ETC5410: Nonparametric smoothing methods

July 2008

MONASH University

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Outline

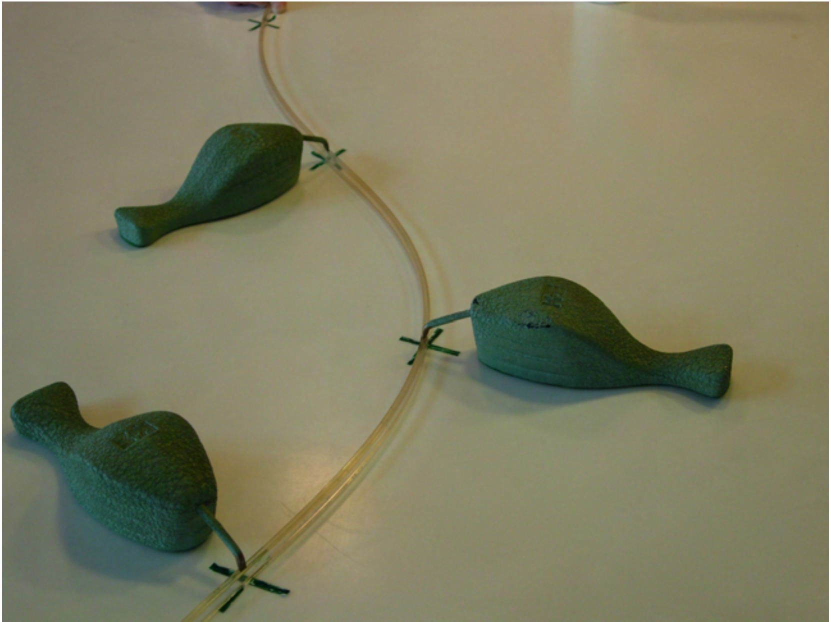
1. Density estimation
2. Kernel regression
3. **Splines**
4. Additive models
5. Functional data analysis

ETC5410: Nonparametric smoothing methods

3. Splines

Outline

Interpolating splines



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- Parameters constrained so that $f(x)$ is continuous.
- Further constraints imposed to give continuous derivatives.

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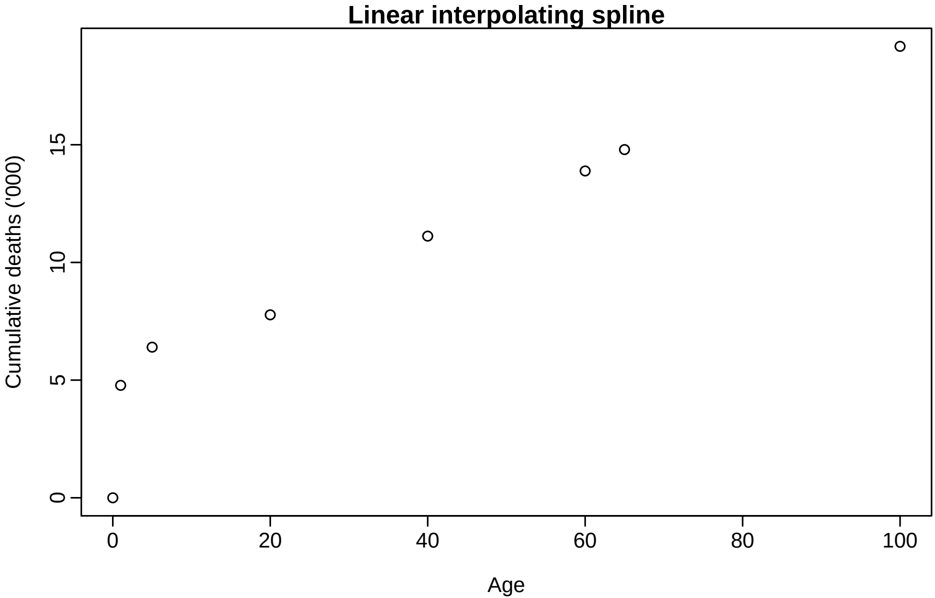

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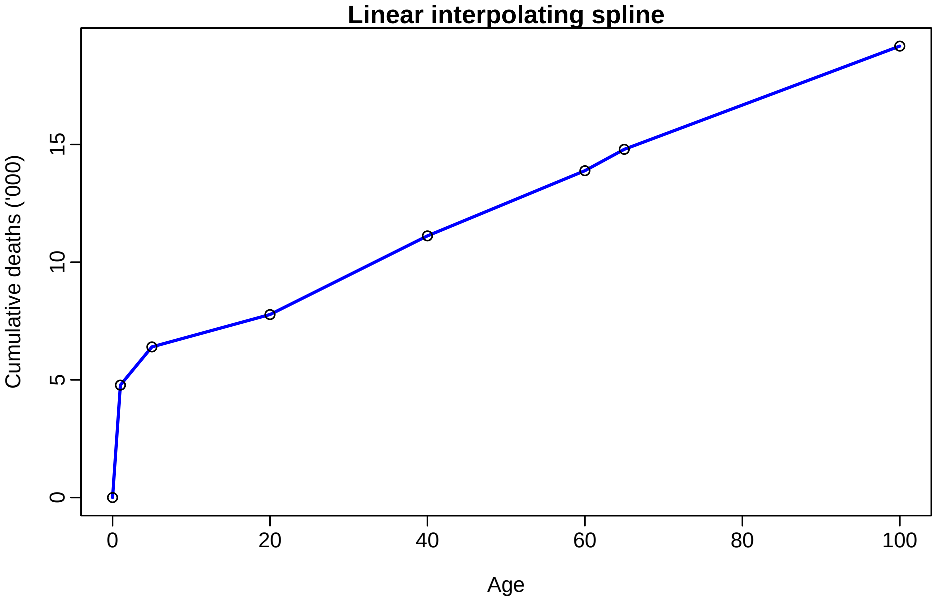

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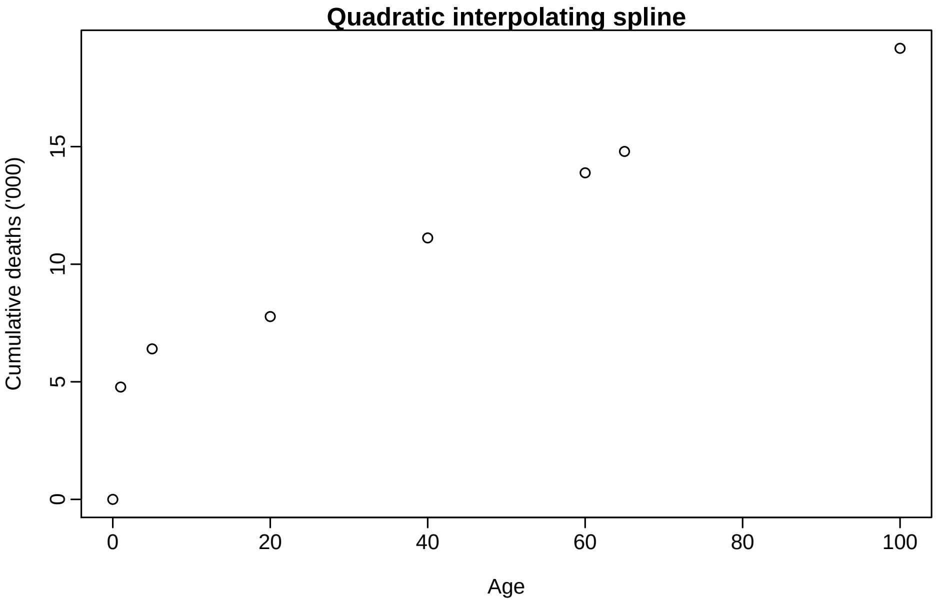

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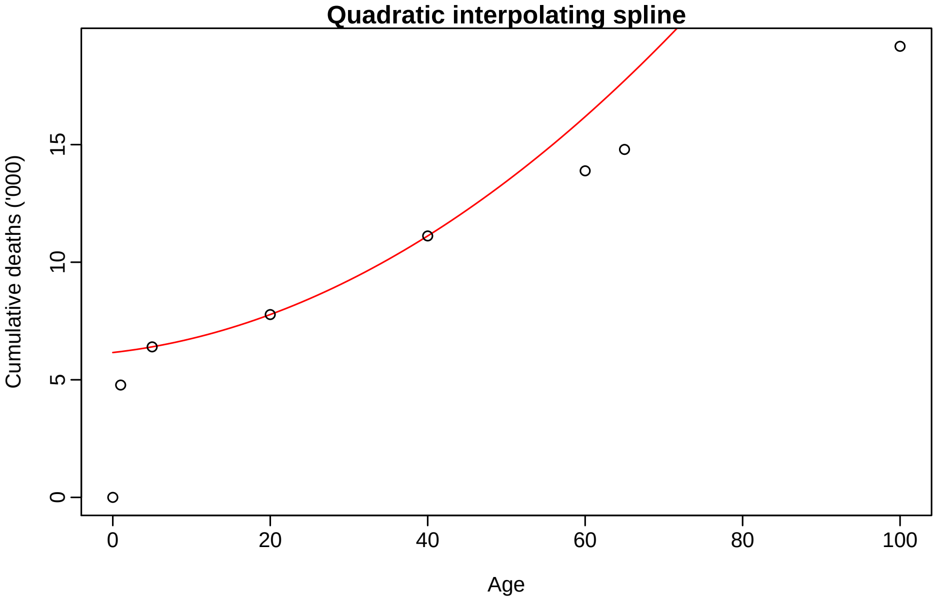

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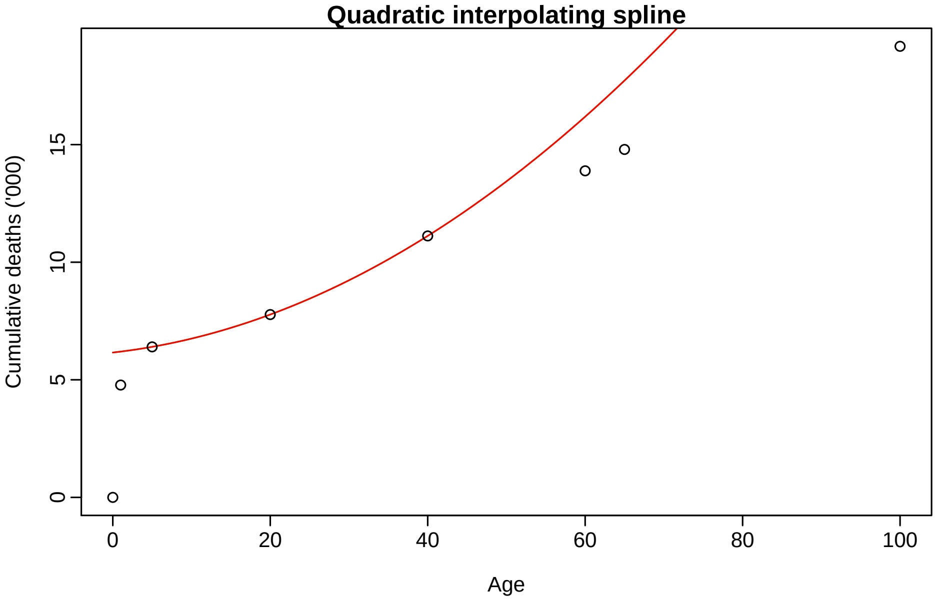

