Locality and Smoothness
or
Wavelets and Splines

May 2, 2018

Motto

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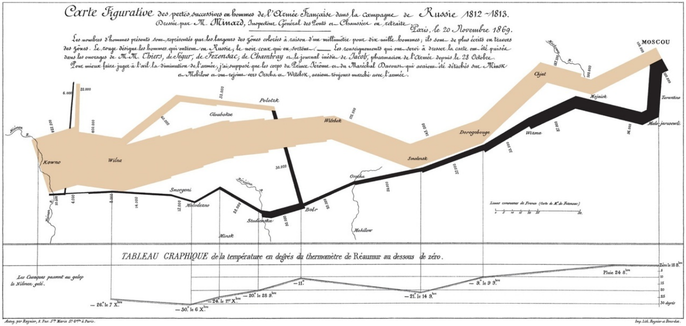
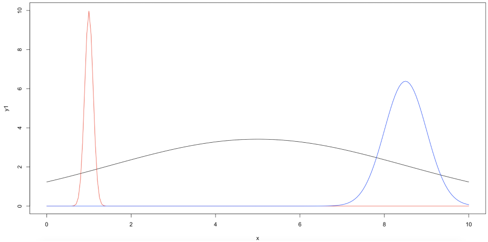


Outline

Overview wavelet bases

- The main idea behind the so called wavelet functions is to represent the local wave like behavior in a signal.
- Inspiration came from physical phenomena but mathematical foundations goes back to Alfréd Haar in 1909.
- The main features of a single wavelet:
    - **a location** – place on horizontal axis (time) where a wavelike disturbance occur
    - **a scale** – how big is the disturbance
    - **a resolution** – how spread is the disturbance around its location, representation of detail
- In a simple approach one could utilize Gaussian curve

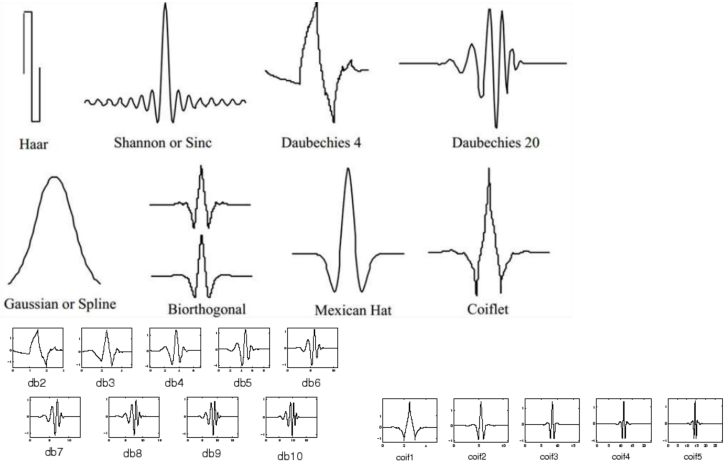
$$f(x; A, m, s) = Ae^{(x-m)^2/s^2}$$



Orthogonalized wavelets

- The only problem with the Gaussian curves that they are not orthogonal
- Can one have curves that have locality and resolution and at the same time to be orthogonal?
- Yes, one can and these are wavelets.
- They are many orthonormal systems with these properties.
- They are generated by the so called **mother wavelets** to which then increasing resolution and scale and locations are added.
- Wavelets in higher dimensions also exist.
- Here we show pictures of them but we will focus from now on only on one system, the oldest and the easiest to understand – Haar wavelets.

Pictures with wavelets



Piecewise constant basis - Haar functions

- Haar functions are the simplest and for most purposes very effective wavelets.
- Define a father wavelet

$$\phi(x) = 1, \;\; x \in [0, 1]$$

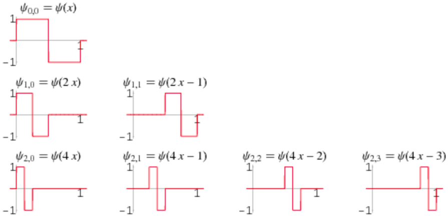
and a mother wavelet

$$\psi(x) = \begin{cases} 1: & 0 \leq x < 1/2; \\ -1: & 1/2 < x \leq 1; \\ 0: & \text{otherwise} \end{cases}$$

and children (orthogonal but not normalized)

$$\psi_{jk}(x) = \psi(2^j x - k)$$

for j a nonnegative integer and $0 \leq k \leq 2^j - 1$.

