# STK-IN4300
# Statistical Learning Methods in Data Science

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## Outline of the lecture

- Basis Expansions and Regularization
  - Piecewise polynomials and splines
  - Smoothing splines
  - Selection of the smoothing parameters
  - Multidimensional splines

## Piecewise polynomials and splines: beyond linear regression

For regression problems:

- usually $f(X) = E[Y|X]$ is considered linear in $X$:
  - easy and convenient approximation;
  - first Taylor expansion;
  - model easy to interpret;
  - smaller variance (fewer parameter to be estimated);
- often in reality $f(X)$ is not linear in $X$;
- IDEA: use transformations of $X$ to capture non-linearity and fit a linear model in the new derived input space.

## Piecewise polynomials and splines: linear basis expansion

Consider the following model (linear basis expansion in $X$),

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

where $h_m(X) : \mathbb{R}^p \to \mathbb{R}$s denote the $m$-th transformation of X.

Note:

- the new variables $h_m(X)$ replace $X$ in the regression;
- the new model is linear in the new variables;
- usual fitting procedures are used.

## Piecewise polynomials and splines: choices of $h_m(X)$

Typical choices of $h_m(X)$:

- $h_m(X) = X_m$: original linear model;
- $h_m(X) = X_j^2$ or $h_m(X) = X_j X_k$: polynomial terms,
  - augmented space to achieve higher-order Taylor expansions;
  - the number of variables grow exponentially ($O(p^d)$, where $d$ is the order of the polynomial, $p$ the number of variables);
- $h_m(X) = \log(X_j), \sqrt{X_j}, \dots$: non-linear transformations;
- $h_m(X) = \mathbb{1}(L_m \leqslant X_k < U_m)$: indicator for a region of $X_k$,
  - breaks the range of $X_k$ into $M_k$ non-overlapping regions;
  - piecewise constant contribution of $X_k$.

## Piecewise polynomials and splines: introduction

Remarks:

- particular functional forms (e.g., logarithm) are useful in specific situations;
- polynomial forms are more flexible but limited by their global nature;

- piecewise-polynomials and splines allow for local polynomials;
- the class of functions is limited,

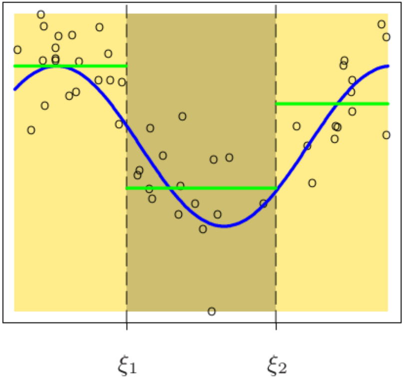
$$f(X) = \sum_{j=1}^{p} f_j(X_j) = \sum_{j=1}^{p} \sum_{m=1}^{M} \beta_{jm} h_{jm}(X_j),$$

by the number of basis $M_j$ used for each component $f_j$.

## Piecewise polynomials and splines: piecewise constant

The **piecewise constant** function:

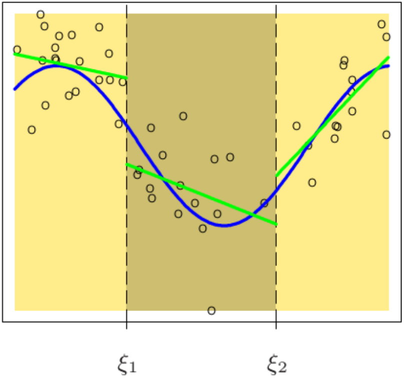
- simplest solution;
- three basis functions:
  - $h_1(X) = \mathbb{1}(X < \xi_1)$
  - $h_2(X) = \mathbb{1}(\xi_1 \leqslant X < \xi_2)$
  - $h_3(X) = \mathbb{1}(\xi_2 \leqslant X)$
- disjoint regions;
- $f(X) = \sum_{m=1}^{3} \beta_m h_m(X)$;
- $\hat{\beta}_m = \bar{Y}_m$, the mean of $Y$ in the region $m$.