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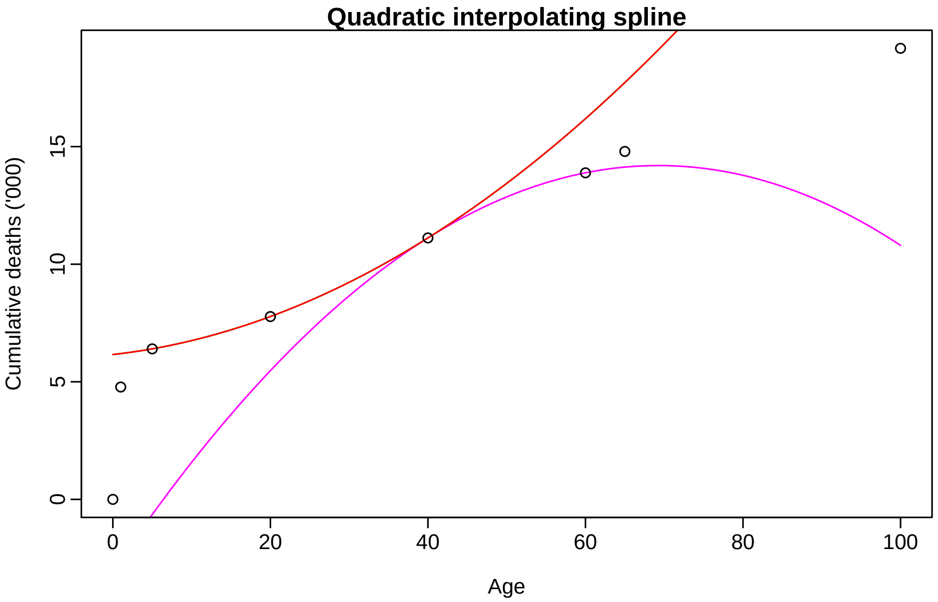

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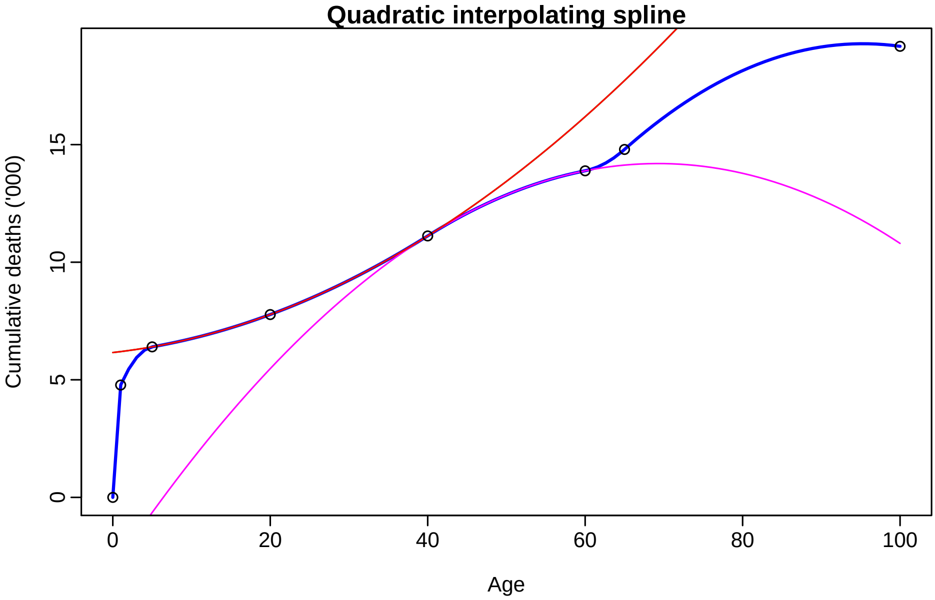

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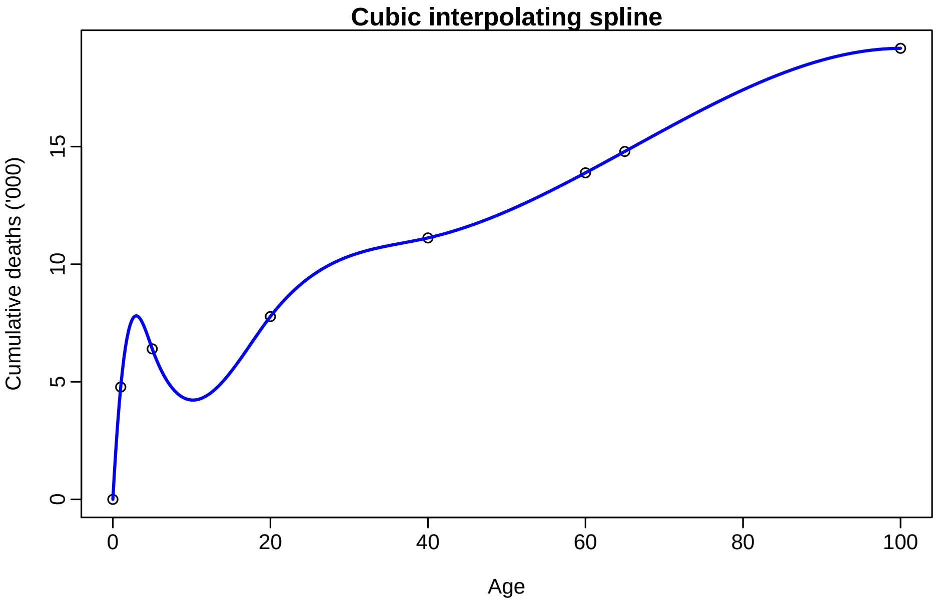

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Implementation in R

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Monotonic interpolation

‘Hyman filter’ ensures spline is monotonic by constraining derivatives while (possibly) sacrificing smoothness.

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Implementation in R

```
require(demography)
plot(x,y)
lines(cm.spline(x,y), col=4)
```

Reference: Smith, Hyndman and Wood (JPR, 2001)

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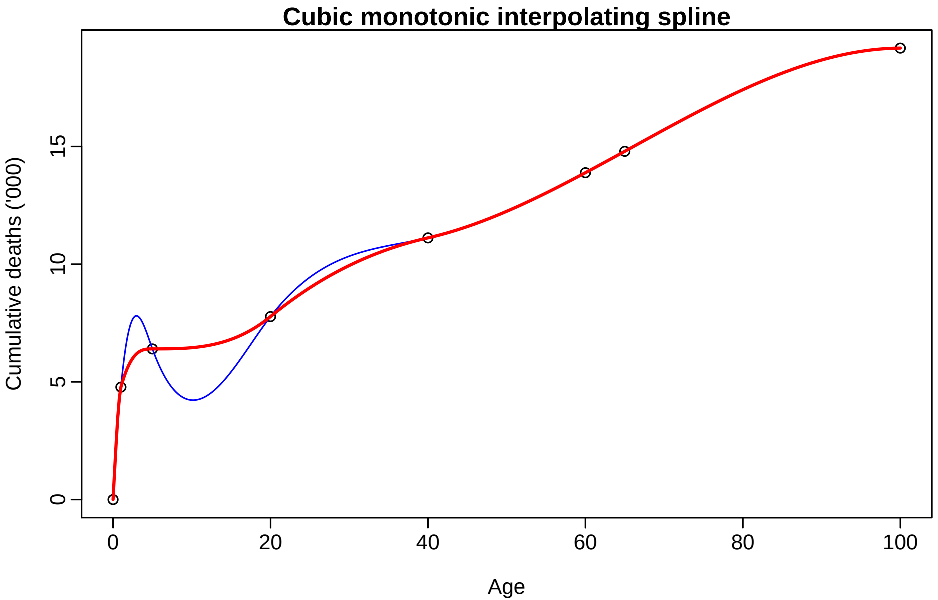

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Spline smoothing

The average squared prediction error is

$$\sum [y_j - r(x_j)]^2.$$

Reduces to zero if r interpolates the data.

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- λ denotes a smoothing parameter.
- First term measures closeness to the data.
- Second term penalizes curvature in the function.

Cubic smoothing splines

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- It consists of piecewise cubic polynomials, with the pieces separated by the x_j values.
- At the design points, x_j, $\hat{r}_\lambda(x)$ and its first two derivatives are continuous. The third derivative may be discontinuous.
- At the minimum and maximum x_j values, the second derivative of $\hat{r}_\lambda(x)$ is zero. Hence, the smoothing spline is linear beyond the extreme data points.

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- At $\lambda \to \infty$, the penalty term dominates $S_\lambda(r)$, forcing $r''(x) = 0$ for all x. So the solution is the least squares straight line.
- As $\lambda \to 0$, the penalty term becomes negligible and the solution tends to an interpolating function which is twice differentiable.

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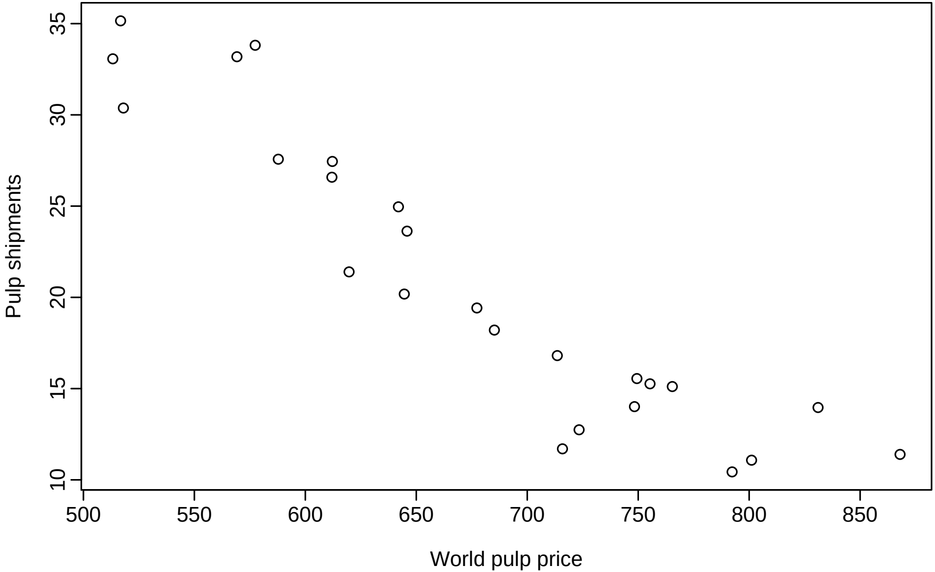

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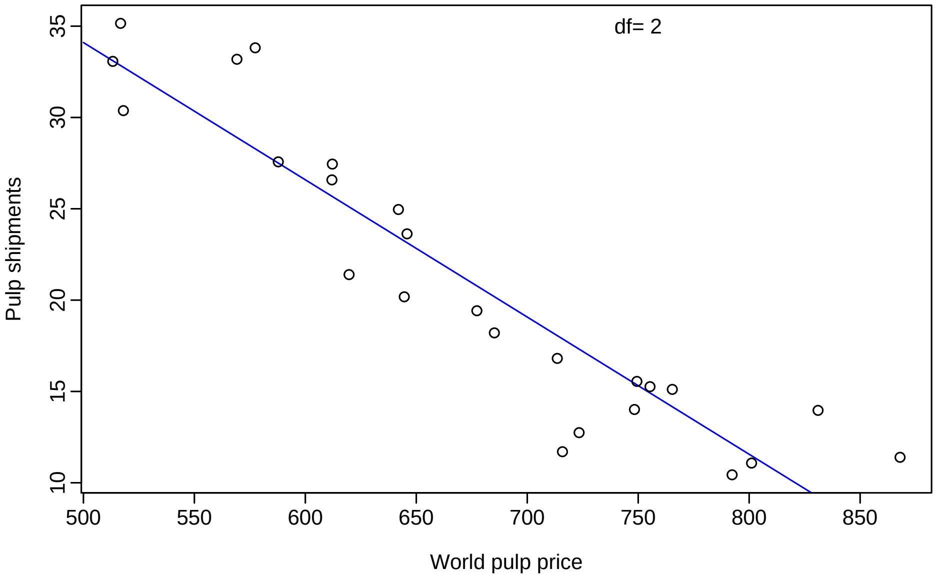