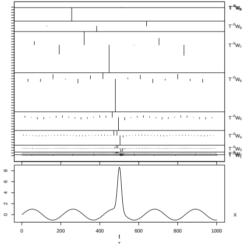


Discrete Wavelet transform – DWT

- Similarly as for the Fourier basis one have FFT for fast computations of the coefficients of decomposition of a signal, there is also a fast algorithm for computing wavelet coefficients.
- It is called the discrete Wavelet transform and is implemented in packages such as `wavelets` in R.

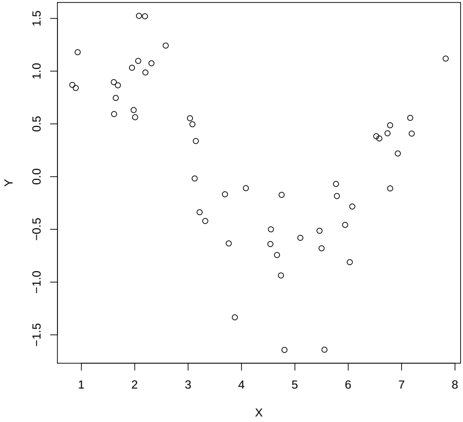
```
install.packages("wavelets")
#Test function and its plot
f=t(8*exp(-5000*(t-1/2)^2)+sin(30*t))
plot(t,f,type="l")


WD=dwt(f,filter="haar")
plot(WD)
```



Outline

A picture



Try to sketch a denoised relation between X and Y.

Noisy sine function

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$$Y = f(X) + \epsilon$$
where X is an explanatory variable, ϵ is a noisy error and Y is an outcome variable (aka response or dependent variable).

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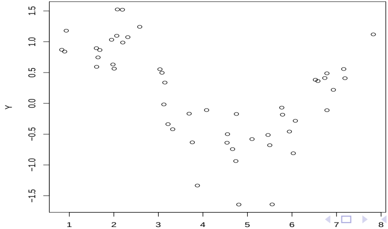
- A sample from such a model



Outline

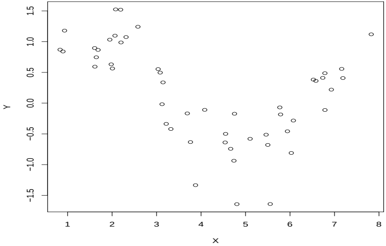
Noisy Sine R-code

```
#Non-linear regression

X=runif(50,0.5,8)
e=rnorm(50,0,0.35)
Y=sin(X)+e

pdf("NoisySine.pdf") #Save a graph to a file
plot(X,Y)
dev.off()            #Closes the graph file
```

How to (re-)discover a non-linear relation



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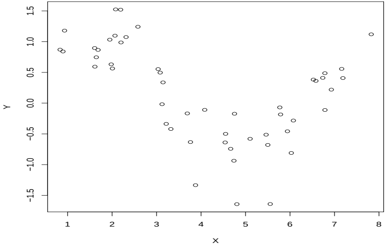

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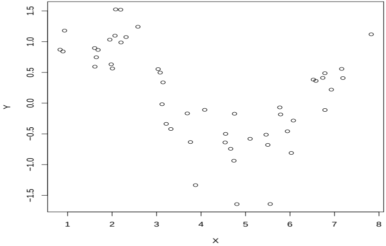

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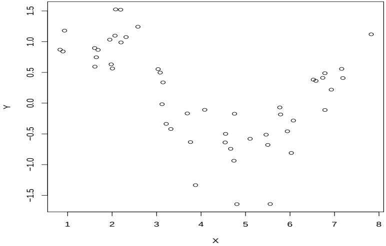

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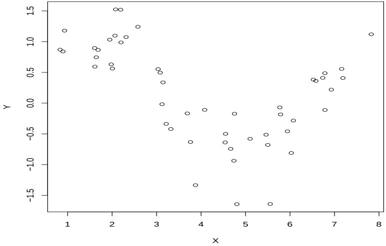

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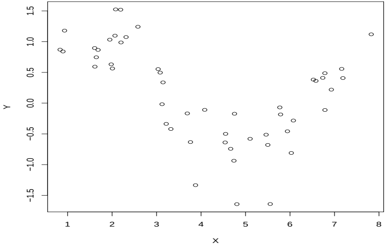

