Lec 12: Overview of various smoothers

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Overview of various smoothers

A scatter plot smoother is a tool for finding structure in a scatter plot: $(x_1, y_1), \ldots, (x_n, y_n)$

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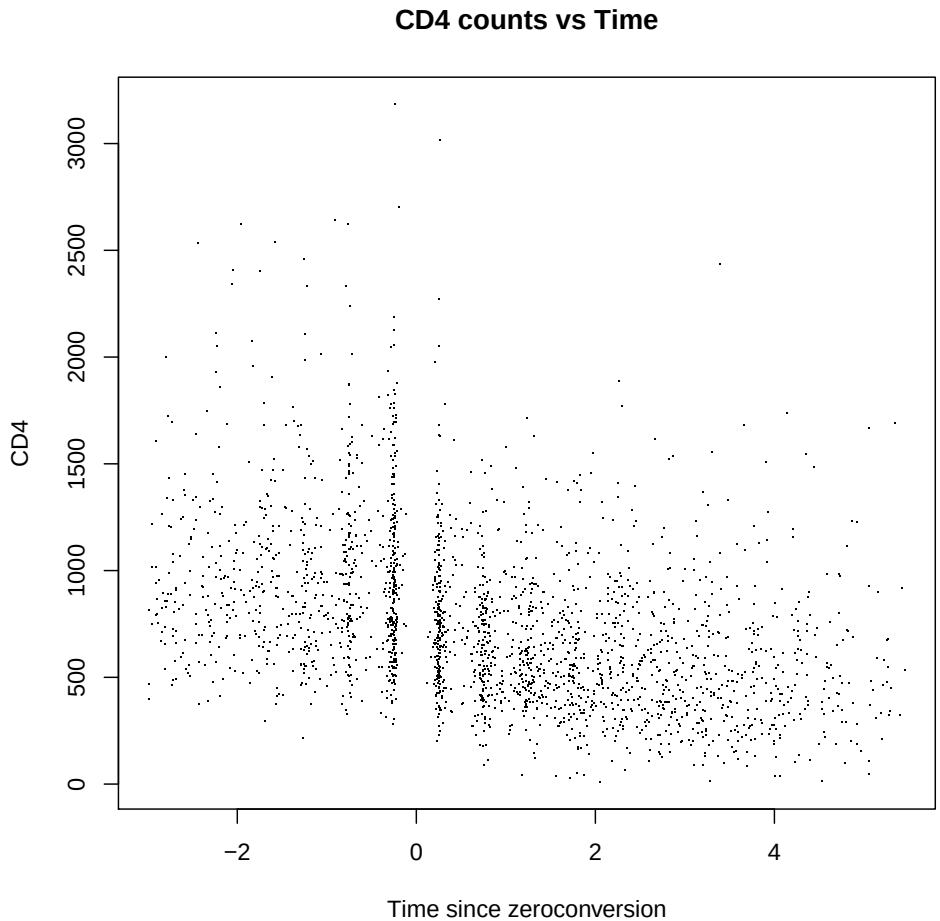

- Suppose that we consider $\mathbf{y} = (y_1, \ldots, y_n)'$ as the *response measurements* and $\mathbf{x} = (x_1, \ldots, x_n)'$ as the *design points*.
- We can think of $\mathbf{x}$ and $\mathbf{y}$ as outcomes of random variable X and Y. However, for scatter plot smoothers we don't really need stochastic assumptions, it can be considered as a descriptive tool.
- A **scatter plot smoother** can be defined as a function (remember the general definition of *function*) of $\mathbf{x}$ and $\mathbf{y}$ with domain at least containing the values in $\mathbf{x}$: $s = \mathbf{S}[\mathbf{y}|\mathbf{x}]$.
- There is usually a "recipe" that gives $s(x_0)$, which is the function $\mathbf{S}[\mathbf{y}|\mathbf{x}]$ evaluated at x_0, for all x_0. We will call x_0 the *target value* when we giving the recipe.

Note: Some recipes don't give an $s(x_0)$ for all x_0, but only for the x's included in $\mathbf{x}$.