## Piecewise polynomials and splines: piecewise linear

A **piecewise linear** fit:

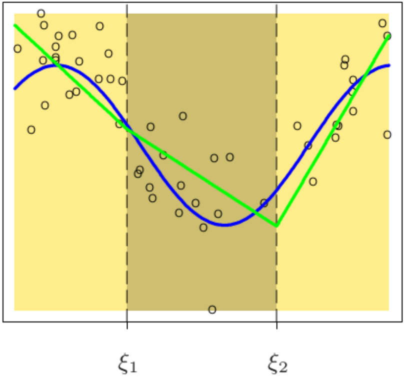
- a linear fit instead of a constant fit in each region;
- three additional basis functions:
  - $h_4(X) = h_1(X)X$
  - $h_5(X) = h_2(X)X$
  - $h_6(X) = h_3(X)X$
- $\hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_3$ are the intercepts;
- $\hat{\beta}_4, \hat{\beta}_5, \hat{\beta}_6$ are the slopes;



## Piecewise polynomials and splines: piecewise linear

A **continuous piecewise linear** fit:

- force continuity at knots;
- generally preferred to the non-continuous version;
- add constrains,
  - $\hat{\beta}_1 + \xi_1 \hat{\beta}_4 = \hat{\beta}_2 + \xi_1 \hat{\beta}_5$;
  - $\hat{\beta}_2 + \xi_2 \hat{\beta}_5 = \hat{\beta}_3 + \xi_2 \hat{\beta}_6$;
- 2 restrictions → 4 free parameters;

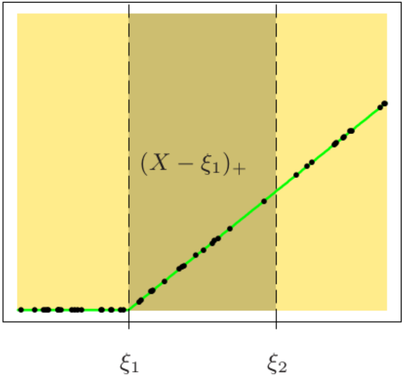


## Piecewise polynomials and splines: piecewise linear

The constrain can be directly incorporated into the basis functions,

- $h_1(X) = 1$
- $h_2(X) = X$
- $h_3(X) = (X - \xi_1)_+$
- $h_4(X) = (X - \xi_2)_+$

where $(\cdot)_+$ denotes the positive part.



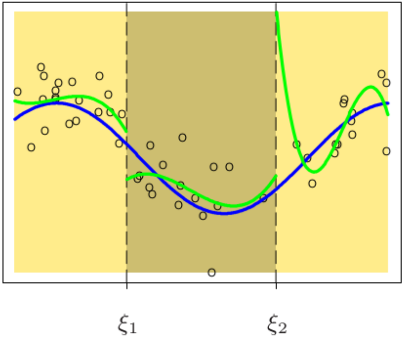
## Piecewise polynomials and splines: piecewise cubic polynomials

Further "improvements":

- smoother functions;
- increase the order of the polynomials;
- e.g., a cubic polynomial in each disjoint region;

↓

**discontinuous piecewise cubic** polynomials.



## Piecewise polynomials and splines: piecewise cubic polynomials

Also in this case:

- we can force the function to be continuous at the nodes;
- by adding constrains;

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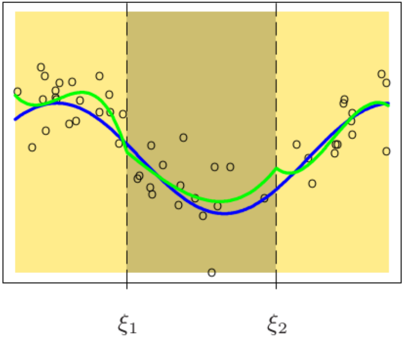
**continuous piecewise cubic** polynomials.



