Week 4: Nonparametric Regression

MATH-517 Statistical Computation and Visualization

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KDE

One-dimensional KDE (from last week):

$$\hat{f}(x) = \frac{1}{nh_n} \sum_{i=1}^{n} K\left(\frac{X_i - x}{h_n}\right)$$

Multidimensional generalization (separable) when $X_1, \ldots, X_n \in \mathbb{R}^d$:

$$\hat{f}(\mathbf{x}) = \frac{1}{nh^d} \sum_{i=1}^{n} K\left(\frac{X_{i,1} - x_1}{h}\right) \cdot \ldots \cdot K\left(\frac{X_{i,d} - x_d}{h}\right)$$

Section 1

Non-parametric Regression

Non-parametric Regression Setup

- we observe i.i.d. copies of a bivariate random vector $(X, Y)^\top$
  - a random sample $(X_1, Y_1)^\top, \dots, (X_n, Y_n)^\top$
- the response variable Y is related to the covariate X through

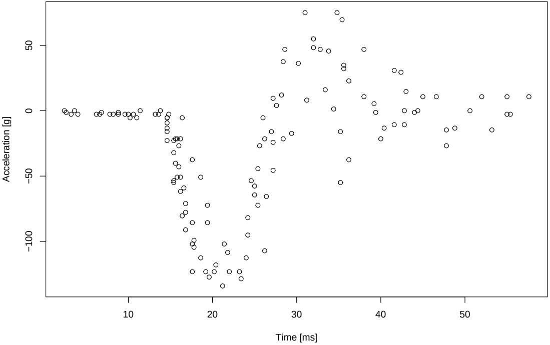
$$Y_i = m(X_i) + \epsilon_i, \quad \mathbb{E}(\epsilon_i) = 0 \quad \text{and } \mathrm{var}(\epsilon_i) = \sigma^2$$

- we are interested in the conditional expectation of Y given X, i.e., the regression function

$$m(x) = \mathbb{E}(Y|X = x)$$

- we want to avoid parametric assumptions

Data Example



- head acceleration Y depending on time X in a simulated motorcycle accident used to test crash helmets

Local average estimator

Goal: estimate $m(x) = \mathbb{E}(Y \big| X = x)$ from $(X_1, Y_1)^\top, \ldots, (X_n, Y_n)^\top$ i.i.d.

Since $m(x) = \mathbb{E}(Y|X = x)$, one can estimate $m(x)$ by averaging the Y_is for which X_i is "close" to x

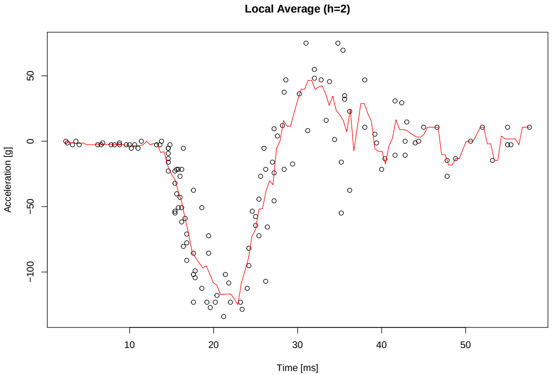
$\Rightarrow$ different averaging methods and different measures of closeness yield different estimators

The local average estimator is

$$\widehat{m}_n(x) = \frac{\sum_{i=1}^n I(x - h < X_i \leq x + h) Y_i}{\sum_{i=1}^n I(x - h < X_i \leq x + h)}$$
$$= \frac{\sum_{i=1}^n \frac{1}{2} \mathbb{1}_{[-1,1)} \left(\frac{x - X_i}{h} \right) Y_i}{\sum_{i=1}^n \frac{1}{2} \mathbb{1}_{[-1,1)} \left(\frac{x - X_i}{h} \right)},$$

