Statistical Learning

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Regression and Smoothing Splines

Introduction

- Let us consider the regression model with a single input X:

$$Y = f(X) + \epsilon,$$

where $f(X) = \mathrm{E}(Y|X)$ is an unknown conditional mean function.

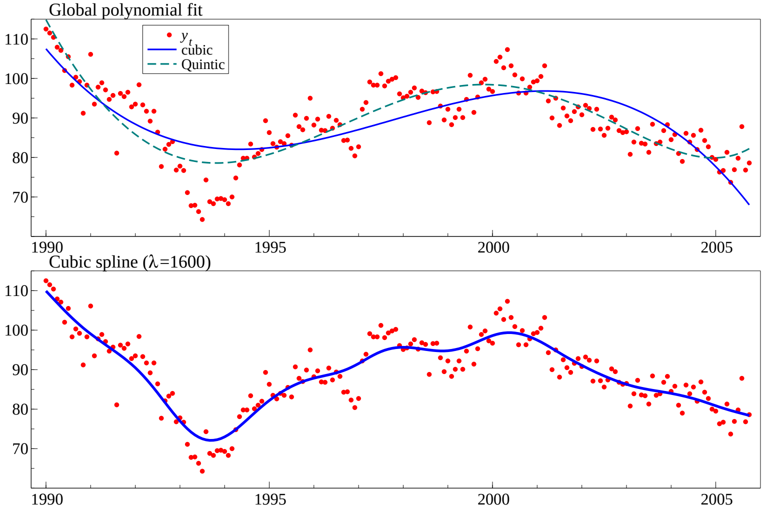
- $f(X)$ is possibly nonlinear and non-additive.
- In the linear regression framework we considered the *global polynomial* approximation

$$f(X) = \beta_0 + \beta_1 X + \beta_2 X^2 \cdots + \beta_p X^p.$$

- Here global means that the coefficients of the polynomial are constant across the sample span of X and it is not possible to control the influence of the individual observations on the fit.

- Global polynomials are amenable to mathematical treatment, but are not very flexible: they can provide bad local approximations and behave rather weirdly at the extremes of the sample.
- This point is illustrated by the first panel of figure 1, which plots the original series, representing the industrial production index for the Italian *Automotive* sector, and the estimate of the trend arising from fitting cubic and quintic polynomials of time.
- In particular, it can be seen that a high order is needed to provide a reasonable fit (the cubic fit being very poor).

Industrial Production Index, Manufacture and Assembly of Motor Vehicles, seasonally adjusted, Italy, January 1990 - October 2005.



Regression splines

- We will discuss the approximation

$$f(X) = \sum_{m=1}^{M} \beta_m h_m(X),$$

  which retains linearity in the regression coefficients and uses a suitable set of transformation or functions of X, $h_m(X)$, called basis.

- In the case of polynomial splines the idea is to add to a global polynomial of order p polynomial pieces at given points, called *knots*, so that the sections are joined together, ensuring that certain continuity properties are fulfilled.
- Given the set of points $\xi_1 < \ldots < \xi_k < \ldots \xi_K$, a polynomial spline function of degree p with K knots $\{\xi_k, k = 1, \ldots, K\}$ is a polynomial of degree p in each of the $k + 1$ intervals $[\xi_k, \xi_{k+1})$, with $p - 1$ continuous derivatives, whereas the p-th derivative has jumps at the knots.

The spline can be represented as follows:

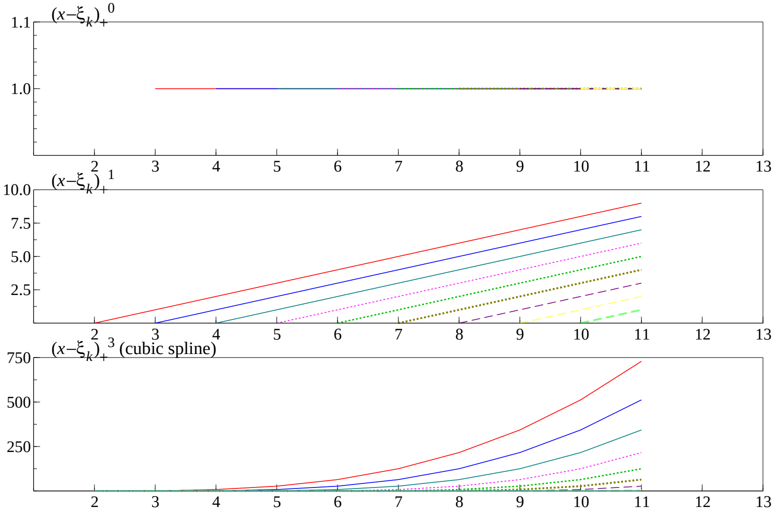
$$f(X) = \beta_0 + \beta_1 X + \cdots + \beta_p X^p + \sum_{k=1}^{K} \beta_{p+k} (X - \xi_k)_+^p, \tag{1}$$