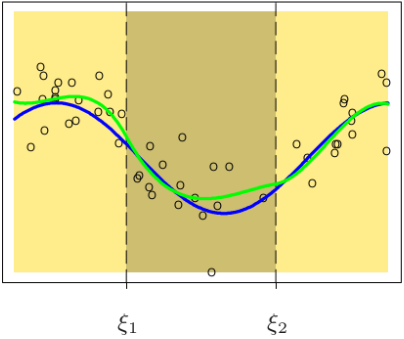
## Piecewise polynomials and splines: piecewise cubic polynomials

Since we have third order polynomials:

- we can increase the order of continuity at knots;
- not only $f(\xi_k^-) = f(\xi_k^+)$;
- additionally, $f'(\xi_k^-) = f'(\xi_k^+)$.

$\downarrow$

**first derivative continuous piecewise cubic** polynomials.



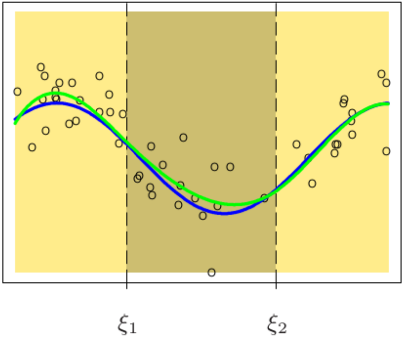
## Piecewise polynomials and splines: piecewise cubic polynomials

Finally,

- further increase the order of continuity;
- constrain $f''(\xi_k^-) = f''(\xi_k^+)$

$\downarrow$

**cubic splines**.




Basis for cubic splines with two knots $\xi_1$ and $\xi_2$:

$$
\begin{aligned}
h_1(X) &= 1, & h_3(X) &= X^2, & h_5(X) &= (X - \xi_1)^3_+ \\
h_2(X) &= X, & h_4(X) &= X^3, & h_6(X) &= (X - \xi_2)^3_+
\end{aligned}
$$

## Piecewise polynomials and splines: general order-M splines

In general, an order-M spline with knots $\xi_j$, $j = 1, \dots, K$:

- is a piecewise-polynomial of degree $M - 1$;
- has continuous derivatives up to order $M - 2$;
- the general form of the basis is:

$$h_j(X) = X^{j-1}, j = 1, \dots, M;$$
$$h_{M+\ell}(X) = (X - \xi_\ell)_+^{M-1}, \ell = 1, \dots, K;$$

- e.g., cubic spline $\rightarrow$ $M = 4$;
- cubic splines are the lowest-order spline for which the discontinuity at the knots cannot be seen by a human eye

$$\Downarrow$$

no reason to use higher-order splines

## Piecewise polynomials and splines: specifications

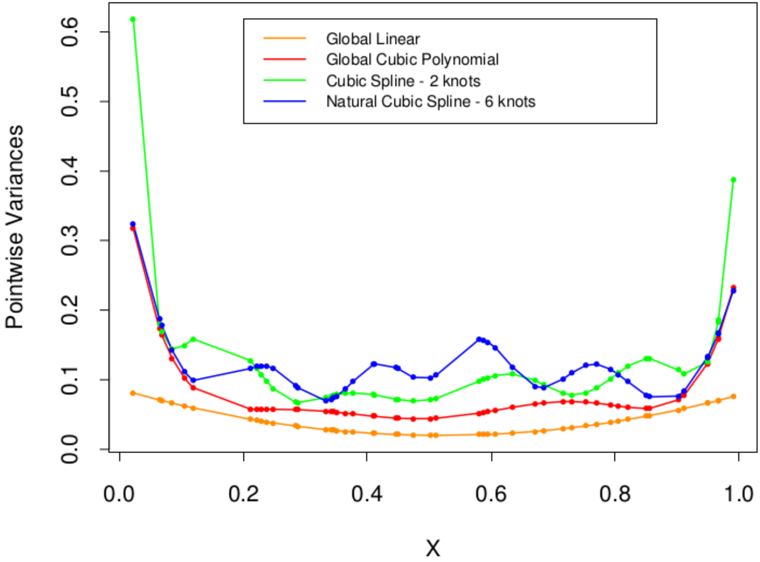
For this kind of splines (a.k.a. regression splines), one needs:

- specify the order of the spline;
- select the number of the knots;
- choose their placement.