for $h > 0$

Local average estimator



Local Constant Regression

Since $m(x) = \int_{\mathbb{R}} y f_{Y|X}(y|x) dy = \frac{\int_{\mathbb{R}} y f_{X,Y}(x,y) dy}{f_X(x)}$ and we can now estimate densities, let's plug in those estimators

$$\hat{f}_X(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right)$$

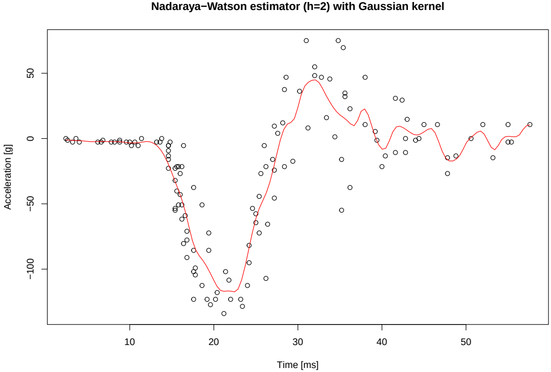
$$\hat{f}_{X,Y}(x,y) = \frac{1}{nh^2} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right) K\left(\frac{y - Y_i}{h}\right)$$

to obtain

$$\widehat{m}(x) = \frac{\sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right) Y_i}{\sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right)}$$

$\Rightarrow$ The "boxcar" kernel is replaced by a general kernel and yields the so-called Nadaraya–Watson kernel estimator

Local Constant Regression



Local Constant Regression

The Nadaraya–Watson kernel estimator

$$\widehat{m}(x) = \frac{\sum_{i=1}^n K\left(\frac{X_i - x}{h}\right) Y_i}{\sum_{i=1}^n K\left(\frac{X_i - x}{h}\right)} = \sum_{i=1}^n \frac{K\left(\frac{X_i - x}{h}\right)}{\sum_{j=1}^n K\left(\frac{X_j - x}{h}\right)} Y_i = \sum_{i=1}^n W_i^0(x) Y_i$$

is a weighted mean of the Y_i and can be considered as a solution to the weighted least squares:

$$\widehat{m}(x) = \underset{\beta_0 \in \mathbb{R}}{\arg\min} \sum_{i=1}^n K\left(\frac{x - X_i}{h}\right) (Y_i - \beta_0)^2$$

For a fixed x, this is a weighted intercept-only regression, with weights given by the kernel $\Rightarrow$ estimate suffers from boundary bias

What if we went for better than intercept-only regression?

Local Polyomial Regression

The aim is to find the local regression parameters $\beta(x)$ s.t.

$$\hat{\beta}(x) = \underset{\beta \in \mathbb{R}^{p+1}}{\arg\min} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right) \{Y_i - \beta_0 - \beta_1(X_i - x) - ... - \beta_p(X_i - x)^p\}^2$$

Local Polyomial Regression

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$$\hat{\beta}(x) = \underset{\beta \in \mathbb{R}^{p+1}}{\arg\min} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right) \{Y_i - \beta_0 - \beta_1(X_i - x) - ... - \beta_p(X_i - x)^p\}^2$$

Why does this make sense?

Recall that the aim is to estimate $m(x) = \mathbb{E}(Y|X = x)$ and hence to minimize the SS

$$\sum_{i=1}^{n} \{Y_i - m(X_i)\}^2$$

A Taylor expansion of m for x close to X_i is

$$m(X_i) \approx m(x) + (X_i - x)m'(x) + \frac{(X_i - x)^2}{2!} m''(x) + ... + \frac{(X_i - x)^p}{p!} m^p(x),$$

Local Polyomial Regression

The SS can be rewritten as

$$\sum_{i=1}^{n}\left\{Y_i - \sum_{j=0}^{p}\frac{m^j(x)}{j!}(X_i - x)^j\right\}^2$$

Thus, $\hat{\beta}_j(x)$ estimates $\frac{m^{(j)}(x)}{j!}$

- $\widehat{m}(x) = \hat{\beta}_0(x)$
- $\widehat{m'}(x) = \hat{\beta}_1(x)$

Finally, add a weighting kernel to make the contributions of X_i dependent on their distance to x

$\Rightarrow \hat{\beta}$ becomes the solution to a weighted least squares problem

$$\hat{\beta} = \arg\min_{\beta\in\mathbb{R}^{p+1}}(\mathbf{Y}-\mathbf{X}\beta)^\top\mathbf{W}(\mathbf{Y}-\mathbf{X}\beta) = (\mathbf{X}^\top\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{W}\mathbf{Y},$$

where $\mathbf{W}$ is a diagonal matrix with entries depending on the kernel!