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- **Any ideas?**

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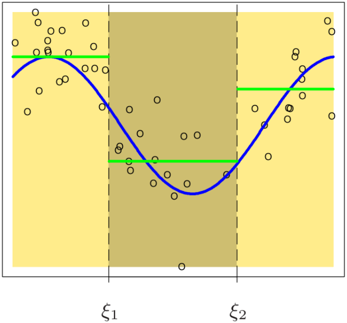
- On each interval we can fit independently.
- For example by constant functions

Piecewise Constant



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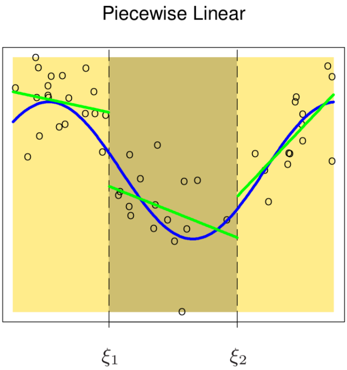

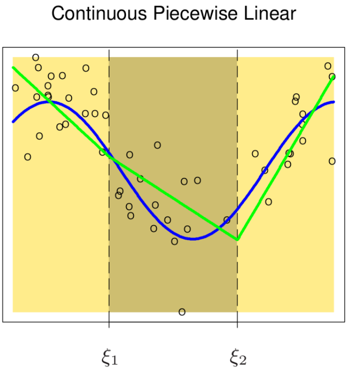

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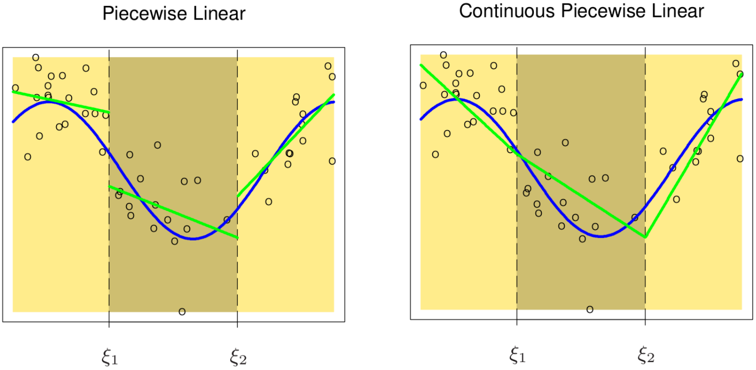

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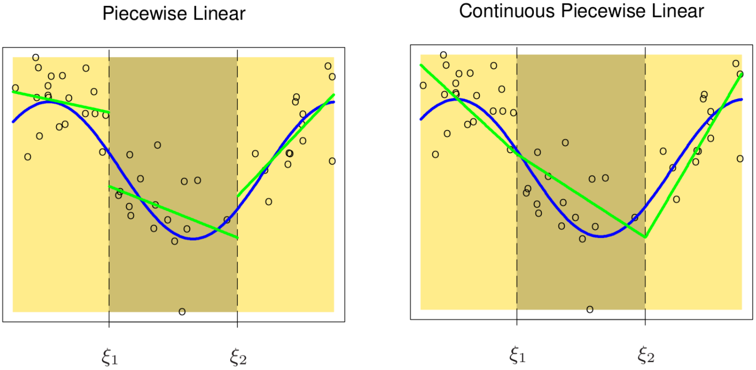

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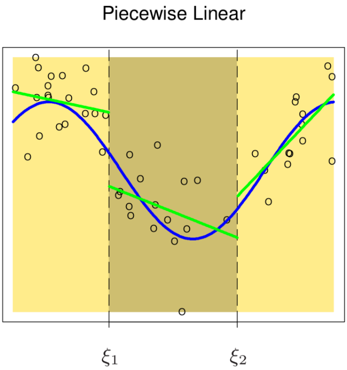