- Note we will call the vector $\{s(x_1), \ldots, s(x_n)\}'$ as **the smooth**.
- Here is a stupid example: If we assume a random design model and take expectations over the empirical distribution $\hat{F}$, defined by the observations, we have for any $x_0 \in \{x_1, \ldots, x_n\}$,

$$E_{\hat{F}}[Y|X = x_0] = ave\{y_i; x_i = x_0\}.$$

- Define $s(x_0) = E_{\hat{F}}[Y|X = x_0]$. What happens if the x_i are unique?

- Since Y and X are, in general, non-categorical, we don't expect to find many replicates at any given value of X. This means that we could end up with the data again, $s(x_0) = y_0$ for all x_0. Not very smooth!
- Note: For convenience, we assume that the data are sorted by X in following sections.
- Many smoothers force $s(x)$ to be a smooth function of x. This is a fancy way of saying we think data points that are close (in x) should have roughly the same expectation.

Parametric smoother

- These are what you have seen already. We force a function defined by "few" parameters on the data and use something like least squares to find the "best" estimates for the parameters.
- For example, a regression line computed with least squares can be thought of as a smoother. In this case

$$S[\mathbf{y}|\mathbf{x}](x_0) = (1, x_0)\,(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

  with $\mathbf{X}$ a design matrix containing a column of 1's and $\mathbf{x}$ (`cbind(1,x)`).
- The lack of flexibility of these types of smoother can make them provide misleading results.

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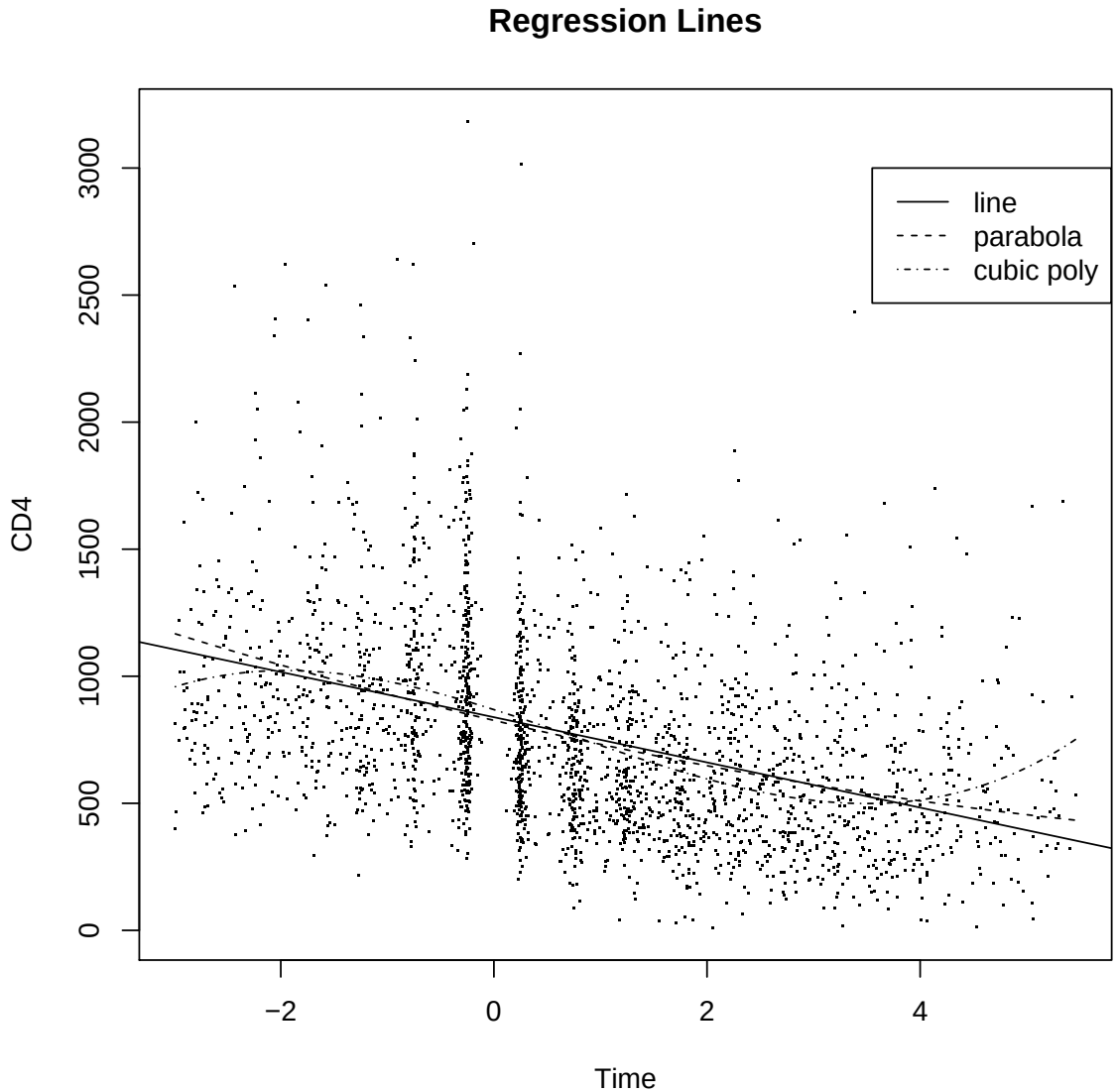