Local Linear Regression

Choosing the order $p = 1$ leads to the local linear estimator

$$(\hat{\beta}_0(x), \hat{\beta}_1(x)) = \arg\min_{\beta \in \mathbb{R}^2} \sum_{i=1}^{n} \{Y_i - \beta_0 - \beta_1(X_i - x)\}^2 K\left(\frac{x - X_i}{h}\right),$$

It can be shown that $\hat{m}(x) = \hat{\beta}_0(x) = \sum_{i=1}^{n} w_{ni}(x) Y_i$, where

$$w_{ni}(x) = \frac{1}{nh} \frac{K\left(\frac{x - X_i}{h}\right)\left\{S_{n,2}(x) - (X_i - x)\, S_{n,1}(x)\right\}}{S_{n,0}(x) S_{n,2}(x) - S_{n,1}^2(x)}$$

with $S_{n,k}(x) = \frac{1}{nh} \sum_{i=1}^{n} (X_i - x)^k K\left(\frac{X_i - x}{h}\right)$

- $\sum_{i=1}^{n} w_{ni}(x) = 1$

$\Rightarrow$ $\hat{m}$ is a linear smoother, i.e., $\forall x$, it can be defined by a weighted average: $\hat{m}(x) = \sum_{i=1}^{n} l_i(x) Y_i$ (valid for Nadaraya–Watson and any p)

Visualization

A shiny App can be found here

Bias and Variance

For local linear regression, similarly to KDE and under regularity assumptions on m, f, K, h, and nh_n,

$$\text{bias}\{\widehat{m}(x)\} = \frac{1}{2}m''(x)h_n^2 \int z^2 K(z)dz + o_P(h_n^2)$$

$$\text{var}\{\widehat{m}(x)\} = \frac{\sigma^2(x)}{f_X(x)} \frac{\int \{K(z)\}^2 dz}{nh_n} + o_P\left(\frac{1}{nh_n}\right)$$

where $\sigma^2(x) = \text{var}(Y_1 | X_1 = x)$ is the conditional/local variance

This implies that

- the bias depends on the curvature of m: negative for concave and positive for convex regions
- the variance decreases at a rate inversely proportional to the effective sample size nh_n

For other orders, similar expressions can be obtained

Nadaraya–Watson vs Local Linear estimator

It can be shown that, under the same smoothing conditions on $f(x)$ and $m(x)$, the Nadaraya–Watson estimator $\tilde{m}$

- has the same variance as the local linear estimator $\hat{m}$
- has bias

$$\text{bias}\{\tilde{m}(x)\} = h_n^2 \left\{ \frac{1}{2} m''(x) + m'(x) \frac{f'(x)}{f(x)} \right\} \int z^2 K(z) dz + o_P(h_n^2)$$

$\Rightarrow$ At the boundary points, the NW estimator bears high value due to the large absolute value of $f'(x)/f(x)$

$\Rightarrow$ Local linear estimation has no boundary bias at it does not depend on $f(x)$ (no design bias)

Bandwidth Selection

Similarly to what we did last week with KDEs, we consider

$$MSE\{\widehat{m}(x)\} = \mathrm{var}\{\widehat{m}(x)\} + \left[\mathrm{bias}\{\widehat{m}(x)\}\right]^2$$

and, dropping the little-o terms, we obtain

$$AMSE\{\widehat{m}(x)\} = \frac{\sigma^2(x)\int\{K(z)\}^2 dz}{f_X(x) n h_n} + \frac{1}{4}\{m''(x)\}^2 h_n^4 \left(\int z^2 K(z) dz\right)^2 .$$