Often:

- use cubic splines ($M = 4$);
- use the degrees of freedom to choose the number of knots;
- e.g., for cubic splines,
  - 4 degrees of freedom for the first cubic polynomial;
  - 1 degree of freedom for each knots $(4 - 1 - 1 - 1)$;
  - number of basis $=$ number of knots $+$ 4;
- use the $x_i$ to place the knots;
  - e.g., with 4 knots, $20^{th}, 40^{th}, 60^{th}, 80^{th}$ percentiles of $x$.

## Piecewise polynomials and splines: natural cubic splines



## Piecewise polynomials and splines: natural cubic splines

At the boundaries:

- same issues saw for kernel density;
- high variance.

Solution:

- force the function to be linear beyond the boundary knots;
- by adding additional constrains;
- it frees up 4 (2 for each boundary) degrees of freedom.

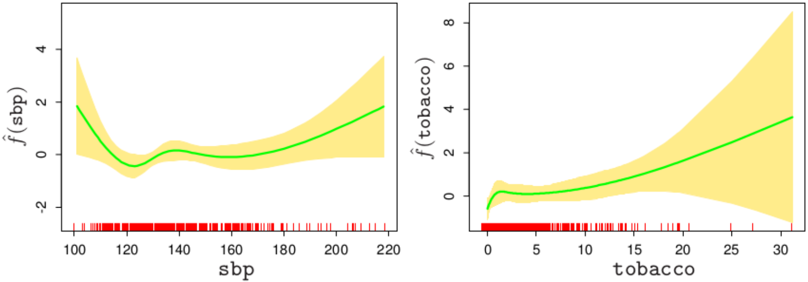
Basis (derived from those of the cubic splines):

$$N_1(X) = 1 \qquad N_2(X) = X \qquad N_{k+2}(X) = d_k(X) - d_{K+1}$$

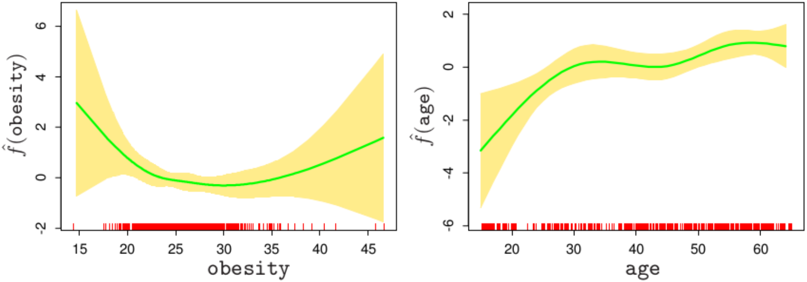
where

$$d_k = \frac{(X - \xi_k)_+^3 - (X - \xi_K)_+^3}{\xi_K - \xi_k}.$$

## Piecewise polynomials and splines: example



# Piecewise polynomials and splines: example



## Smoothing splines: introduction

To avoid choosing the number of knots and their placement:

- use the maximal number (one for each observation);
- control the complexity with a penalty term.

## Smoothing splines: minimizer

Consider the minimization problem,

$$\hat{f}(x) = \text{argmin}_{f(x)} \left\{ \sum_{i=1}^{N} (y_i - f(x_i))^2 + \lambda \int \{f''(t)\}^2 dt \right\}$$

such that $f(x)$ has two continuous derivatives.
Here $\lambda$ is the smoothing parameter:

- $\lambda = 0 \rightarrow$ no constrain ($f(x)$ can be any function interpolating the data);
- $\lambda = \infty \rightarrow$ least squares line fit (no curvature tolerated).

It can be shown that the unique minimizer is a natural cubic spline with knots at the unique values $x_i$, $i = 1, \dots, N$.

## Smoothing splines: solution

If we consider the natural spline

$$f(x) = \sum_{j=1}^{N} N_j(x)\theta_j,$$

then

$$\hat{\theta} = \text{argmin}_\theta \left\{(y - N\theta)^T(y - N\theta) + \lambda\theta^T\Omega_N\theta\right\},$$

where:

- $\{N\}_{ij} = N_j(x_i)$, and $N_j(\cdot)$ are the basis functions;
- $\{\Omega\}_{jk} = \int N_j''(t)N_k''(t)\,dt$.

