooth estimate of $\hat{f}^{(k)}(x)$, we need $w_j(x)$ to have continuous derivatives up to order k. This rules out many of the standard kernel weighting functions.

Derivative estimation

For an asymptotically unbiased estimator of $f'(x)$, we require

$$\sum_{j=1}^{n} w_j^{(1)}(x) = 0$$

and $$\sum_{j=1}^{n} w_j^{(1)}(x)(x - x_j) = 1.$$

- Local polynomials of degree $p \geq 1$ will satisfy these constraints.
- So will cubic splines (of any flavour)
- But not kernel smooths.

Derivative estimation

For an asymptotically unbiased estimator of $f''(x)$, we require

$$\sum_{j=1}^{n} w_j^{(2)}(x) = 0$$

$$\sum_{j=1}^{n} w_j^{(2)}(x)(x - x_j) = 0$$

and $$\sum_{j=1}^{n} w_j^{(2)}(x)(x - x_j)^2 = 2.$$

- Local polynomials of degree $p \geq 2$ will satisfy these constraints.
- So will cubic splines (of any flavour)
- But not kernel or locally linear smoothers.

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3. Derivative estimation
4. **Multidimensional smoothers**
5. Penalized regression splines

Multidimensional kernel smoothing

If $m \geq 2$ predictors, need to fit surface rather than line.

Multidimensional kernel smoothing

$$\hat{f}(\mathbf{z}) = \sum_{j=1}^{n} w_j(\mathbf{z}) y_j \quad \text{where} \quad w_j(\mathbf{z}) = \frac{K_m(\mathbf{z} - \mathbf{x}_j)}{\sum_{j=1}^{n} K_m(\mathbf{z} - \mathbf{x}_j)}.$$

$\mathbf{z}$ and $\mathbf{x}_j$ are m-dimensional vectors and $K_m(\mathbf{u})$ is an m-dimensional function.

Product kernel: $K_m(\mathbf{u}) = \prod_{i=1}^{m} \frac{1}{h_i} K(u_i/h_i)$ where $K(u)$ is univariate kernel and h_i is smoothing parameter in ith dimension.

Multidimensional distance: $K_m(\mathbf{u}) = \frac{1}{h} K(\|u\|/h)$ where $\|u\|$ is distance metric (e.g. Euclidean distance). Only one smoothing parameter, h, used.

Multidimensional kernel smoothing

- If multidimensional distance used, it is usually necessary to standardise each predictor by dividing by its standard deviation or some other measure of spread.
- If $m = 1$, both methods give the standard univariate results.

Local polynomial surfaces

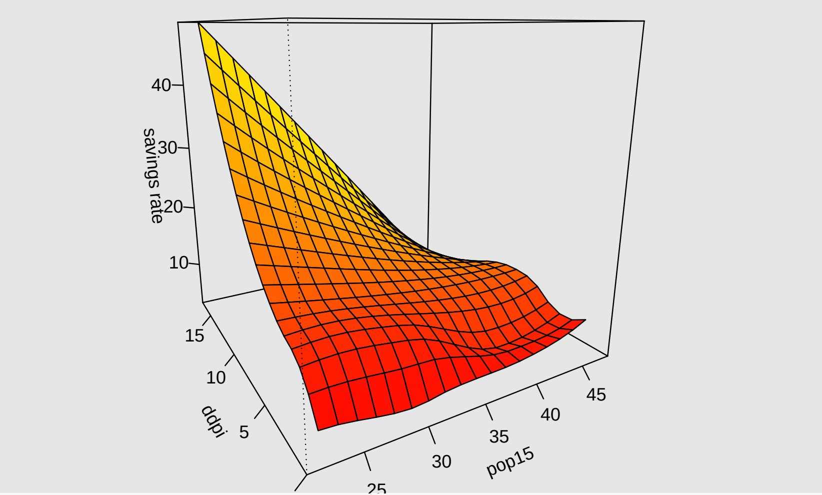
Locally weighted lines generalise easily to higher dimensions.

- Instead of computing local lines, compute a local plane.
- If predictors are w and v, local plane is computed using multiple regression on w and v.
- Local quadratic surfaces computed using multiple regression on w, v, wv, w^2 and v^2.

```
fit <- loess(y ~ x + z, span)
```

Bivariate smoothing

```
lomod <- loess(sr ~ pop15 + ddpi, data=savings)
```



Bivariate splines

Smoothing splines can be generalized to thin-plate splines in two dimensions.

- Minimize

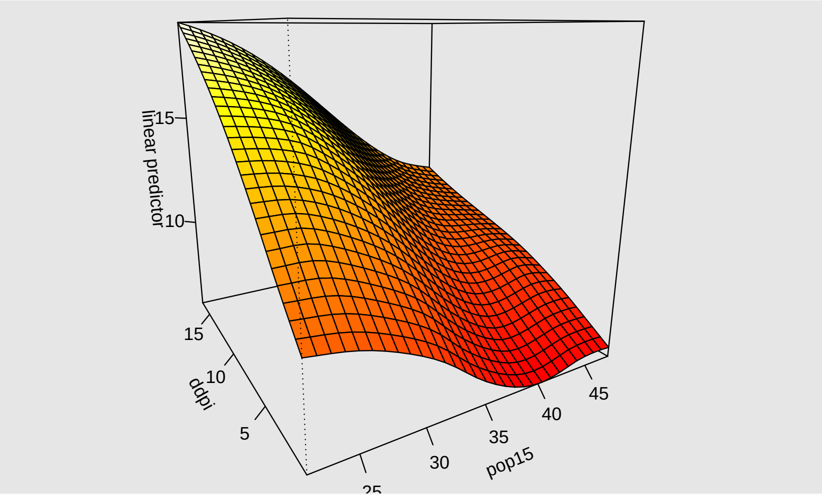
$$\sum_{i=1}^{n}(y_i - f(\boldsymbol{x}_i))^2 + \lambda \iint \left[\left(\frac{\partial^2 f}{\partial x_1^2} \right) + 2 \left(\frac{\partial^2 f}{\partial x_1 \partial x_2} \right) + \left(\frac{\partial^2 f}{\partial x_2^2} \right) \right] dx_1\, dx_2$$