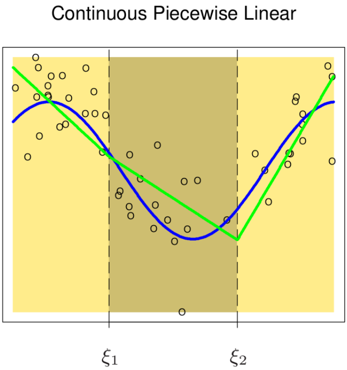

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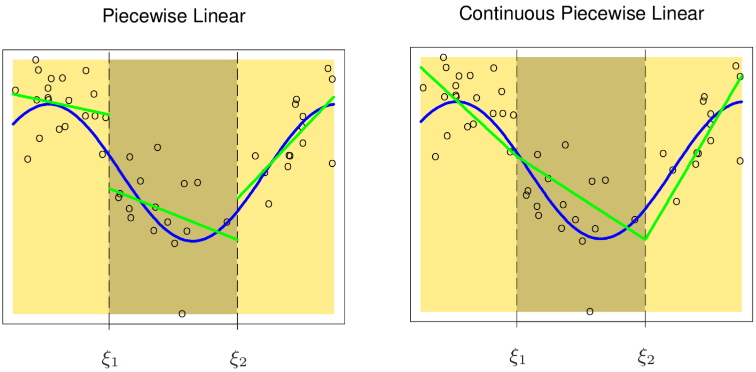

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- How to do it?

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- 3-intercepts $+$ 3-slopes $-$ 2-knots $=$ 4 (we subtract knots because each knot sets one equation to fulfill the continuity assumption.
- The problem should be fitted with four parameters.

From now on we assume the knots locations are decided for and not changing.

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- There are four parameters, so that any continuous piecewise linear function should be fitted by proper choice of β_j's.

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$$Y_i = \beta_1 h_{i1} + \cdots + \beta_r h_{ir} + \varepsilon_i,$$

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- Fitting problem is solved by fitting the **linear regression problem** (the least squares method).

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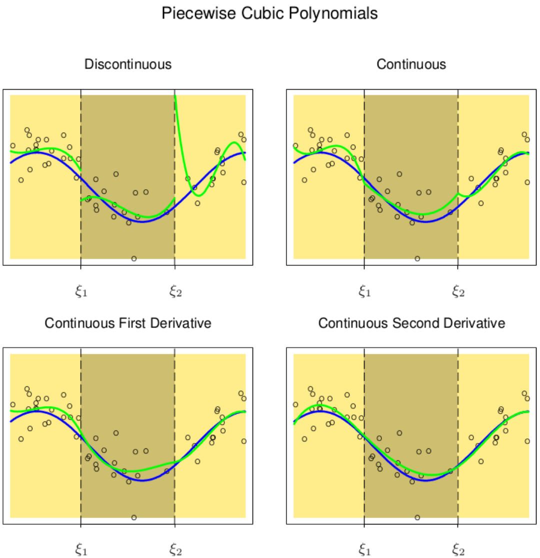
- We can increase the order of **smoothness at the knots** by increasing the degree of polynomial that is fitted in each region and then imposing the **continuity constraints at each knot**.
- The cubic splines are quite popular for this purpose.

Illustration – cubic splines



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- Example of the basis

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- Define recursively functions $B_{i,m}$ that are splines of the $(m-1)$th order of smoothness (0 smoothness is discontinuity at the knots), $i = 1, \dots, K+8$, $m = 1, \dots, 4$

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- Higher $(m-1)$ order of smoothness , $i = 1, \ldots, K+8-m$,

$$B_{i,m}(x) = \frac{x - \tau_i}{\tau_{i+m-1} - \tau_i} B_{i,m-1}(x) + \frac{\tau_{i+m} - x}{\tau_{i+m} - \tau_{i+1}} B_{i+1,m-1}(x).$$

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- The piecewise constant (0-smooth), $i = 1, \dots, K+7$,

$$B_{i,1}(x) = \begin{cases} 1 & \text{if } \tau_i \leq x < \tau_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

- Higher $(m-1)$ order of smoothness , $i = 1, \dots, K+8-m$,

$$B_{i,m}(x) = \frac{x - \tau_i}{\tau_{i+m-1} - \tau_i} B_{i,m-1}(x) + \frac{\tau_{i+m} - x}{\tau_{i+m} - \tau_{i+1}} B_{i+1,m-1}(x).$$

- $B_{i,4}$ are cubic order splines that constitutes basis for all cubic splines.