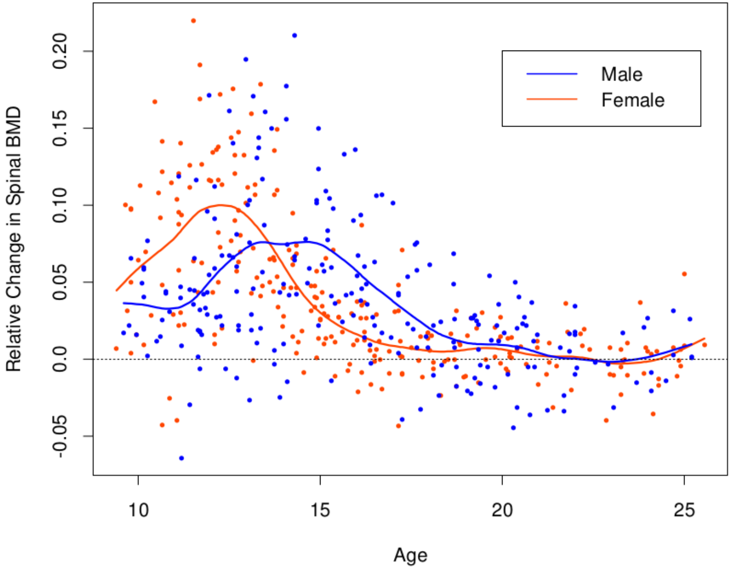
Therefore,

$$\hat{\theta} = (N^TN + \lambda\Omega_N)^{-1}N^Ty$$

and

$$\hat{f}(x) = \sum_{j=1}^{N} N_j(x)\hat{\theta}_j.$$

## Smoothing splines: example



## Selection of the smoothing parameters: linear operators

Polynomial splines and smoothing splines are linear operators:

- cubic splines: $\hat{f}(x) = \underbrace{B_\xi(B_\xi^T B_\xi)^{-1}B_\xi^T}_{H_\xi} y$;
- smoothing splines: $\hat{f}(x) = \underbrace{N(N^T N + \lambda\Omega_N)^{-1}N^T}_{S_\lambda} y$.

$H_\xi$ is called hat matrix, $S_\lambda$ smoothing matrix:

- they do not depend on $y$ (linear [operator / smoother]);
- are symmetric and semidefinite positive;
- $H_\xi H_\xi = H_\xi$ (idempotent), $S_\lambda S_\lambda \leq S_\lambda$ (shrinking);
- $H_\xi$ has rank $M$, $S_\lambda$ has rank $N$.

## Selection of the smoothing parameters: degrees of freedom

The expression $M = \text{trace}(H_\xi)$ gives:

- the dimension of the projection space;
- number of basis function;
- number of parameters involved in the fit.

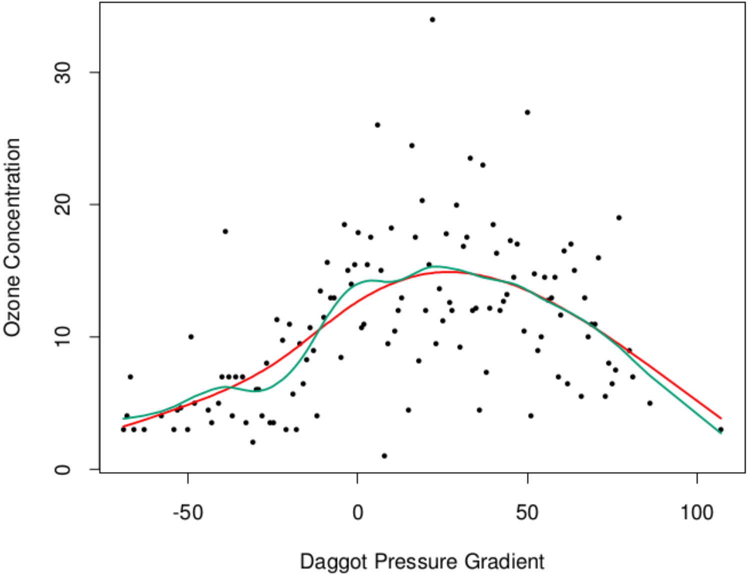
Similarly, we define the **effective degrees of freedom** as