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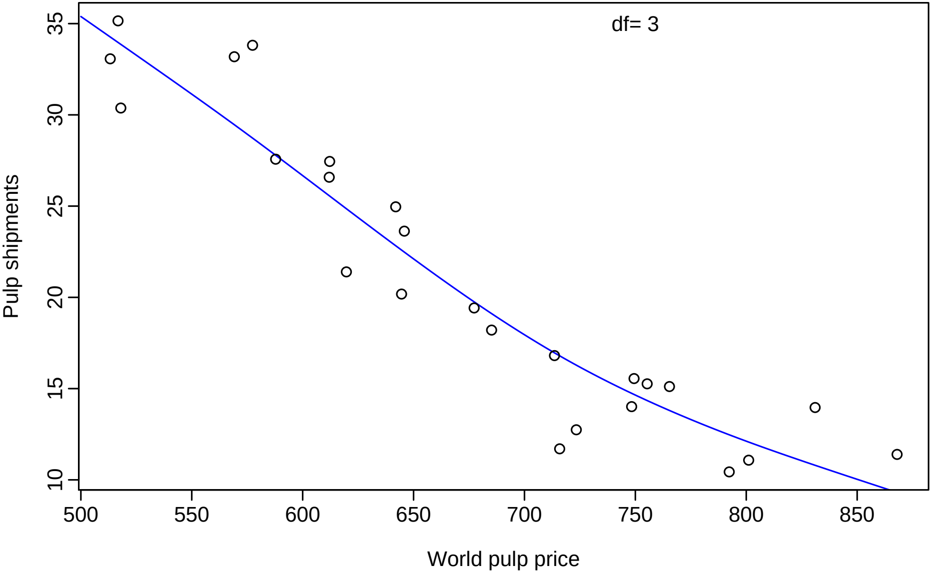

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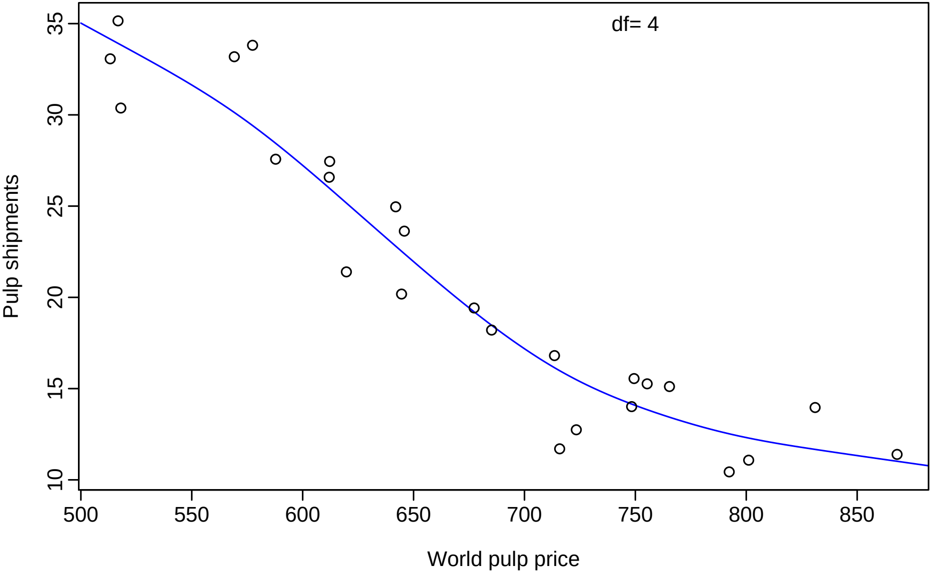

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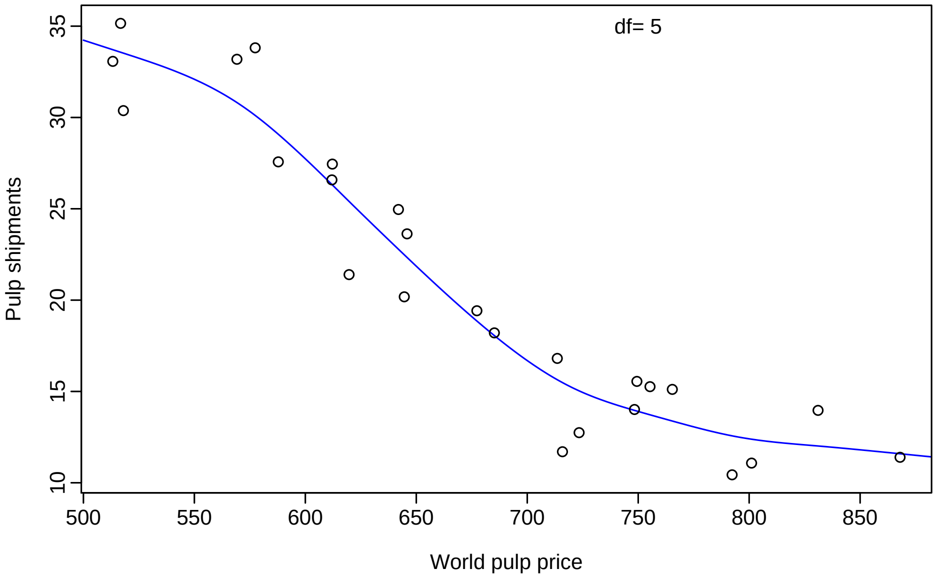

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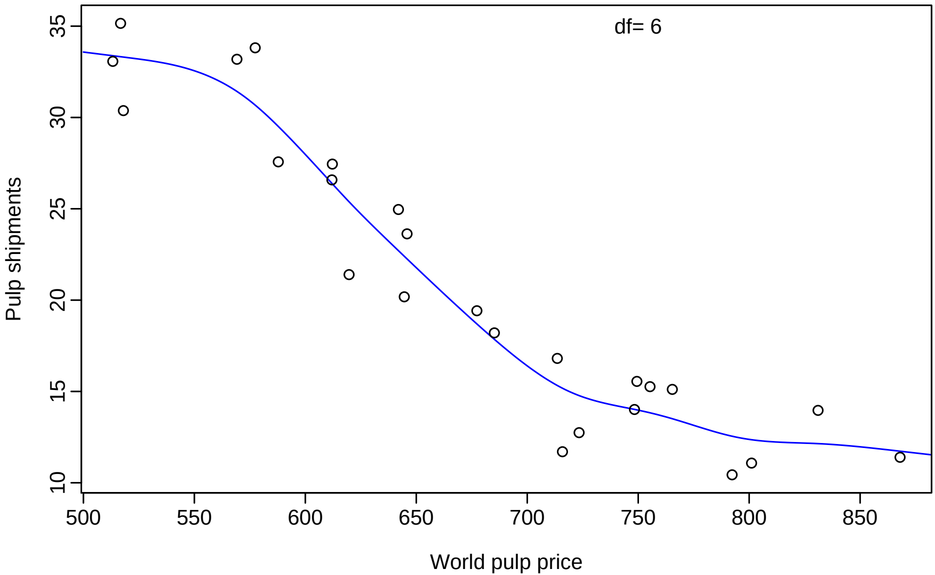

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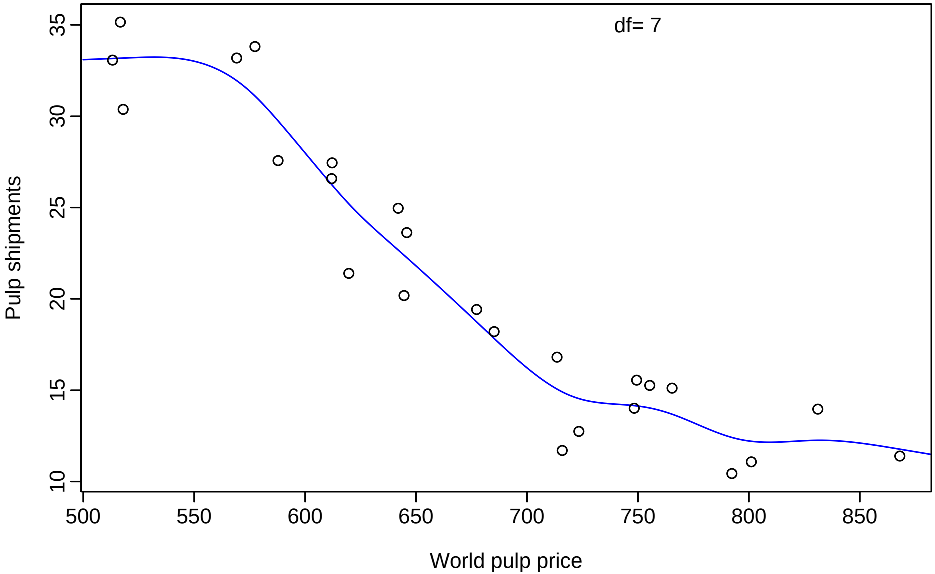

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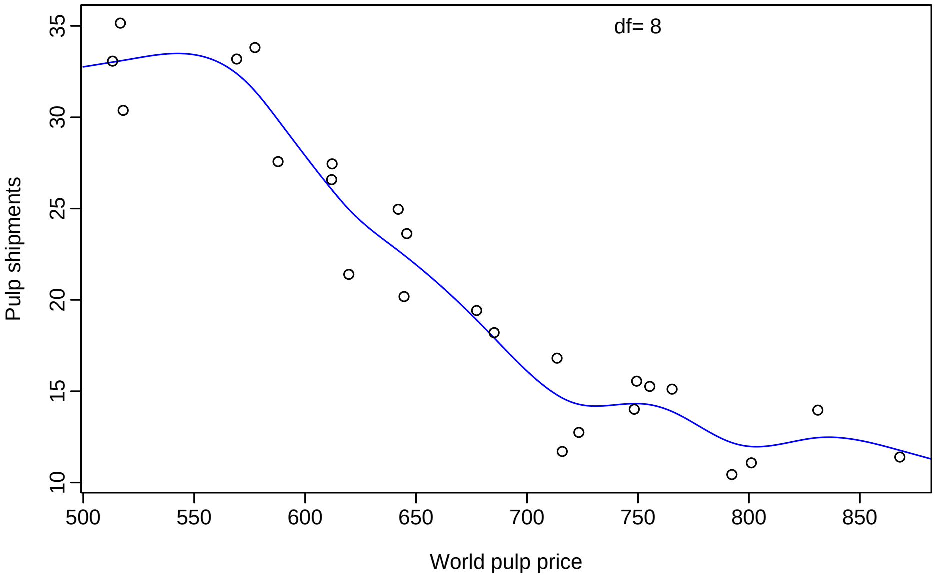