Bin smoothers

- A bin smoother, also known as a **regressogram**(Regression+Histgram), mimics a categorical smoother by partitioning the predicted value into disjoint and exhaustive regions, then averaging the response in each region.
- Formally, we choose cut-points $c_0 < \cdots < c_K$ where $c_0 = -\infty$ and $c_K = \infty$, and define

$$R_k = \{i : c_k \leq x_i < c_{k+1}\}; k = 0, \ldots, K$$

the indexes of the data points in each region. Then $S[\mathbf{y}|\mathbf{x}]$ is given by

$$s(x_0) = ave_{i \in R_k}\{y_i\} \text{ if } x_0 \in R_k$$

Notice that the bin smoother will have discontinuities.

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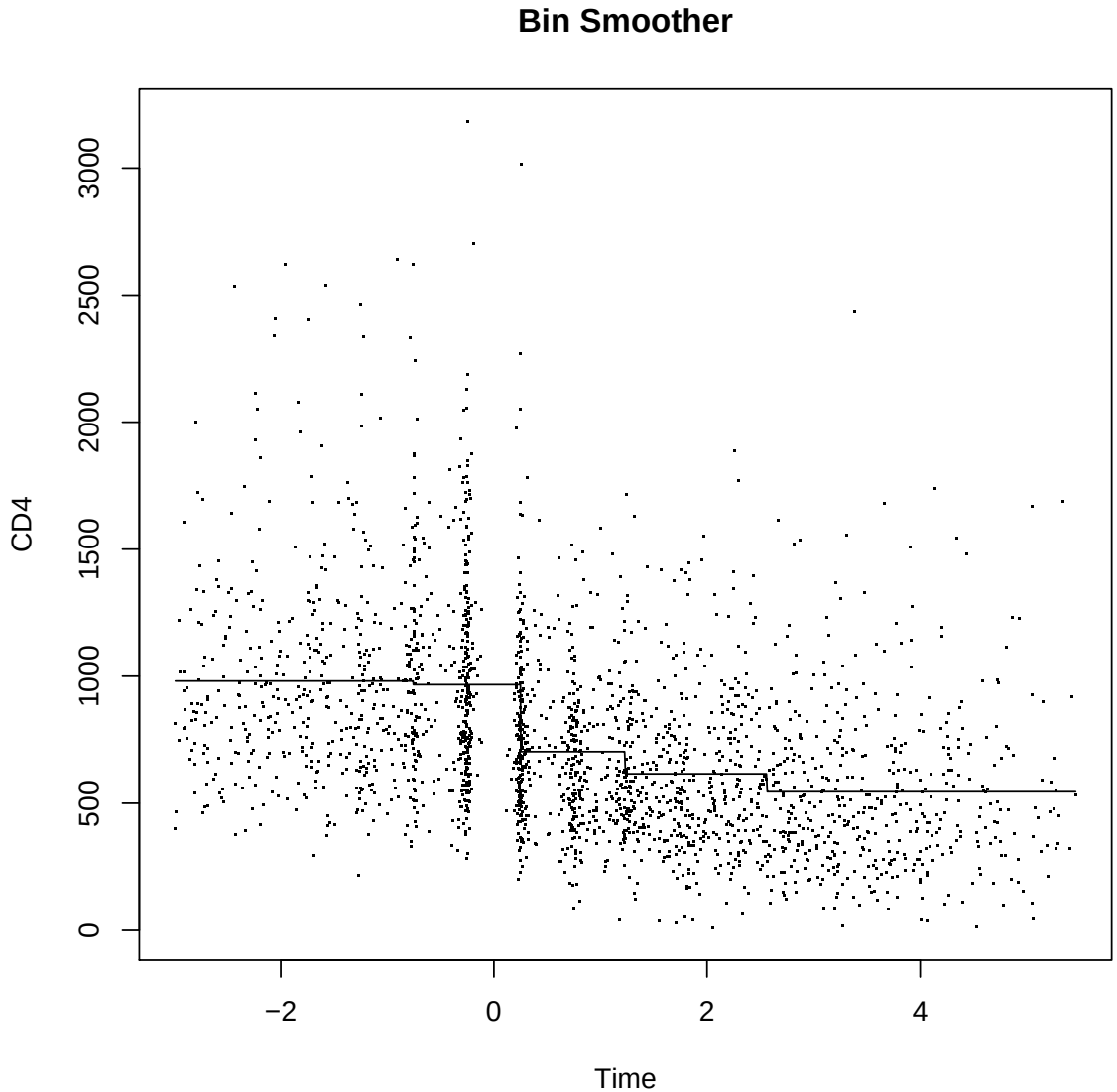