$$\text{df}_\lambda = \text{trace}(S_\lambda).$$

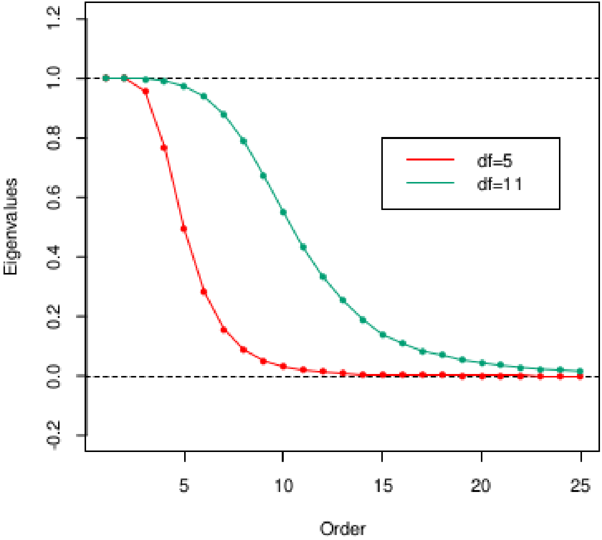
We can fix the degrees of freedom and find the value of $\lambda$:

- e.g., in the last example, $\text{df}_\lambda = 12 \rightarrow \lambda = 2.2 \times 10^{-4}$.

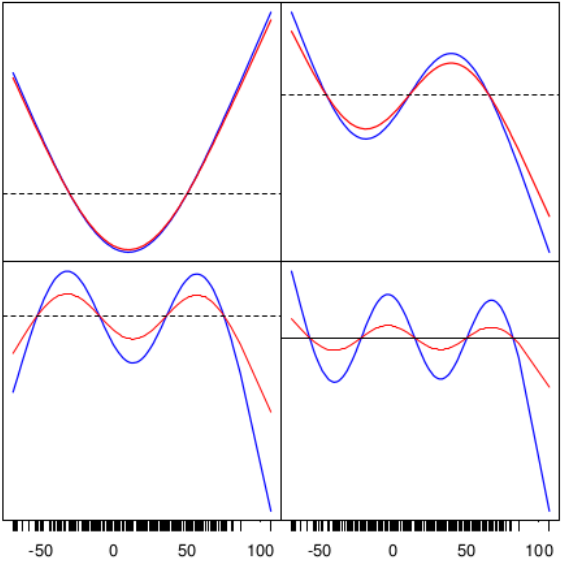
## Selection of the smoothing parameters: example



## Selection of the smoothing parameters: example



# Selection of the smoothing parameters: example



## Selection of the smoothing parameters: smoother matrices

Let us rewrite $S_\lambda$ in his Reinsch form,

$$S_\lambda = (I + \lambda K)^{-1},$$

where $K$ (penalty matrix) does not depend on $\lambda$.

The eigen-decomposition of $S_\lambda$ is

$$S_\lambda = \sum_{k=1}^{N} \rho_k(\lambda) u_k u_k^T$$

with $\rho_k(\lambda) = \frac{1}{1+\lambda_k}$.

## Selection of the smoothing parameters: smoother matrices

Note that:

- the eigenvectors are not affected by changes in $\lambda$,
  - the whole family of smoothing splines indexed by $\lambda$ has the same eigenvectors;
- $S_\lambda y = \sum_{k=1}^{N} u_k \rho_k(\lambda) \langle u_k, y \rangle$,
  - smoothing splines decompose $y$ w.r.t. the basis $u_k$;
  - differentially shrink the contribution using $\rho_k(\lambda)$;
- the eigenvalues $\rho_k(\lambda) = 1/(1 + \lambda_k)$ are inverse function of the eigenvalues $d_k$ of the penalty matrix $K$, moderated by $\lambda$,
  - $\lambda$ controls the rate at which $\rho_k(\lambda)$ decreases to 0.