- In R:

```
library(mgcv)
fit <- gam(y ~ s(x, z), data)
vis.gam(fit)
```

Bivariate smoothing

```r
library(mgcv)
smod <- gam(sr ~ s(pop15, ddpi), data=savings)
```



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Recall cubic regression splines

$$y = f(x) + \varepsilon$$

$$f(x) = \beta_0 + \sum_{k=1}^{K+3} \beta_k \phi_k(x)$$

where $\phi_1(x), \dots, \phi_{K+3}(x)$ is a family of spline functions.

Example:

- Knots: $\kappa_1 < \kappa_2 < \cdots < \kappa_K$.
- $\phi_1(x) = x$, $\phi_2(x) = x^2$, $\phi_3(x) = x^3$,
  $\phi_k(x) = (x - \kappa_{k-3})_+^3 \quad$ for $k = 4, \dots, K + 3$.
- Choice of knots can be difficult and arbitrary.

Penalized spline regression

Idea: Use many knots, but constrain their influence by

$$\sum_{k=4}^{K+3} \beta_k^2 < C.$$

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Let $D = \begin{bmatrix} \mathbf{0}_{4\times 4} & \mathbf{0}_{4\times K} \\ \mathbf{0}_{K\times 4} & \boldsymbol{I}_{K\times K} \end{bmatrix}.$

Then we want to minimize

$$\|\boldsymbol{y} - \boldsymbol{X}\beta\|^2 \qquad \text{subject to} \qquad \beta'\mathbf{D}\beta \leq C.$$

Penalized regression splines

A Lagrange multiplier argument shows that this is equivalent to minimizing

$$\|\boldsymbol{y} - \boldsymbol{X}\beta\|^2 + \lambda^2\beta'\boldsymbol{D}\beta$$

for some number $\lambda \geq 0$.

Solution: $\hat{\beta}_\lambda = (\boldsymbol{X}'\boldsymbol{X} + \lambda^2\boldsymbol{D})^{-1}\boldsymbol{X}'\boldsymbol{y}$.

- A type of ridge regression.

Mixed model representation

Split $\boldsymbol{X}$ matrix in two:

$$\boldsymbol{X} = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 \end{bmatrix} \text{ and } \boldsymbol{Z} = \begin{bmatrix} (x_1-\kappa_1)_+^3 & \dots & (x_1-\kappa_K)_+^3 \\ \vdots & \ddots & \vdots \\ (x_n-\kappa_1)_+^3 & \dots & (x_n-\kappa_K)_+^3 \end{bmatrix}$$

and let $\boldsymbol{\beta} = [\beta_0, \beta_1, \beta_2, \beta_3]'$ and $\boldsymbol{u} = [u_1, \dots, u_K]'$.

Then we want to minimize

$$\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta} - \boldsymbol{Z}\boldsymbol{u}\|^2 + \lambda^2\|\boldsymbol{u}\|^2$$

This is equivalent to estimating the mixed model

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{Z}\boldsymbol{u} + \boldsymbol{\varepsilon}$$

where $u_i \sim \mathrm{N}(0, \sigma_u^2)$ and $\varepsilon_j \sim \mathrm{N}(0, \sigma_\varepsilon^2)$.

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Let $\lambda = \sigma_\varepsilon / \sigma_u$ and $\boldsymbol{V} = \mathrm{Cov}(\boldsymbol{y}) = \sigma_u^2 \boldsymbol{Z}\boldsymbol{Z}' + \sigma_\varepsilon^2 \boldsymbol{I}$.

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Formulas

Let $\lambda = \sigma_\varepsilon / \sigma_u$ and $\boldsymbol{V} = \text{Cov}(\boldsymbol{y}) = \sigma_u^2 \boldsymbol{Z}\boldsymbol{Z}' + \sigma_\varepsilon^2 \boldsymbol{I}$. Then

$$\hat{\beta} = (\boldsymbol{X}\boldsymbol{V}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{V}^{-1}\boldsymbol{y}.$$

$$\hat{\boldsymbol{u}} = \sigma_u^2 \boldsymbol{Z}'\boldsymbol{V}^{-1}(\boldsymbol{y} - \boldsymbol{X}\hat{\beta}).$$

$\boldsymbol{V}$ estimated using profile log-likelihood methods.

Choice of knots

- Provided the set of knots is relatively dense with respect to the $\{x_j\}$, the result hardly changes.
- Choose enough knots to model structure, but not too many knots to cause computational problems.
- Ruppert, Wand and Carroll recommend:
  - $\max(n/4, 35)$ knots where n = number of unique observations.
  - $\kappa_j = \left(\frac{j+1}{K+1}\right)$th sample quantile of the unique $\{x_j\}$.
- `mgcv` package uses penalized regression splines by default.