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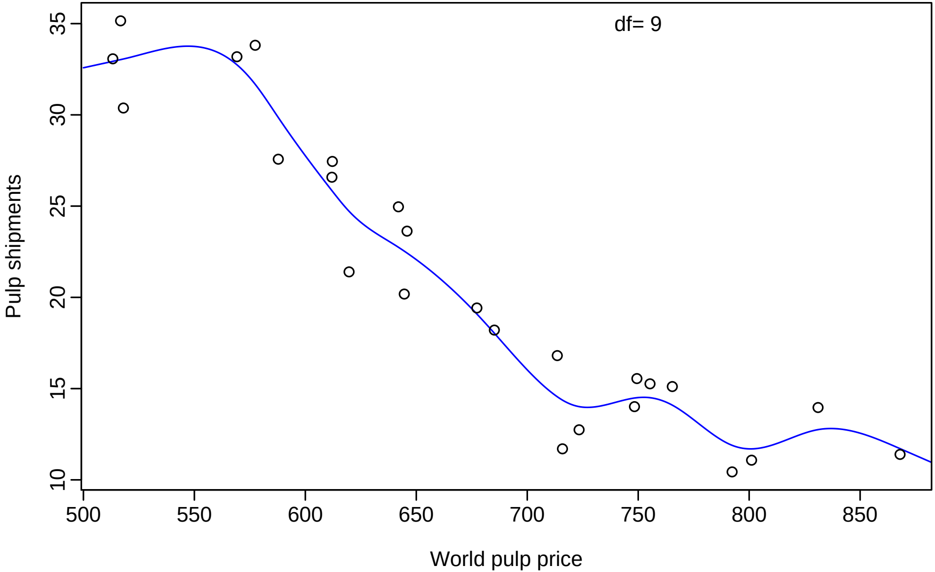

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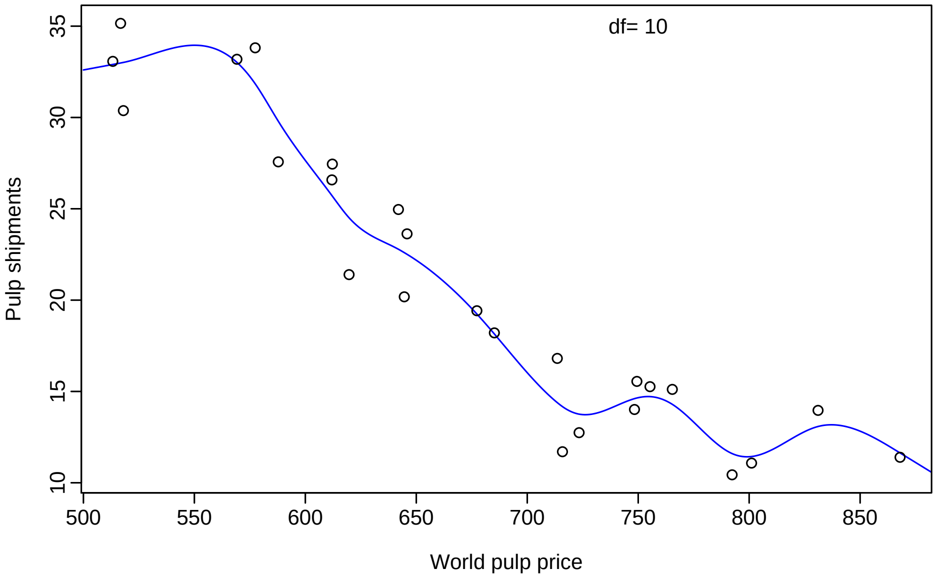

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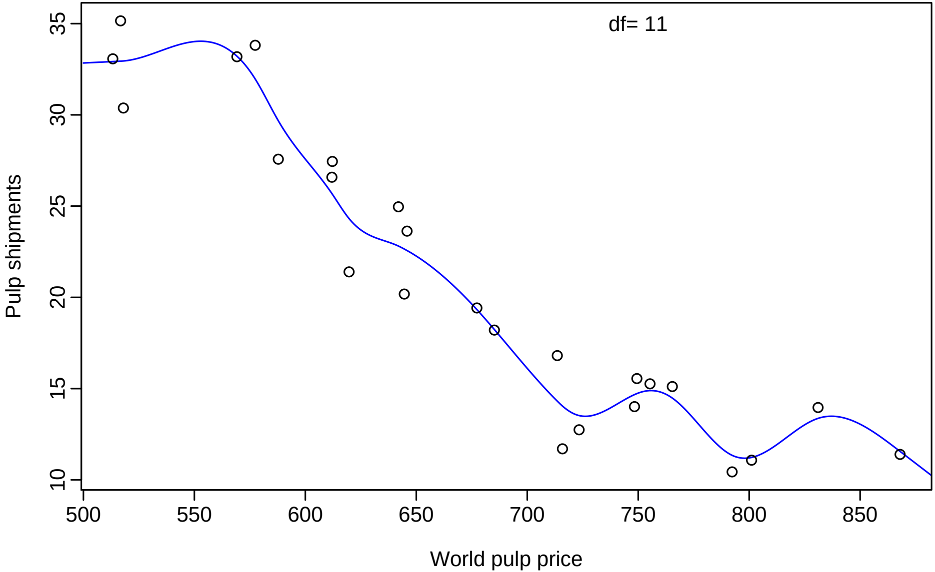

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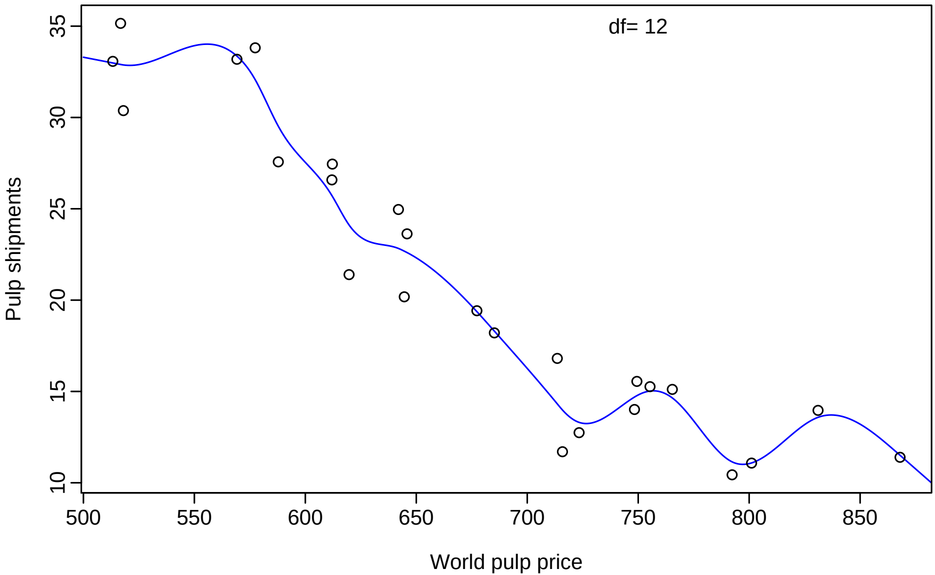

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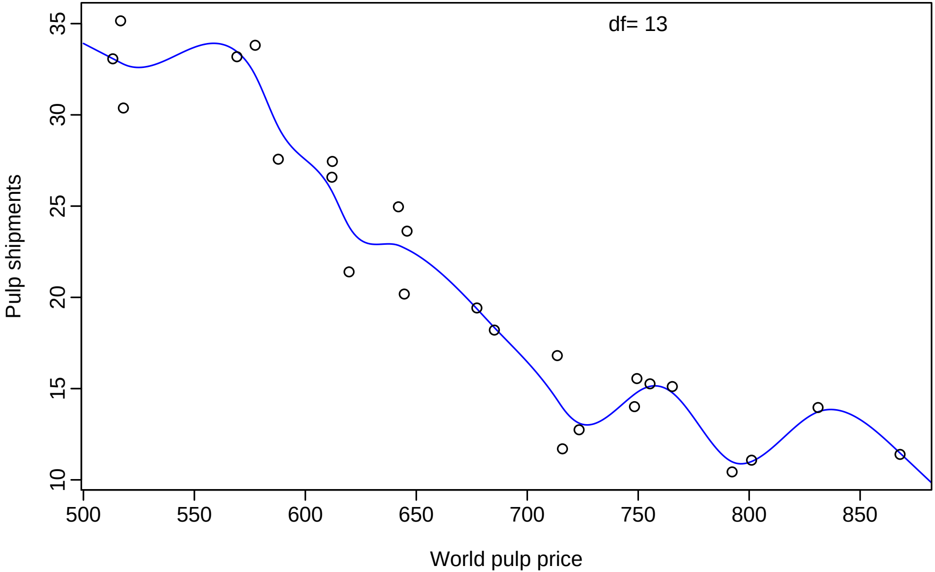

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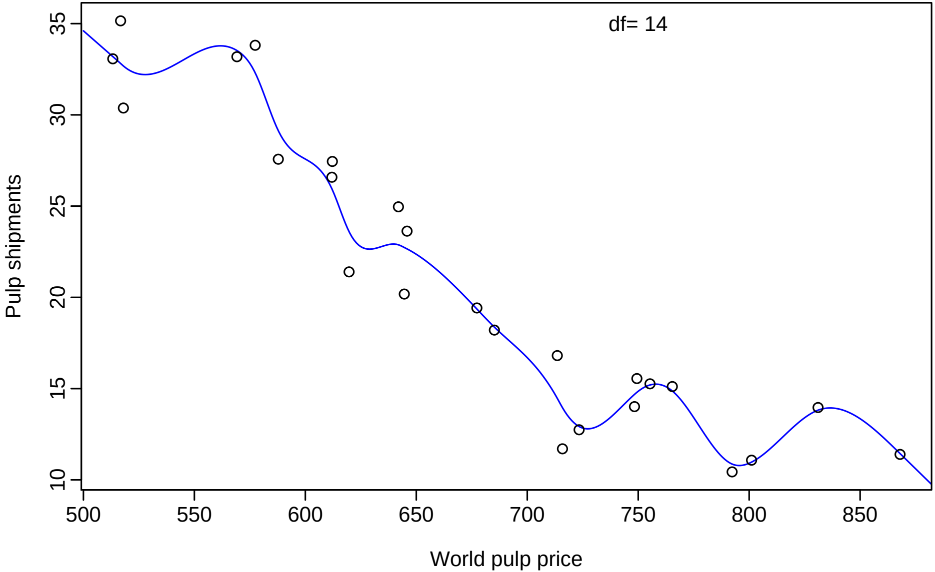

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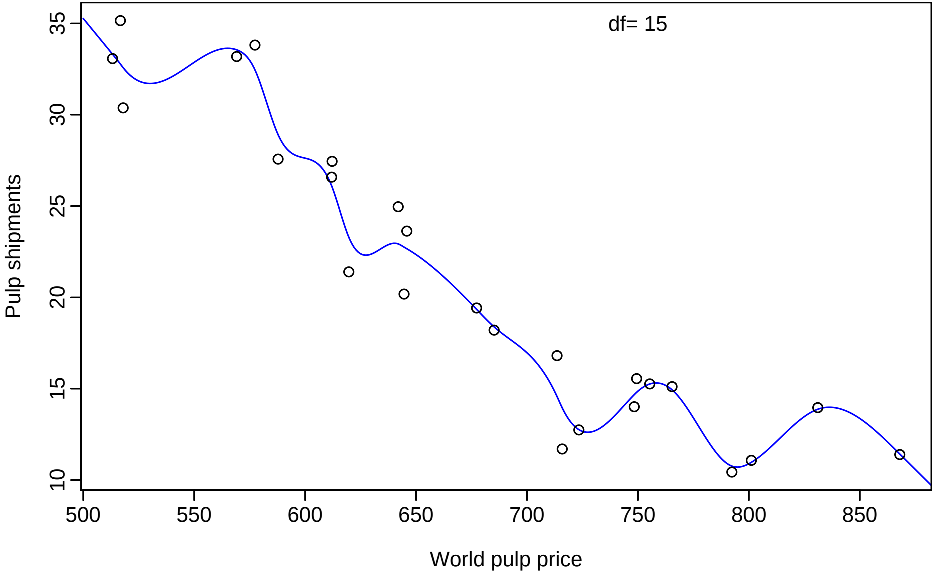