Now, a local bandwidth choice can be obtained by optimizing AMSE. Taking derivatives and setting them to zero, we obtain

$$h_{opt}(x) = n^{-1/5} \left[\frac{\sigma^2(x)\int\{K(z)\}^2 dz}{\left\{m''(x)\int z^2 K(z) dz\right\}^2 f_X(x)}\right]^{1/5}$$

Bandwidth Selection

$$h_{opt}(x) = n^{-1/5} \left[\frac{\sigma^2(x) \int \{K(z)\}^2 dz}{\left\{m''(x) \int z^2 K(z) dz\right\}^2 f_X(x)} \right]^{1/5}$$

This is somewhat more complicated compared to the KDE case, because we have to estimate

- the marginal density $f_X(x)$,
  - let's say that we already know how to do this, e.g., by KDE even though that requires a choice of yet another bandwidth
- the local variance function $\sigma^2(x) = \mathrm{var}(Y_1 | X_1 = x)$, and
- the second derivative of the regression function $m''(x)$

Again, like in the case of KDEs, the global bandwidth choice can be obtained by integration:

- calculate $AMISE(\widehat{m}) = \int AMSE\{\widehat{m}(x)\} dx$, and
- set $h_{AMISE} = \underset{h>0}{\arg\min}\ AMISE(\widehat{m})$

Rule of Thumb Plug-in Algorithm

Replace the unknown quantities in

$$h_{AMISE} = n^{-1/5} \left[\frac{\int K^2(z)dz \int \sigma^2(x)dx}{\int z^2 K(z)dz \int \{m''(x)\}^2 f_X(x)dx} \right]^{1/5}$$

by parametric OLS estimators

- Assume homoscedasticity and a quartic kernel, then

$$h_{AMISE} = n^{-1/5} \left(\frac{35\sigma^2 |supp(X)|}{\theta_{22}} \right)^{1/5}, \quad \theta_{22} = \int \{m''(x)\}^2 f_X(x)dx$$

- Block the sample in N blocks and fit, in each block j, the model

$$y_i = \beta_{0j} + \beta_{1j}x_i + \beta_{2j}x_i^2 + \beta_{3j}x_i^3 + \beta_{4j}x_i^4 + \epsilon_i$$

to obtain estimate $\hat{m}_j(x_i) = \hat{\beta}_{0j} + \hat{\beta}_{1j}x_i + \hat{\beta}_{2j}x_i^2 + \hat{\beta}_{3j}x_i^3 + \hat{\beta}_{4j}x_i^4$

Rule of Thumb Plug-in Algorithm

- Estimate the unknown quantities by

$$\hat{\theta}_{22}(N) = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{N}\hat{m}_j''(X_i)\hat{m}_j''(X_i)\mathbb{1}_{X_i\in\mathcal{X}_j}$$

$$\hat{\sigma}^2(N) = \frac{1}{n-5N}\sum_{i=1}^{n}\sum_{j=1}^{N}\{Y_i - \hat{m}_j(X_i)\}^2\mathbb{1}_{X_i\in\mathcal{X}_j}$$

Remark Unknown quantities can also be replaced by non-parametric estimates, using a pilot bandwidth (see lecture notes for details).

Why Local Linear?

Bias and variance can be calculated similarly also for higher order local polynomial regression estimators. In general:

- bias decreases with an increasing order
- variance increases with increasing order, but only for $p = 2k + 1 \to p + 1$, i.e., when increasing an odd order to an even one

For this reason, odd orders are preferred to even ones

- $p = 1$ is easy to grasp as it corresponds to locally fitted simple regression line
- increasing p has a similar effect to decreasing the bandwidth h
  - hence $p = 1$ is usually fixed and only h is tuned