- Since we have no replicates and we want to force $s(x)$ to be smooth we can use the motivation that under some statistical model, for any x_0 values of $f(x) = E[Y|X = x]$ for x close to x_0 are similar.
- How do we define close? A formal definition is the *symmetric nearest neighborhood*

$$N^S(x_i) = \{\max(i-k,1), \ldots, i-1, i, i+1, \min(i+k,n)\}$$

- We may now define running mean as:

$$s(x_i) = ave_{j \in N^S(x_i)}\{y_j\}$$

We can also forget about the symmetric part and simply define the nearest k neighbors.

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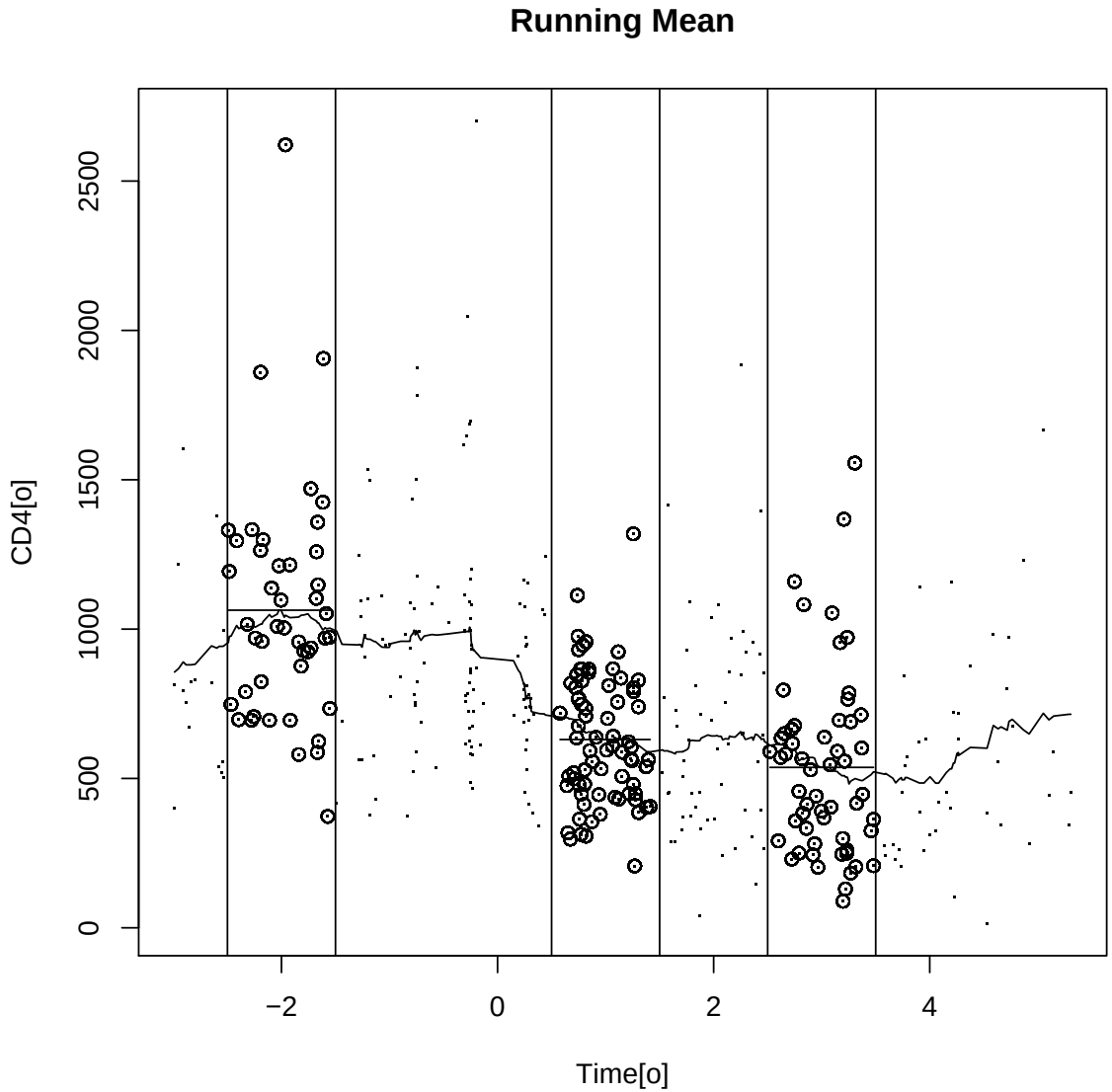