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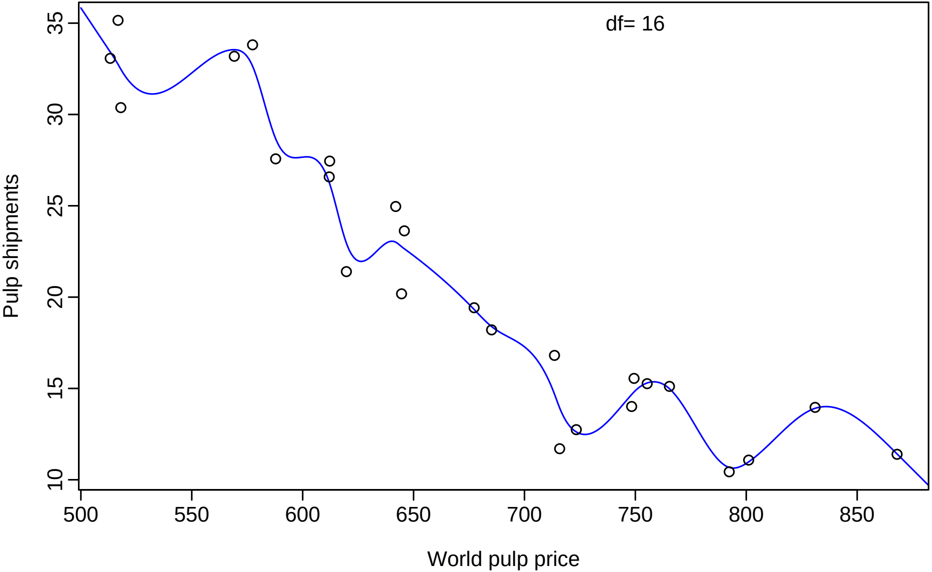

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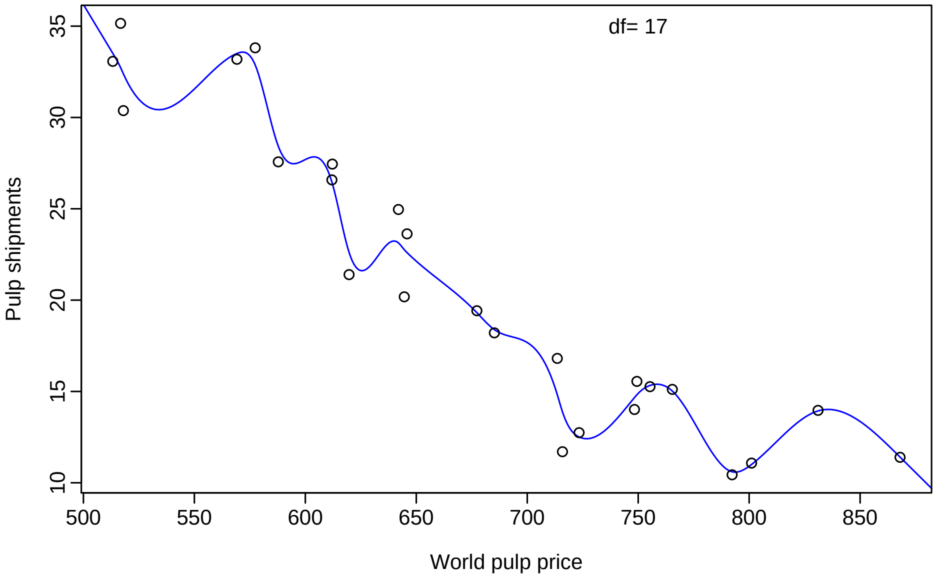

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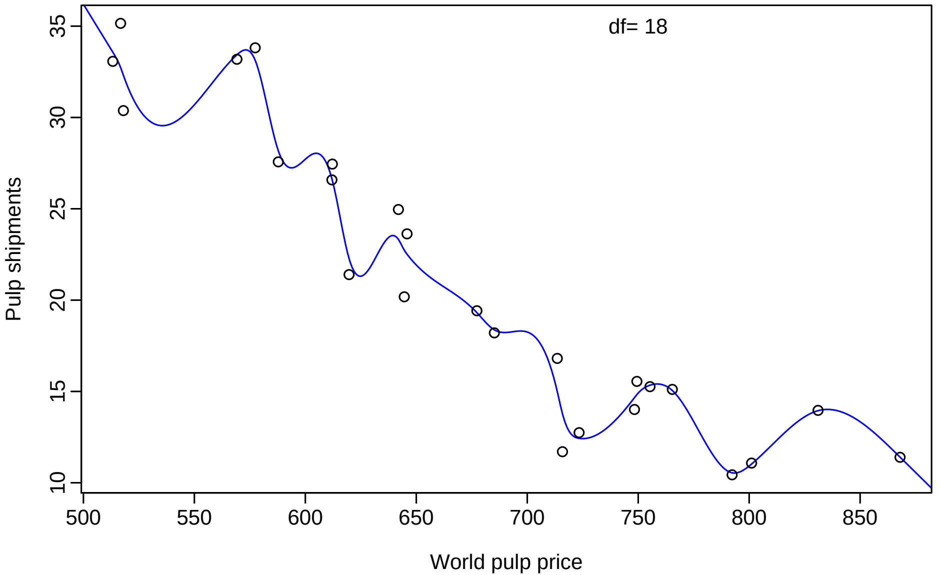

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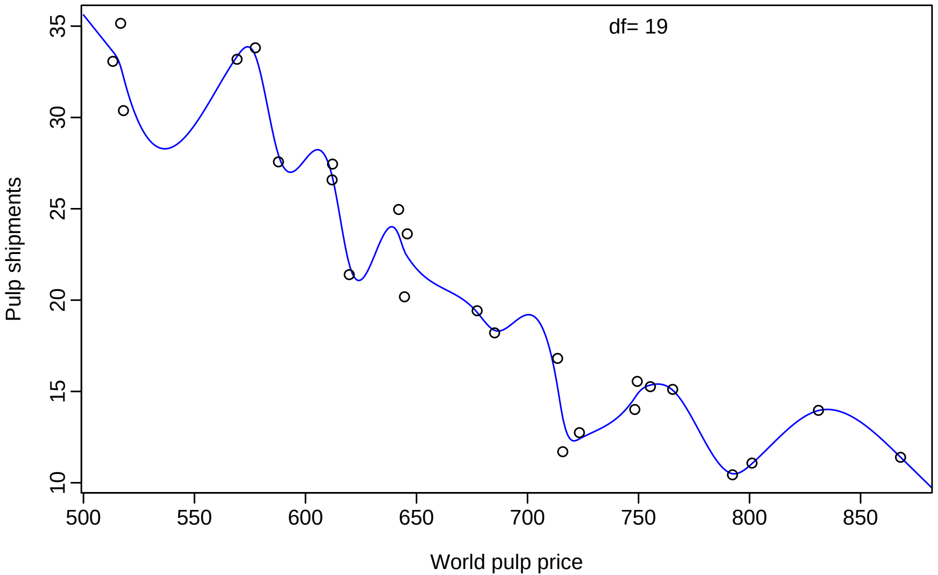

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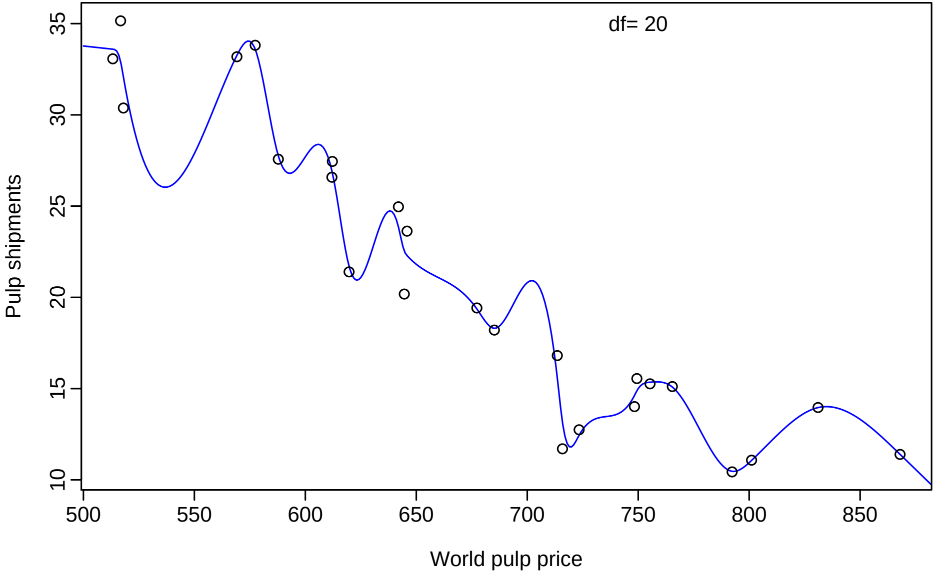

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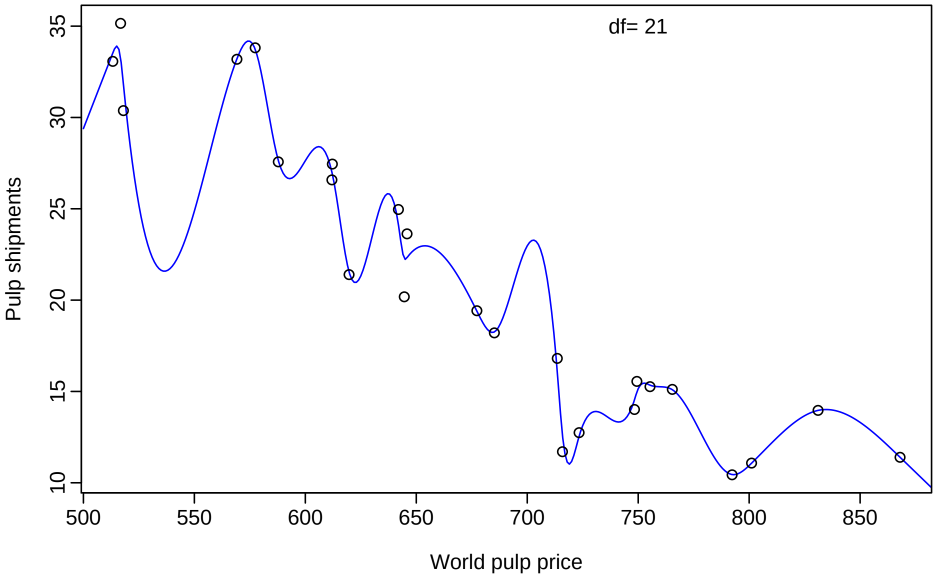

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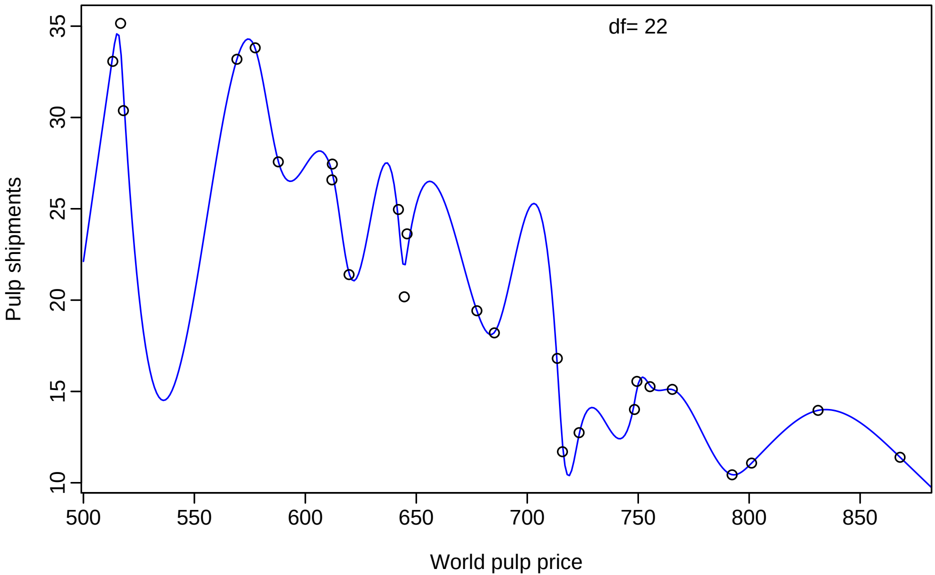