where the set of functions

$$(X - \xi_k)_+^p = \begin{cases} (X - \xi_k)^p, & X - \xi_k \geq 0, \\ 0, & X - \xi_k < 0 \end{cases}$$

defines what is usually called the *truncated power basis* of degree p.

Figure: Truncated power basis for polynomial spline models.



- According to (1) the spline is a linear combination of polynomial pieces; at each knot a new polynomial piece, starting off at zero, is added so that the derivatives at that point are continuous up to the order $p-1$.
- The truncated power representation has the advantage of representing the spline as a multivariate regression model.
- The piecewise nature of the spline "reflects the occurrence of structural change" (Poirer, 1973). The knot ξ_i is the location of a structural break. The change is "smooth", since certain continuity conditions are ensured.
- The coefficients β_k determines the size of the break.

Cubic splines and natural boundary conditions

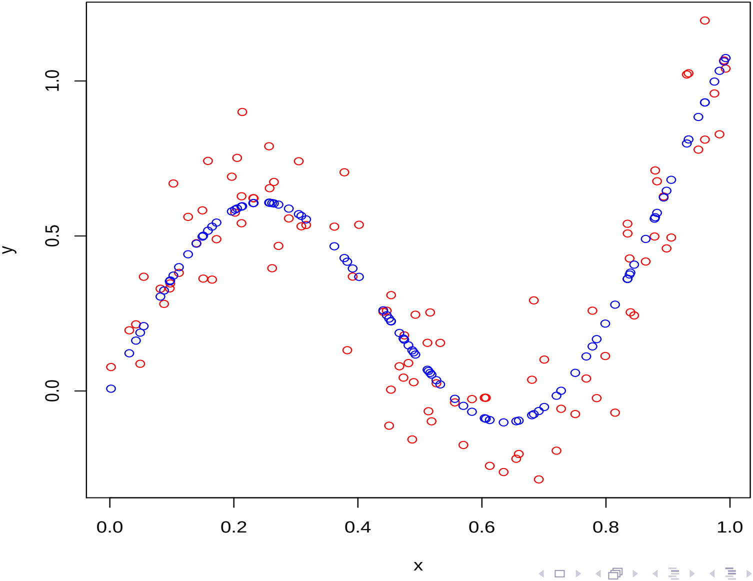
The cubic spline model arises when $p = 3$:

$$f(X) = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \beta_4 (X - \xi_1)_+^3 + \cdots + \beta_{K+3} (X - \xi_K)_+^3.$$

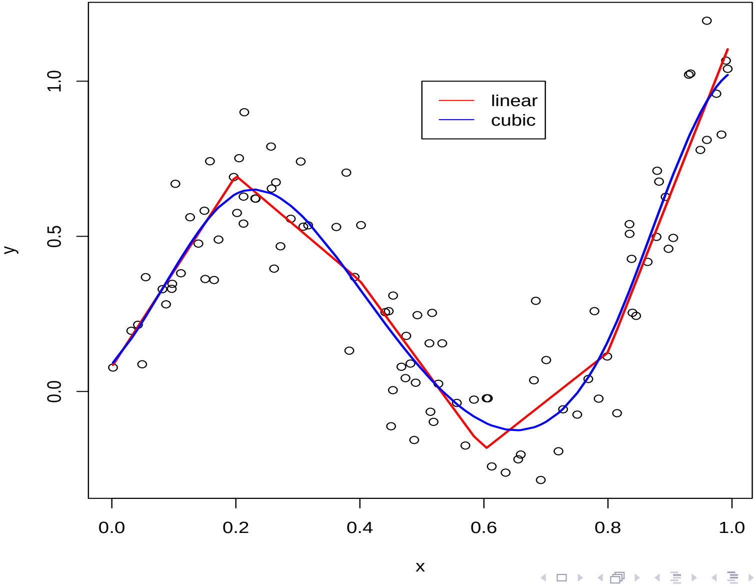
The model has $K + 4$ parameters and the number of effective degrees of freedom is $df = 4 + K$.