## Selection of the smoothing parameters: bias variance trade-off

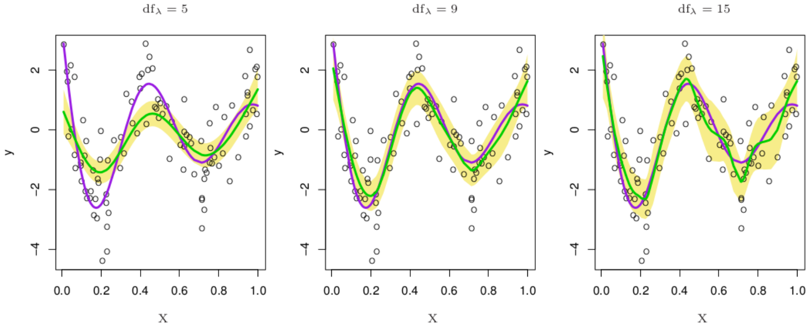
Consider the following example:

- $Y = f(X) + \epsilon$;
- $f(X) = \frac{\sin(12(X+0.2))}{X+0.2}$;
- $\epsilon \sim N(0,1)$;
- $X \sim \text{Unif}[0,1]$;
- $N = 100$.

We fit smoothing splines with three different values of $\text{df}_\lambda$:

- $\text{df}_\lambda = 5$;
- $\text{df}_\lambda = 9$;
- $\text{df}_\lambda = 15$.

## Selection of the smoothing parameters: bias variance trade-off



## Selection of the smoothing parameters: bias variance trade-off

In yellow it is shown the area $\hat{f}_\lambda(x) \pm 2 \cdot se(\hat{f}_\lambda(x))$.

Since $\hat{f}(x) = S_\lambda(x)y$,

$$\text{Cov}(\hat{f}(x)) = S_\lambda \text{Cov}(y) S_\lambda^T = S_\lambda S_\lambda^T$$

The diagonal contains the pointwise variances at the points $x_i$.

About the bias,

$$\text{Bias}(\hat{f}(x)) = f(x) - E(\hat{f}_\lambda(x)) = f - S_\lambda^T f.$$

We can estimate bias and variance via Monte Carlo methods.

## Selection of the smoothing parameters: bias variance trade-off

Note from the last figure:

- $\text{df}_\lambda = 5$: strong bias, low variance;
  - *trim down the hills and fill the valleys* behaviour;
- $\text{df}_\lambda = 9$: the bias is strongly reduces, paying a relatively low price in terms of variance;
- $\text{df}_\lambda = 15$: close to the true function (i.e., low bias), but somehow wiggly $\rightarrow$ high variance.

Here the term "bias" is used loosely, in the picture it is actually shown $\hat{f}(x)$, not $E[\hat{f}(x)]$.

## Selection of the smoothing parameters: bias variance trade-off

We want to minimize the expected prediction error,

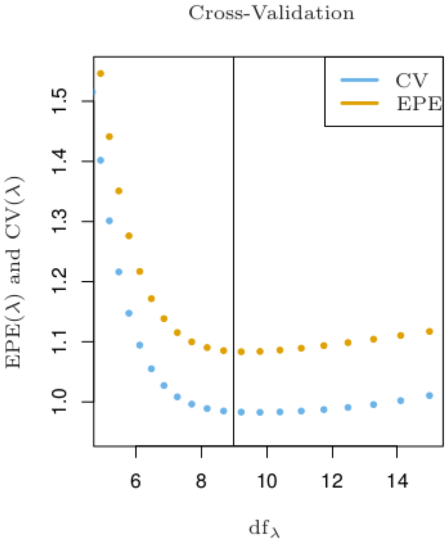
$$EPE(\hat{f}_\lambda(x)) = \mathrm{Var}(Y) + E[\mathrm{bias}^2(\hat{f}_\lambda(x)) + \mathrm{Var}(\hat{f}_\lambda(x))]$$

We do not know the true function $\rightarrow$ cross-validation:

- $K$-fold cross-validation;
- leave-one-out cross validation,

$$\begin{aligned}\mathrm{CV}(\hat{f}_\lambda(x)) &= \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{f}_\lambda^{(-i)}(x_i))^2 \\ &= \frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i - \hat{f}_\lambda(x_i)}{1 - S_{\lambda\,[i,i]}}\right)^2\end{aligned}$$

## Selection of the smoothing parameters: bias variance trade-off



## Multidimensional splines: multidimensional splines

All spline models generalize to multidimensional cases.