- This usually too wiggly to be considered useful. Why do you think?
- Notice we can also fit a line instead of a constant. This procedure is called running-line.
- Can you write out the recipe for $s(x_i)$ for the running-line smoother?

- One of the reasons why the previous smoothers is wiggly is because when we move from x_i to x_{i+1} two points are usually changed in the group we average.
- If the new two points are very different then $s(x_i)$ and $s(x_{i+1})$ may be quite different. One way to try and fix this is by making the transition smoother. That's the idea behind kernel smoothers.
- Generally speaking a kernel smoother defines a set of weights $\{W_i(x)\}_{i=1}^n$ for each x and defines

$$s(x) = \sum_{i=1}^{n} W_i(x) y_i.$$

- We will see that most scatter plot smoothers can be considered to be kernel smoothers in this very general definition.
- What is called a kernel smoother in practice has a simple approach to represent the weight sequence $\{W_i(x)\}_{i=1}^n$ by describing the shape of the weight function $W_i(x)$ by a density function with a scale parameter that adjusts the size and the form of the weights near x.
- It is common to refer to this shape function as a *kernel* K. The kernel is a continuous, bounded, and symmetric real function K which integrates to one,

$$\int K(u)\,du = 1.$$

- For a given scale parameter h, the weight sequence is then defined by

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

  Notice: $\sum_{i=1}^{n} W_{hi}(x_i) = 1$

- The kernel smoother is then defined for any x as before by

$$s(x) = \sum_{i=1}^{n} W_{hi}(x) Y_i.$$

- Notice: if we consider x and y to be observations of random variables X and Y then one can get an intuition for why this would work because

$$E[Y|X] = \int y \frac{f_{X,Y}(x,y)}{f_X(x)} dy,$$

with $f_X(x)$ the marginal distribution of X and $f_{X,Y}(x,y)$ the joint distribution of (X,Y), and

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

- Because we think points that are close together are similar, a kernel smoother usually defines weights that decrease in a smooth fashion as one moves away from the target point.
- Running mean smoothers are kernel smoothers that use a "box" kernel. A natural candidate for K is the standard Gaussian density. (This is very inconvenient computationally because its never 0). This smooth is shown in the following figure for $h = 1$ year.