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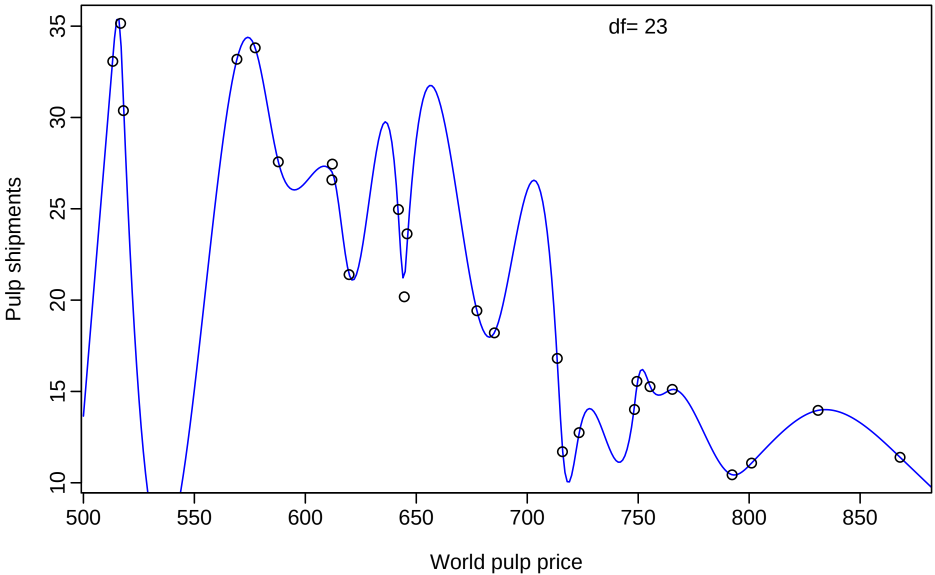

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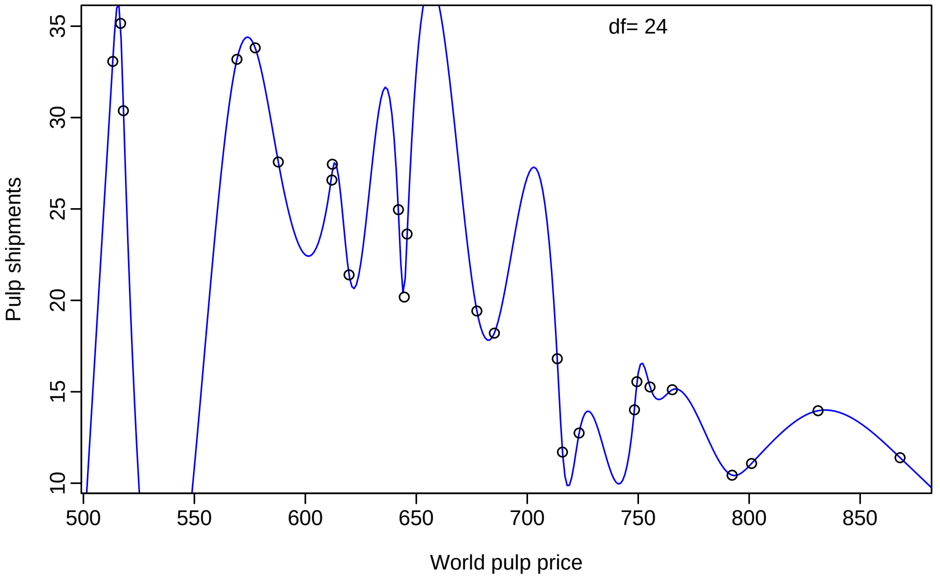

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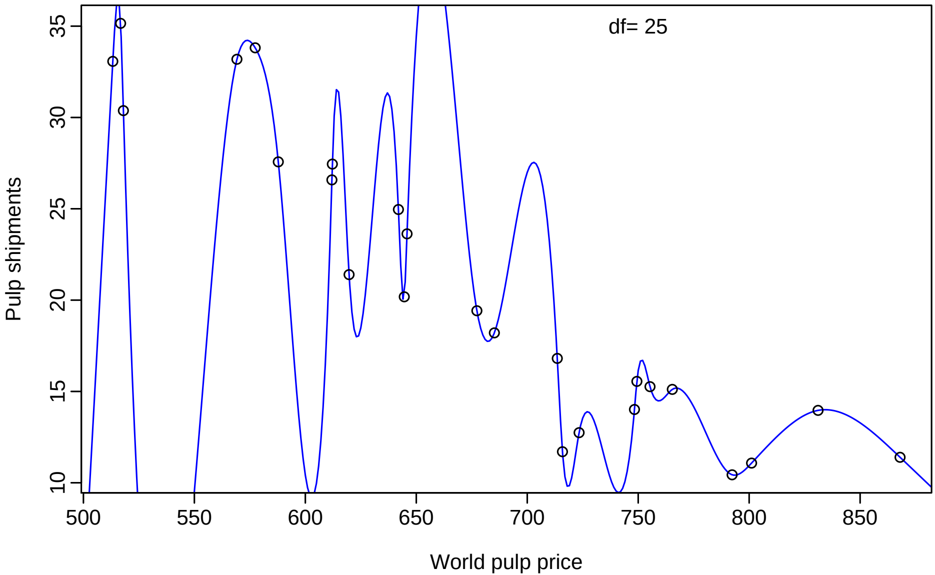

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Implementation in R

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- The value of λ is selected automatically using cross-validation.
- The argument `df` can be supplied and then λ is chosen to give approximately `df` degrees of freedom.

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- HP recommended $\lambda = 1600$ for quarterly data. There is no theoretical justification for this.
- Better to use proper bandwidth selection tools.

Cross-validation again

Recall: Find smoothing parameter which minimises

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

where $\hat{r}_j(x_j)$ uses all data *except* (x_j, y_j).

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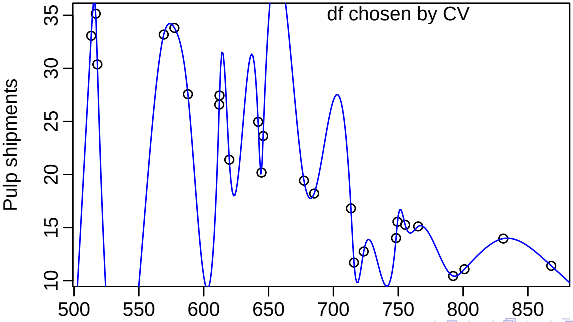

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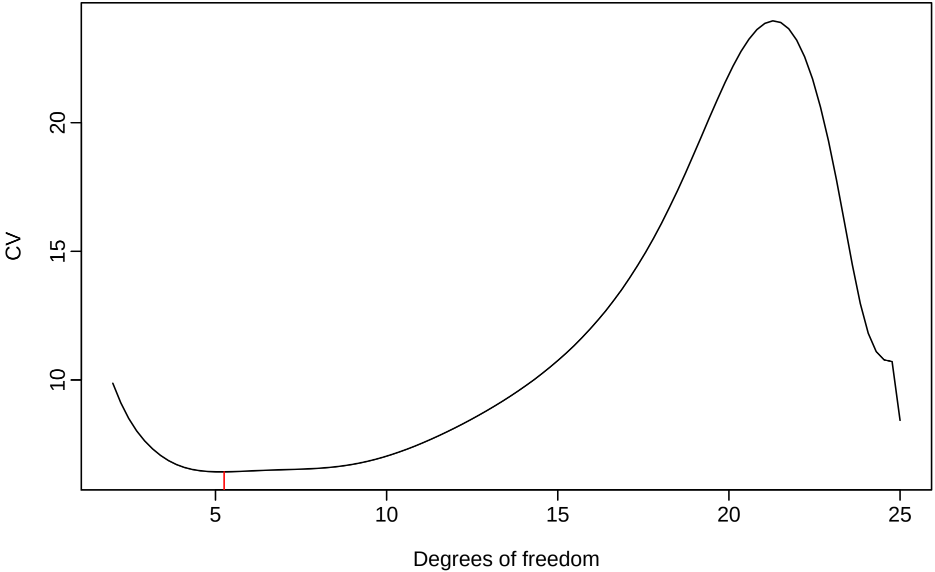

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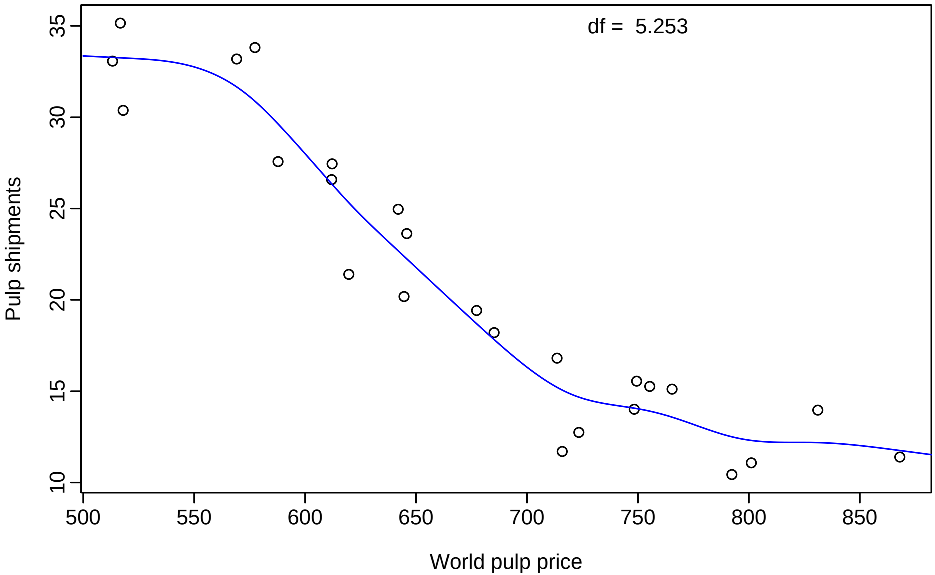

General cubic splines

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Let $h_1(x) = 1$, $h_2(x) = x$, $h_3(x) = x^2$, $h_4(x) = x^3$,
$h_j(x) = (x - \kappa_{j-4})_+^3$ for $j = 5, \dots, k + 4$.

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$\{h_1, \ldots, h_{k+4}\}$ form a basis for the set of cubic splines at these knots, called the **truncated power basis**.

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$$r(x) = \sum_{j=1}^{k+4} \beta_j h_j(x).$$

A cubic smoothing spline is obtained by setting $\kappa_j = x_j$, $j = 1, \ldots, n$.

Matrix form

Let $B_{ij} = h_j(x_i)$ be the basis matrix. Then for smoothing splines we need to minimize

$$(Y - B\boldsymbol{\beta})'(Y - B\boldsymbol{\beta}) + \lambda\boldsymbol{\beta}'\Omega\boldsymbol{\beta}$$

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This gives $\hat{\beta} = (B'B + \lambda\Omega)^{-1}B'\mathbf{Y}.$

Inference

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Any cubic smoothing spline can be written as a linear smoother with smoothing matrix $\mathbf{S} = B(B'B + \lambda\Omega)^{-1}B'$.