A cubic spline (like any other high order spline) behaves too erratically at the boundary of the X support, i.e. the variance of the fit is very high.

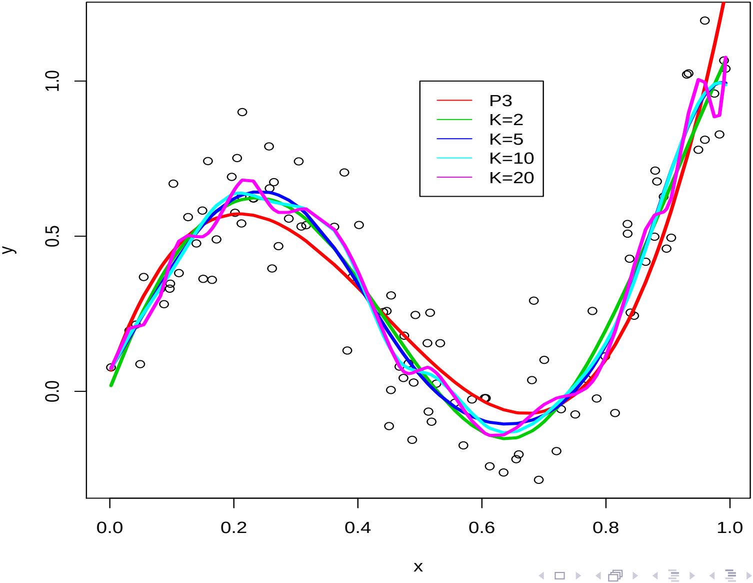
Training sample (x_i, y_i) and true regression function $f(X) = [\exp(1.2X) + 1.5\sin(7X) - 1]/3$.



Comparison of cubic and linear spline fit with 4 internal equally spaced knots at 0.2, 0.4, 0.6, 0.8.



Cubic spline fit with different K and global cubic fit (knots are located automatically at quantiles of the X distribution.



- This is the reason why it is preferable to impose the so called *natural boundary conditions*, which constrain the spline be linear outside the boundary knots.
- The natural boundary conditions require that the second and the third derivatives are zero for $x \leq \xi_1$ and $x \geq \xi_K$. This amounts to imposing 4 restrictions, and this frees 4 df.
- The complexity of the spline model is measured by the degrees of freedom, which is the trace of the hat matrix. This is equal to $p + 1 + K$ for polynomial splines and K for a natural cubic spline.

Natural boundary conditions

The 2nd and 3rd derivatives of

$$f(X) = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \sum_{k=1}^{K} \beta_{k+3}(X - \xi_k)_+^3$$

are respectively

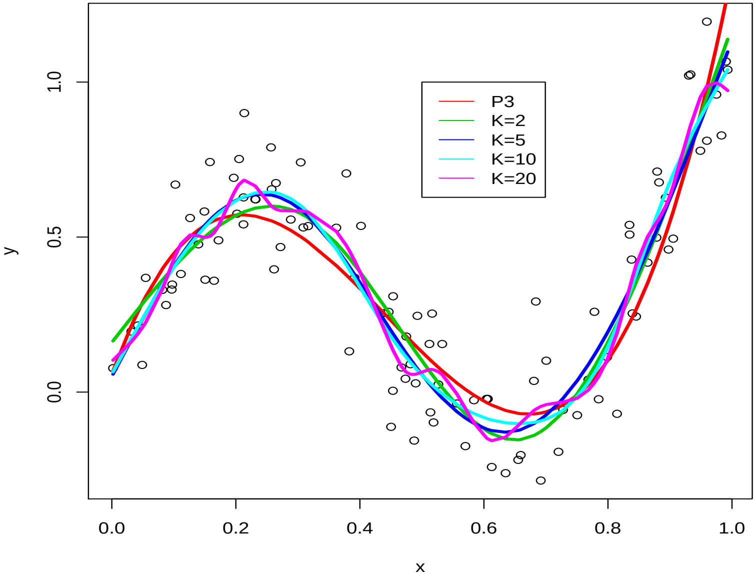
$$f^{''}(X) = 2\beta_2 + 6\beta_3 X + 6\sum_{k=1}^{K} \beta_{k+3}(X - \xi_k)_+$$

$$f^{'''}(X) = 6\beta_3 + 6\sum_{k=1}^{K} \beta_{k+3}(X - \xi_k)_+^0.$$

The natural boundary conditions imply the following constraints on the coefficients:

$$\beta_2 = \beta_3 = 0; \sum_{k=1}^{K} \beta_{k+3} = 0; \sum_{k=1}^{K} \xi_k \beta_{k+3} = 0$$

Natural cubic splines. Comparison of fit with different K and global cubic fit.