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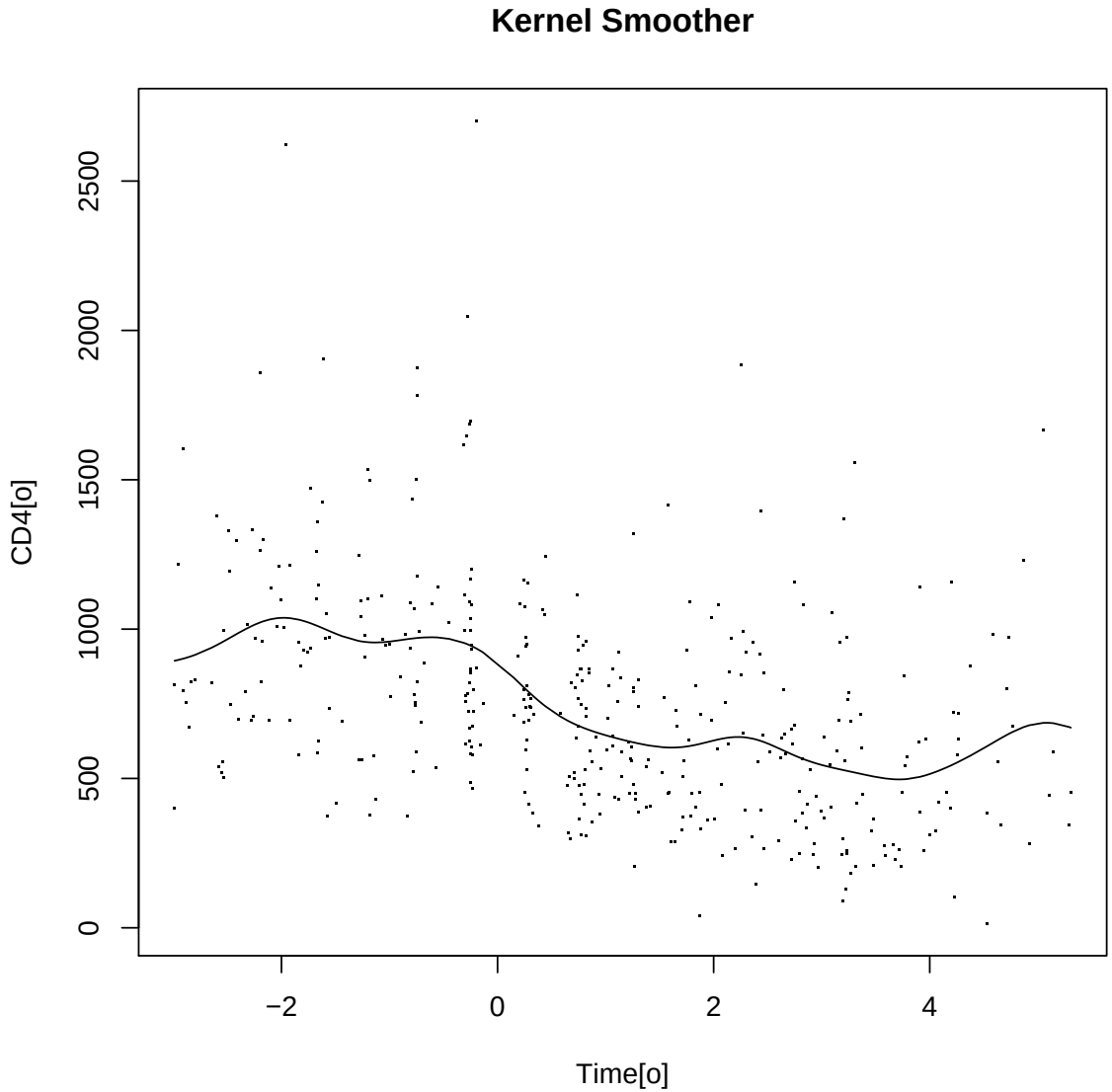