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- $\text{df} = \text{trace}(\mathbf{S})$

Outline

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$$\hat{\beta} = (B'B)^{-1}B'\mathbf{Y}.$$

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Penalized spline regression

$$r(x) = \sum_{j=1}^{K} \beta_j h_j(x).$$

Idea: retain all the knots but constrain their influence by

$$\sum \beta_j^2 < C.$$

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Let

$$D = \begin{bmatrix} \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times K} \\ \mathbf{0}_{K\times 2} & \mathbf{I}_{K\times K} \end{bmatrix}.$$

Then we want to

minimize $\|\mathbf{y} - \mathbf{B}\beta\|^2$ subject to $\beta'\mathbf{D}\beta \leq C$.

Penalized regression splines

A Lagrange multiplier argument shows that this is equivalent to minimizing

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

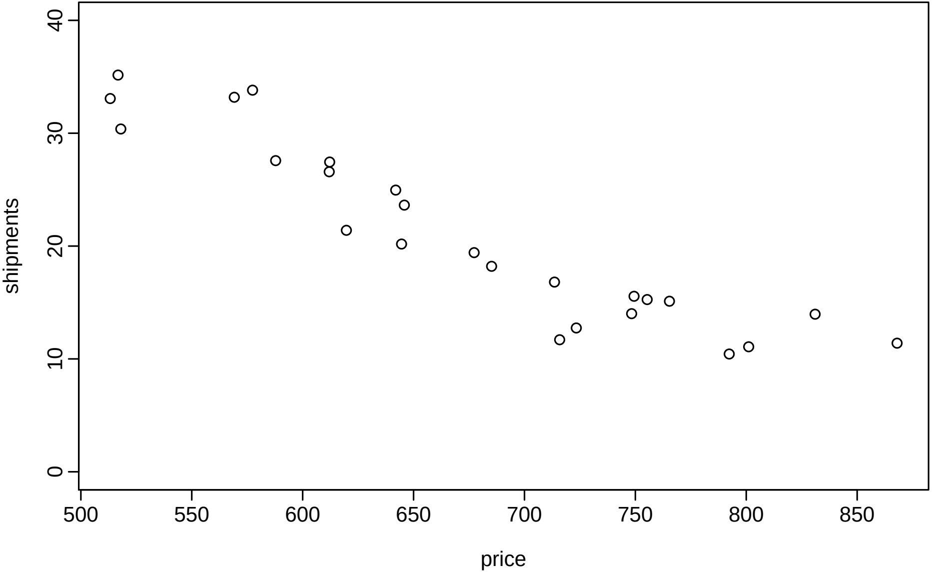
for some number $\lambda \geq 0$.

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

Fitted values: $\hat{\mathbf{y}} = \mathbf{X}(\mathbf{X}'\mathbf{X} + \lambda^2 \mathbf{D})^{-1} \mathbf{X}'\mathbf{y}$.

- A type of ridge regression.

Penalized regression splines



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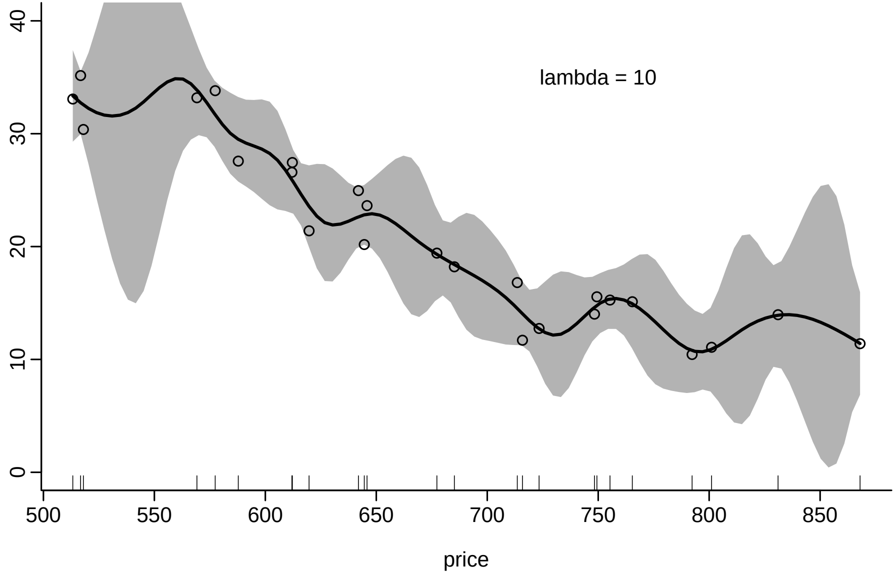

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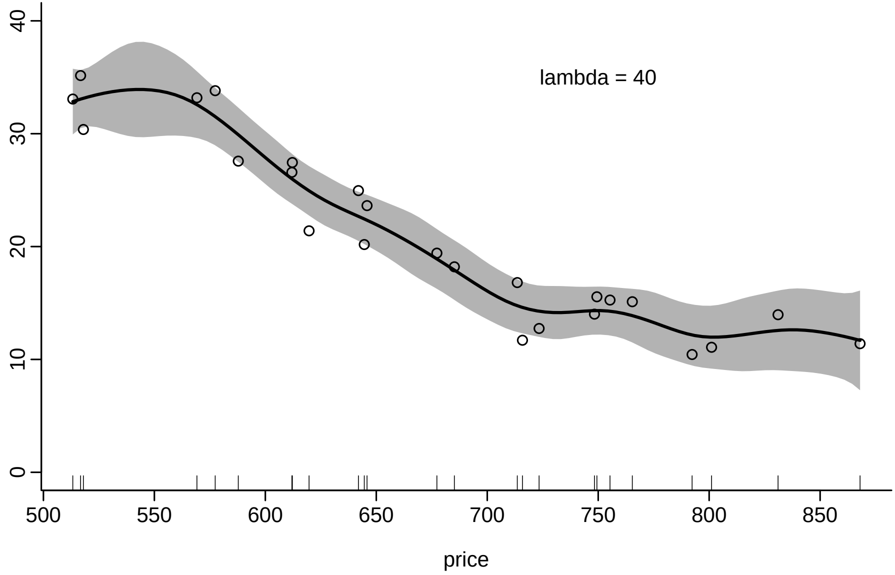

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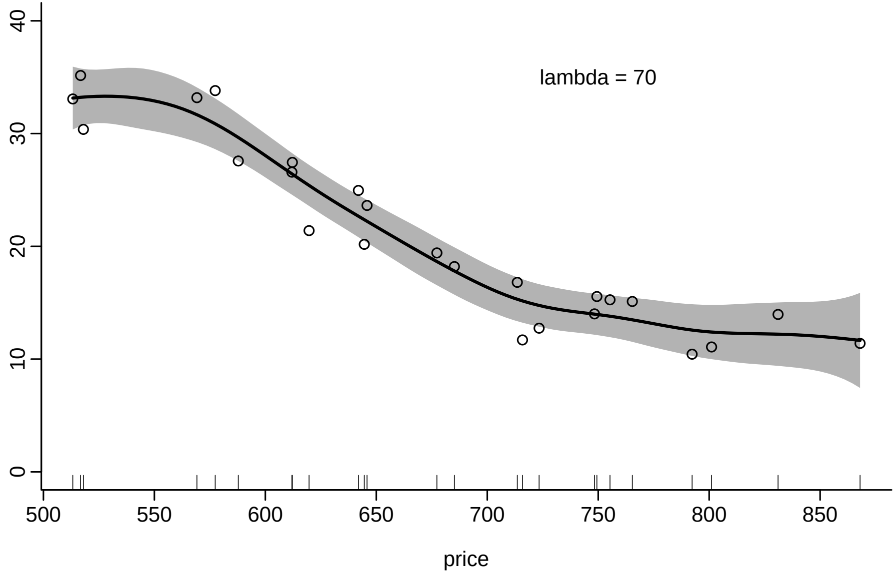

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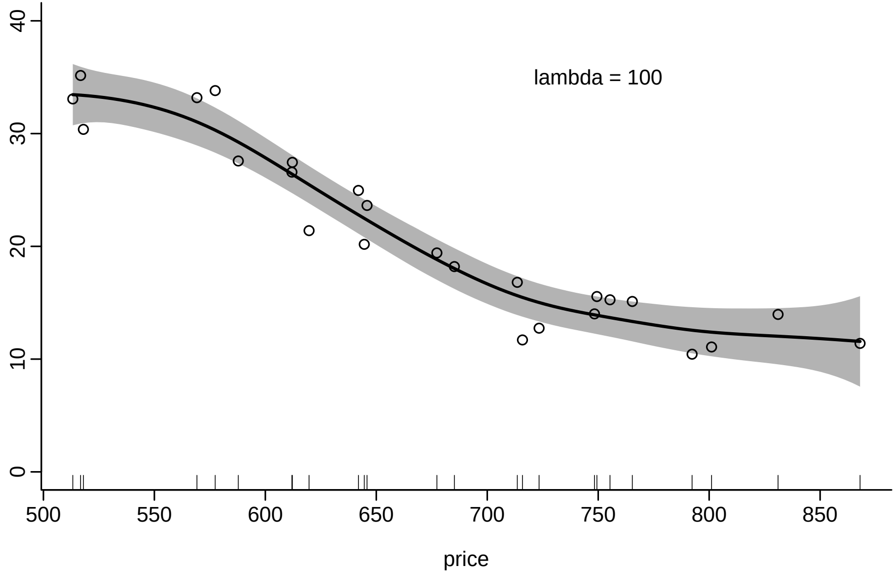

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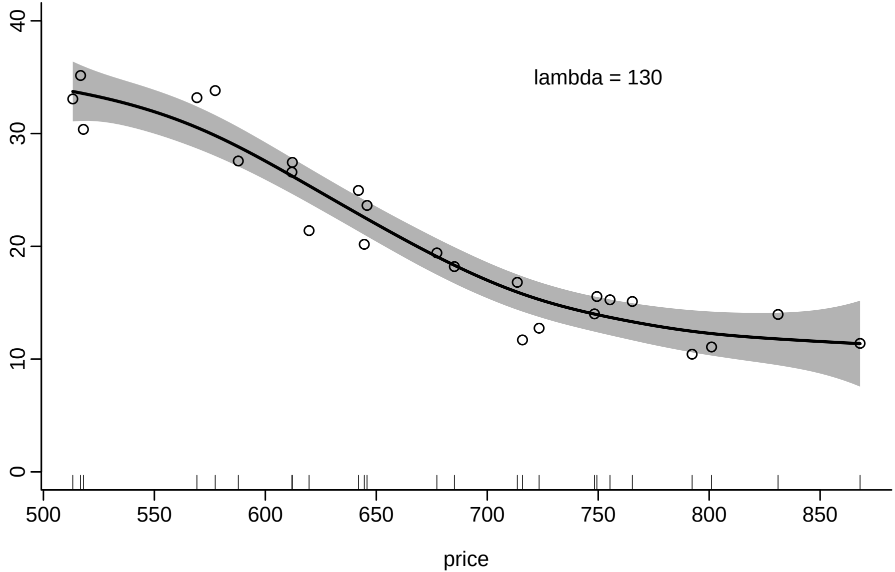