Illustration – evenly distributed knots

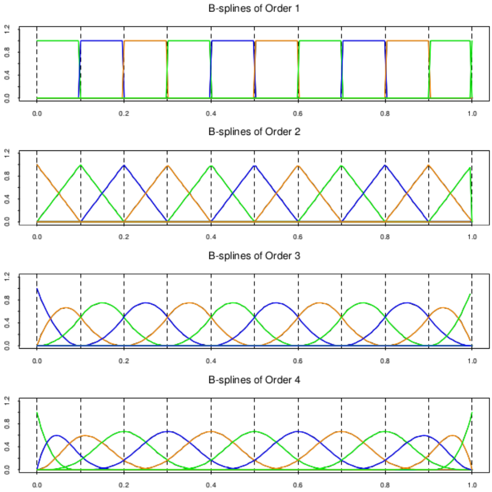
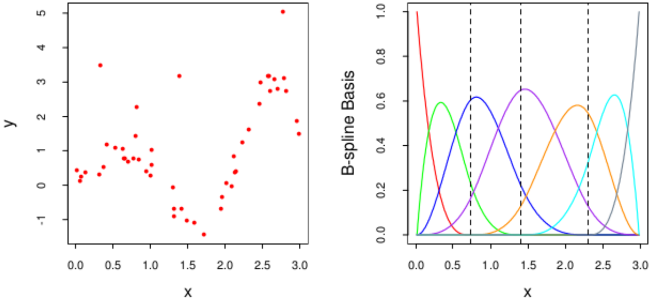


Illustration – non-evenly distributed knots

Illustration – non-evenly distributed knots

- Another data set and B-spline basis



Outline

Splines without knot selection

The regression problem with one predictor

$$y = \alpha + f(x) + \epsilon.$$

- The maximal set of knots: a knot is located at each abscissa location in the data.
- Clearly, without additional restrictions this leads to overfitting and non-identifiability.

Splines without knot selection

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- The maximal set of knots: a knot is located at each abscissa location in the data.
- Clearly, without additional restrictions this leads to overfitting and non-identifiability. **Why?**
- These issues are taken care of since irregularity is penalized.
- Outside the range of predictors it is estimated by a linear function (smoothing on the boundaries).

Penalty for being non-smooth

- Minimize the penalized residual sum of squares

$$PRSS(f,\lambda) = \sum_{i=1}^{N} (y_i - f(x_i))^2 + \lambda \int f''(t)^2 dt$$

- $\lambda = 0$: any fit that interpolates data exactly.
- $\lambda = \infty$: the least square fit (second derivative is zero)
- We fit by the cubic splines with knots set at all the values of x's and the solution has the form

$$f(x) = \sum_{j=1}^{N+4} \gamma_j B_j(x), \tag{1}$$

where γ_j's have to be found.

B-spline basis

- The splines $B_j(x)$, $j = 1, \ldots, N+4$, are used in the smoothing splines, where the initial x_i, $i = 1, \ldots, N$ are augmented by 2 end points defining the range of interest for the total of $N+2$ knots.
- We have seen that if there is N internal points, then there have to be $N+4$ of the third order splines in order for them to constitute basis.
- One can compute explicitly the coefficients of the following matrix

$$\boldsymbol{\Omega}_B = \left[\int B_i''(t) B_j''(t)\, dt \right]$$

Solution

- The solution has the following explicit form

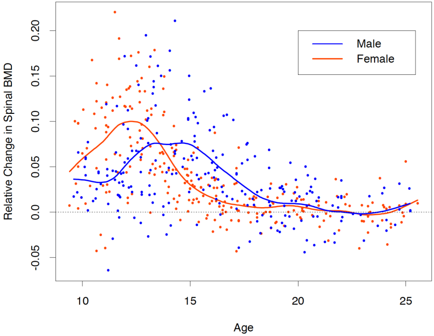
$$\hat{\gamma} = \left(\mathbf{B}^T\mathbf{B} + \lambda\mathbf{\Omega}_B\right)^{-1}\mathbf{B}^T\mathbf{y},$$

  where

$$\mathbf{\Omega}_B = \left[\int B_i''(t)B_j''(t)\,dt\right]$$

- To see this substitute to the PRSS – it becomes a regular least squares problem that is solved by $\hat{\gamma}$.
- Further details in Discussion Sesssion 2.

Example – bone mineral density



The response is the relative change in bone mineral density mea- sured at the spine in adolescents, as a function of age. A separate smoothing spline was fit to the males and females, with $\lambda = 0.00022$. It can be argued that this choice of λ corresponds to about 12 degrees of freedom (the number of parameters in a comparable standard spline fit of the solution). See the textbook for the discussion of transformation from the degrees of freedom to λ and vice versa.