Model selection: how many knots? Where?

- Model selection is carried out by the same methods considered for regression.
- It entails not only the selection of the number of knots, K, but also their location along the support of X.
- The automatic option is to locate them at the $100k/(K+1), k = 1, \dots, K$-th percentiles of the distribution of X.
- If there are K candidate knots, there are 2^K possible models to select. Stepwise selection has been proposed. An alternative is to use a regularization approach, i.e. smoothing splines.
- Model complexity is measured by the degrees of freedom, e.g. $df = \text{trace}(\boldsymbol{H}) = p + 1 + K$ for a polynomial spline.

Note: the truncated power basis is easily interpretable; however, for computational efficiency a linear transformation of this basis, the B-spline basis, is used for estimation (the regressors are less collinear and more 'sparse').

Smoothing splines

- A smoothing spline is a natural cubic spline with N knots placed at each observation $x_i, i = 1, \dots, N$. Hence each new observation carries "news".
- Obviously, such a model is overparameterized, as the number of parameters is N, i.e. there is one parameter for each observation.
- We can write $f(X) = \sum_{k=1}^{N} \theta_k N_k(X)$, where $N_k(X)$ are the elements of the natural spline basis corresponding to the knots x_k's.
- The coefficients θ_k are estimated by minimising the following penalised residual sum of squares function:

$$PRESS(\lambda) = \min \left\{ \sum_{i=1}^{N} [y_i - f(x_i)]^2 + \lambda \int [f''(x)]^2 dx \right\}, \tag{2}$$

where $\lambda \geq 0$ is the smoothness parameter, $f''(x)$ is second derivative of the function, and $\int [f''(x)]^2 dx$ is the curvature of the function.

- The parameter λ regulates the complexity of the model.
- For $\lambda = 0$, the spline fits the observations perfectly ($y_i = \hat{f}(x_i)$).
- For $\lambda \to \infty$ we obtain the linear fit $\hat{f}(x_i) = \hat{\beta}_0 + \hat{\beta}_1 x_i$ (the linear function has zero second derivative and so $\int [f''(x)]^2 dx = 0$).

In vector notation, writing $\boldsymbol{f} = \boldsymbol{N\theta}$,

$$PRESS(\lambda) = (\boldsymbol{y} - \boldsymbol{N\theta})'(\boldsymbol{y} - \boldsymbol{N\theta}) + \lambda\boldsymbol{\theta}'\boldsymbol{\Omega\theta},$$

where $\boldsymbol{N}$ is the regression matrix of the natural spline and $\boldsymbol{\Omega}$ has elements $\int N_h^{''}(x) N_k^{''}(x) dx$.

For a fixed value of λ, the solution is

$$\hat{\boldsymbol{\theta}} = (\boldsymbol{N}'\boldsymbol{N} + \lambda\Omega)^{-1}\boldsymbol{N}'\boldsymbol{y}$$

(notice the analogy with ridge regression).

- The estimated regression function is $\hat{\boldsymbol{f}} = \boldsymbol{H}_\lambda \boldsymbol{y}$, where $\boldsymbol{H}_\lambda = \boldsymbol{N}(\boldsymbol{N}'\boldsymbol{N} + \lambda\boldsymbol{\Omega})^{-1}\boldsymbol{N}'$.
- The effective degrees of freedom (complexity) of the spline fit is

$$df(\lambda) = \text{tr}(\boldsymbol{H}_\lambda).$$

- When $\lambda \to \infty$, $df(\lambda) \to 2$ (minimal complexity), whereas as $\lambda \to 0$ $df(0) \to N$ (maximum complexity).
- The estimation of λ is carried out either by minimizing an information criterion or by crossvalidation. Denoting