Consider $X \in \mathbb{R}^2$, then

$$g(X) = \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \theta_{jk} g_{jk}(X),$$

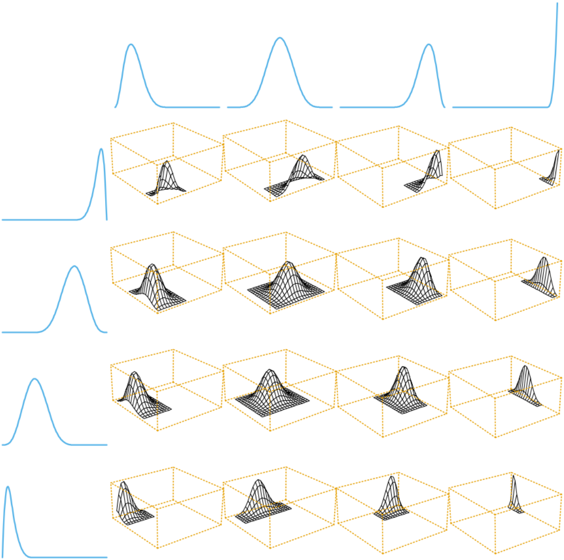
where:

- $g_{jk}(X)$ is an element of the $M_1 \times M_2$ tensor product basis

$$g_{jk}(X) = h_{1j}(X_1) h_{2k}(X_2), j = 1, \dots, M_1, k = 1, \dots, M_2;$$

- $h_{1j}(X_1)$ is a set of $M_1$ basis for the coordinate $X_1$;
- $h_{2j}(X_2)$ is a set of $M_2$ basis for the coordinate $X_2$;
- $\theta = \theta_{jk}$ is the $M_1 \times M_2$-dimensional vector of coefficients.

## Multidimensional splines: multidimensional splines



## Multidimensional splines: multidimensional smoothing splines

Smoothing splines can be extended to more than one dimension as well, by generalizing

$$\hat{f}(x) = \text{argmin}_{f(x)} \sum_{i=1}^{N} \{y_i - f(x_i)\}^2 + \lambda J[f(x)],$$

where $J[f(x)]$ takes care of the "smoothness" in $\mathbb{R}^d$.

For example, in the case $d = 2$,

$$J[f(x)] = \int_{\mathbb{R}} \int_{\mathbb{R}} \left[ \left( \frac{\partial^2 f(x)}{\partial x_1^2} \right)^2 + 2 \left( \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} \right)^2 + \left( \frac{\partial^2 f(x)}{\partial x_2^2} \right)^2 \right] dx_1 dx_2.$$

## Multidimensional splines: multidimensional smoothing splines

The minimizer $\hat{f}(x)$ (in $\mathbb{R}^2$) is known as **thin-plate spline**:

- for $\lambda \to 0$, $\hat{f}(x) \to$ interpolation function;
- for $\lambda \to \infty$, $\hat{f}(x) \to$ least square hyperplane;
- for intermediate values of $\lambda$, linear expansion of basis with their coefficients computed by a form of generalized ridge.

The solution has the form

$$f(x) = \beta_0 + \beta^T x + \sum_{j=1}^{N} \alpha_j h_j(x),$$

where $h_j(x) = ||x - x_j|| \log ||x - x_j||$ (radial basis function).

## Multidimensional splines: multidimensional smoothing splines

Remarks:

- the computational complexity is $O(N^3)$;
- often the thin-plate splines are only computed on a grid of $K$ knots distributed on the domain (see figure);
- the computational complexity reduces to $O(NK^2 + K^3)$;

Simplification:

- by imposing a specific structure;
- e.g., additivity:
  - $f(x) = \alpha + f_1(x_1) + \cdots + f_d(x_d)$ (GAM, see next lecture);
  - then

$$J[f(x)] = J(f_1(x_1) + \cdots + f_d(x_d))$$
$$= \sum_{j=1}^{d} \int f_j''(t_j) dt_j.$$

# Multidimensional splines: multidimensional smoothing splines