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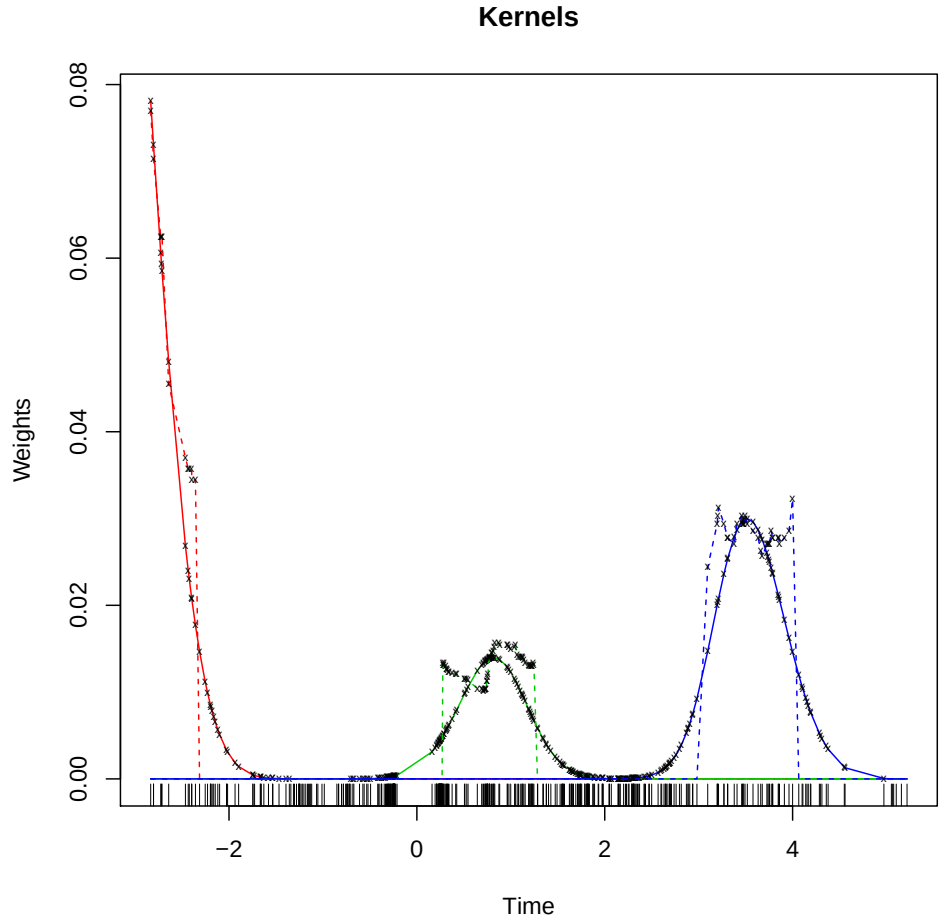

We can see the weight sequence for the box and Gaussian kernels for three values of x.

An Asymptotic result

- For the asymptotic theory presented here we will assume the stochastic design model with a one-dimensional covariate.
- For the first time in this Chapter we will set down a specific stochastic model. Assume we have n i.i.d observations of the random variables (X, Y) and that

$$Y_i = m(X_i) + \varepsilon_i, i = 1, \ldots, n \tag{1}$$

  where X has marginal distribution $f_X(x)$ and the ε_i i.i.d errors independent of the X. A common extra assumption is that the errors are normally distributed.
- For each n we define an estimate for $m(x)$ using the kernel smoother with scale parameter h_n. We are now going to let n go to infinity.

Theorem

Under the following assumptions

1. $\int |K(u)|\, du < \infty$
2. $\lim_{|u|\to\infty} uK(u) = 0$
3. $E(Y^2) \leq \infty$
4. $n \to \infty, h_n \to 0, nh_n \to \infty$

Then, at every point of continuity of $m(x)$ *and* $f_X(x)$ *we have*

$$\frac{\sum_{i=1}^n K\left(\frac{x-x_i}{h}\right) y_i}{\sum_{i=1}^n K\left(\frac{x-x_i}{h}\right)} \to m(x) \text{ in probability.}$$

Linear smoothers

- Most of the smoother presented here are linear smoothers which means that the fit at any point x_0 can be written as

$$s(x) = \sum_{j=1}^{n} S_j(x) y_j.$$

- In practice we usually have the model

$$Y_i = m(X_i) + \epsilon_i$$

and we have observations $\{(x_i, y_i)\}$. Many times it is the vector $m = \{m(x_1), \ldots, m(x_n)\}'$ we are after.

- In this case the vector of estimates $\hat{m} = \{\hat{m}(x_1), \ldots, \hat{m}(x_n)\}'$ can be written as

$$\hat{m} = \mathbf{Sy}$$

with $\mathbf{S}$ a matrix with the i, j-th entry $S_j(x_i)$. We will call $\hat{m}$ the *smooth*.

- This makes it easy to figure out things like the variance of $\hat{m}$ since

$$var[\mathbf{Sy}] = \mathbf{S}var[\mathbf{y}]\mathbf{S}'$$

which in the case of i.i.d data is $\sigma^2\mathbf{SS}'$.