$$RSS(\lambda) = \sum_{i=1}^{N}[y_i - f(x_i)]^2,$$

$$AIC(\lambda) = \ln[RSS(\lambda)] + 2df(\lambda)/N.$$

Crossvalidation

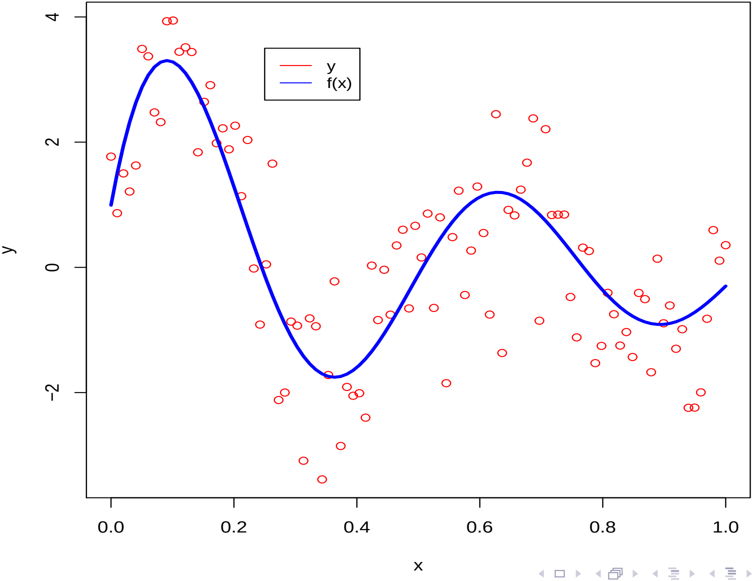
We seek the value of λ which minimises

$$CV(\lambda) = \sum_{i=1}^{N} \left(\frac{y_i - \hat{f}(x_i)}{1 - h_{i,\lambda}} \right)^2$$

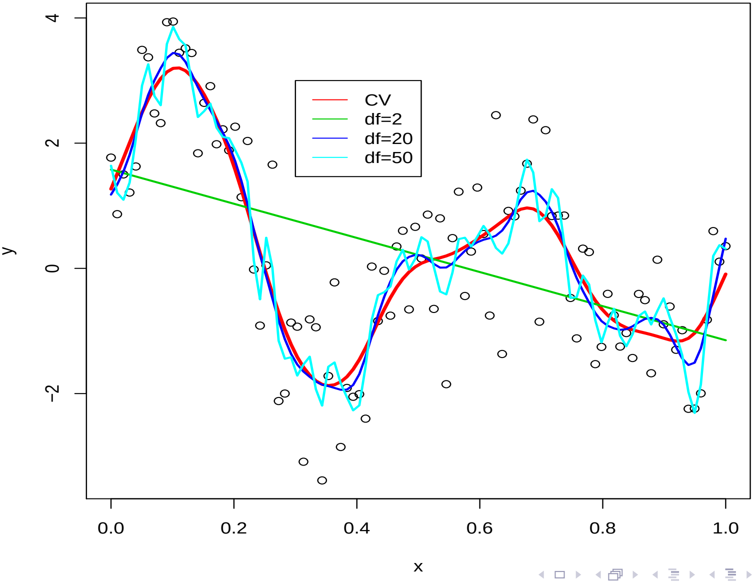
where $h_{i,\lambda}$ is the i-th diagonal element of $\boldsymbol{H}_\lambda$, or

$$GCV(\lambda) = \frac{RSS(\lambda)}{[1 - N^{-1} df(\lambda)]^2}.$$

Simulated example: $N = 100$, $f(X) = \sin[12(X + 0.2)]/(X + 0.2)$, $\epsilon \sim \mathrm{N}(0, 1)$, $Y = f(X) + \epsilon$.



Simulated example: $N = 100$, $f(X) = \sin[12(X+0.2)]/(X+0.2)$, $\epsilon \sim \mathrm{N}(0,1)$, $Y = f(X) + \epsilon$. Smoothing spline fit.



Nonparametric logistic regression

- Polynomial splines can be easily adapted to logistic regression.
- In particular, we specify

$$\ln \frac{P(G=1|X=x)}{P(G=0|X=x)} = f(x).$$

- As for spline smoothing, the function f can be estimated by minimizing the penalized log-likelihood, where the additional term penalizes the curvature of the function.
- Again, for large values of λ the logits are a linear function of X, whereas for small values a more complex fit is obtained.

Multiple predictors

- Multidimensional generalizations of regressions and smoothing splines are difficult.
- They suffer from the curse of dimensionality.
- Restricted approaches, that impose additivity, like Generalized Additive Models (GAMs, see later), are preferred.
- We model only the main effects and leave out interactions.