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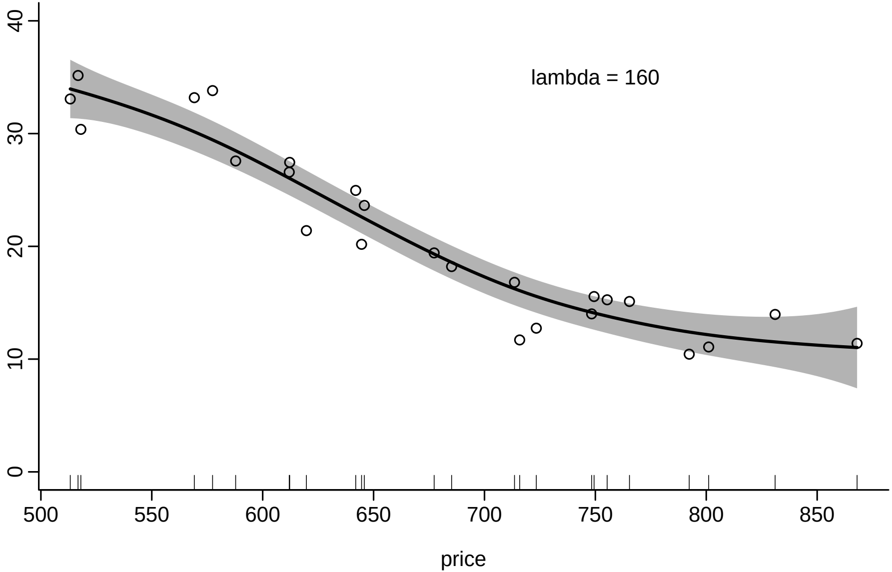

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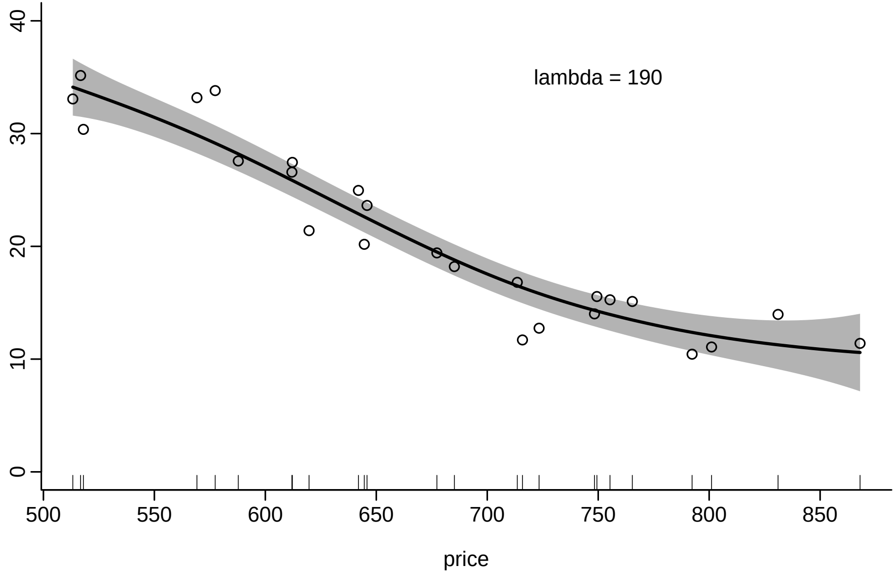

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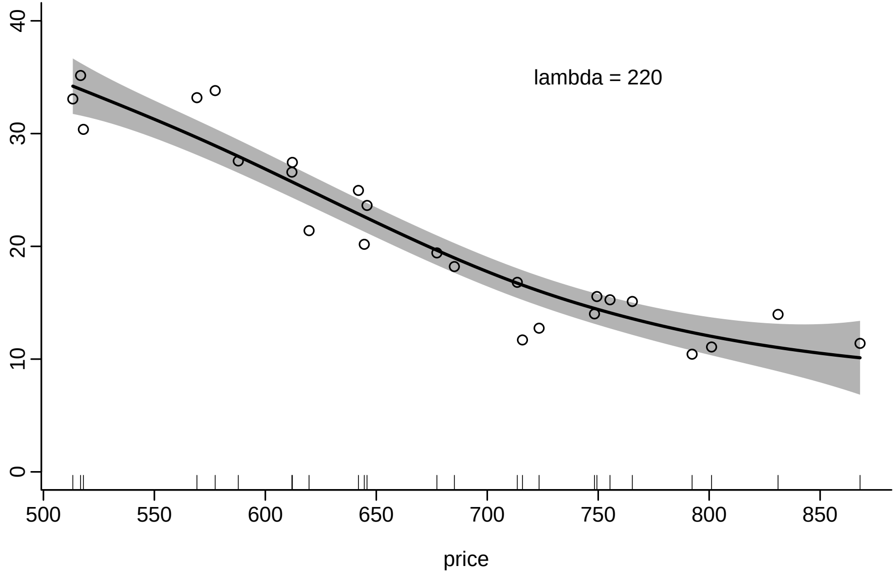

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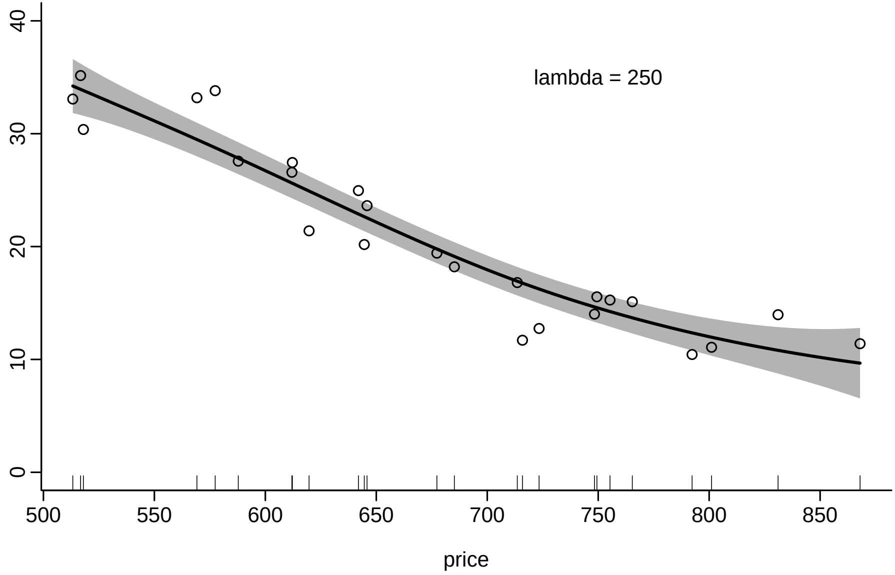

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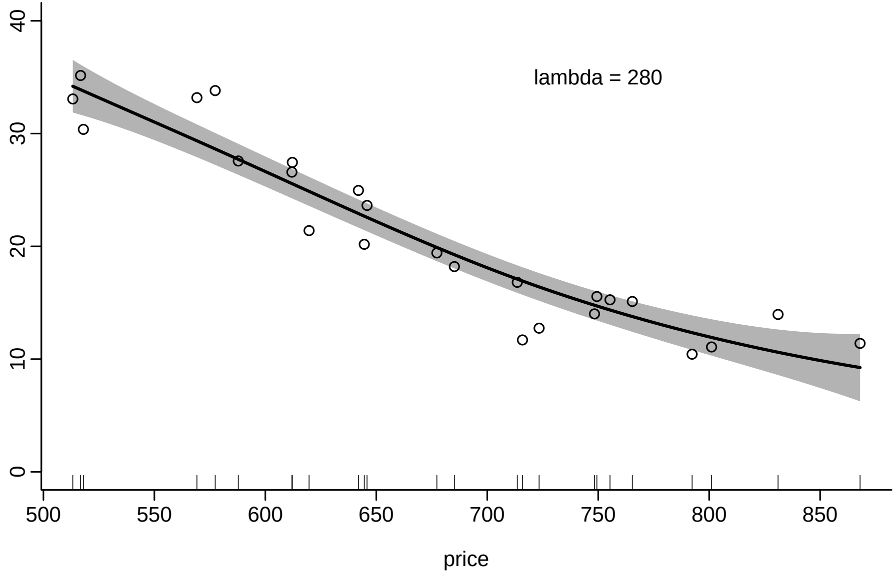

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Implementation in R

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For lots of examples and an introduction to the theory:

http://www.uow.edu.au/~mwand/SPmanu.pdf

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Spline bases

Truncated power basis of degree p

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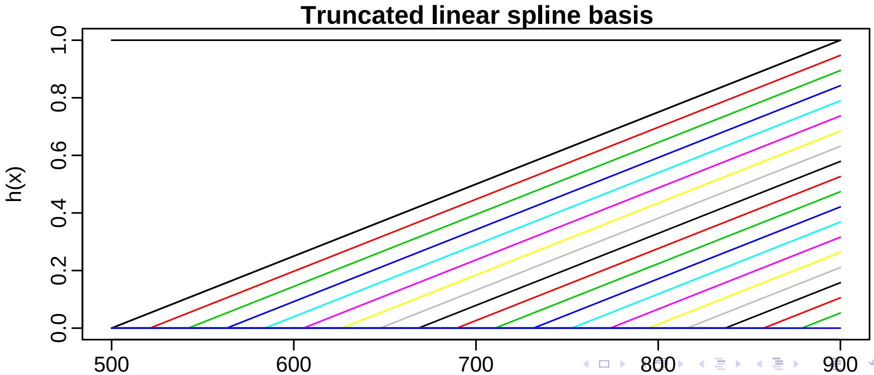

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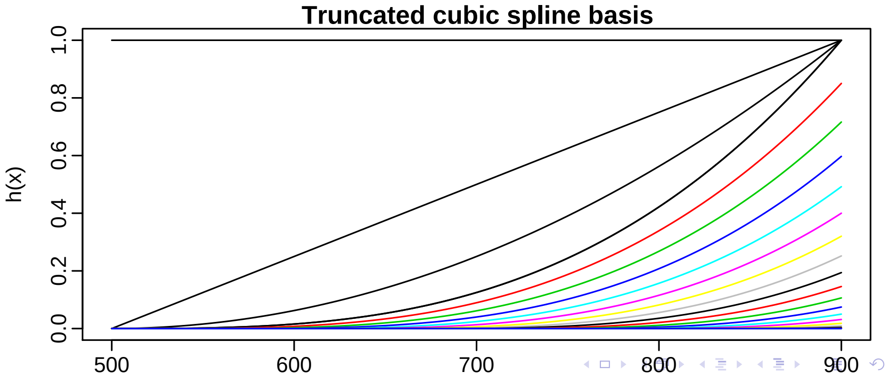

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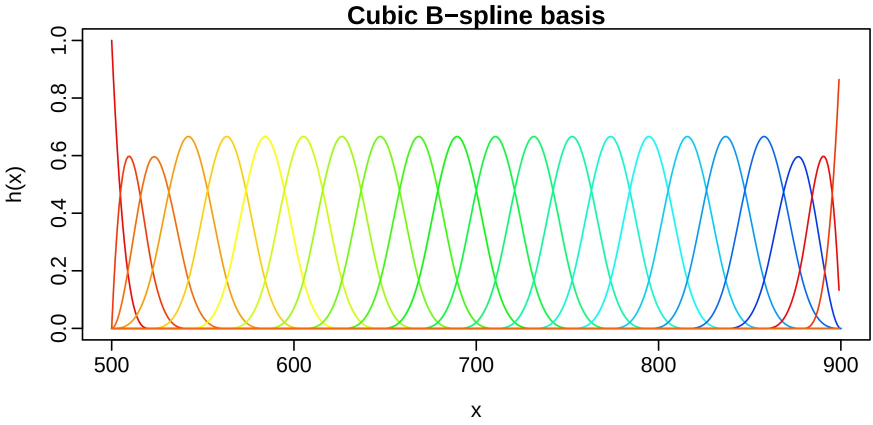

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