Section 2

Other Smoothers

Smoothing Splines

Consider the optimization problem

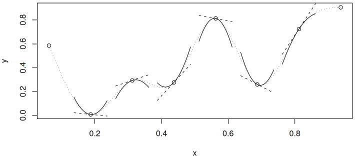
$$\arg\min_{g \in C^2} \sum_{i=1}^{n} \{Y_i - g(X_i)\}^2 + \lambda \int \{g''(x)\}^2 dx$$

- measure of closeness to the data, and
- smoothing penalty: $\lambda > 0$ controls the trade-off between fit and smoothness

Unique solution: the **natural cubic spline**

- piece-wise cubic polynomial between
- knots at X_i, $i = 1, \ldots, n$
- two continuous derivatives at the knots
- $\hat{m}''(x_1) = \hat{m}''(x_n) = 0$

$\Rightarrow$ it has n free parameters

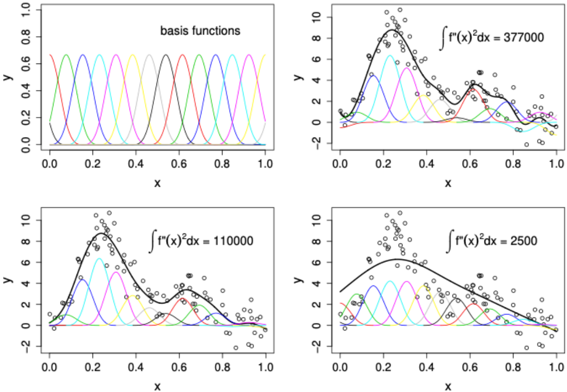


Source: Wood (2017)

Cubic Spline Basis

A natural cubic spline g with n knots can be expressed w.r.t. the natural cubic spline basis $\{e_j\}$ (a set of basis functions) as

$$m(x) = \sum_{j=1}^{n} \gamma_j e_j(x)$$



Smoothing Splines

A natural cubic spline g with n knots can be expressed w.r.t. the natural cubic spline basis $\{e_j\}$ (a set of basis functions) as

$$m(x) = \sum_{j=1}^{n} \gamma_j e_j(x)$$

Let

- $\gamma = (\gamma_1, \dots, \gamma_n)^\top \in \mathbb{R}^n$ be unknown coefficients
- $E := (e_{ij}) := \{e_j(x_i)\}_{i,j=1}^{n} \in \mathbb{R}^{n \times n}$ and
- $\Omega = (\omega_{ij}) \in \mathbb{R}^{n \times n}$ with $\omega_{ij} = \int e_i''(x) e_j''(x) dx$

Then, the optimisation problem becomes

$$\sum_{i=1}^{n} \{Y_i - m(X_i)\}^2 + \lambda \int \{m''(x)\}^2 dx \quad \equiv \quad (Y - E\gamma)^\top (Y - E\gamma) + \lambda \gamma^\top \Omega \gamma$$

Smoothing Splines

The solution is obtained in closed form

$$\hat{\gamma} = (E^\top E + \lambda\Omega)E^\top Y$$

The fitted values are

$$\widehat{Y} = (\hat{m}_\lambda(x_1), \dots, \hat{m}_\lambda(x_n))^\top = E\hat{\gamma} = S_\lambda Y, \quad \text{with } S_\lambda = E(E^\top E + \gamma\Omega)E^\top$$

$\Rightarrow$ smoothing splines are linear smoothers

The matrix S_λ is the hat matrix and $tr(S_\lambda)$ plays the role of the degrees of freedom (how many effective parameters you have in the model)

- Although there are n unknown coefficients, many are shrunken towards zero through the smoothness/roughness penalty
- λ encodes the bias-variance trade-off ($\lambda = 0:$ very rough, $\lambda = \infty$: very smooth)
- λ is chosen by CV (next week's lecture)

Orthogonal Series: Regression Splines

- take a pre-defined set of orthogonal functions $\{e_j\}_{j=1}^{\infty}$
  - customarily some basis, e.g., Fourier basis, B-splines, etc.
- truncate it to $\{e_j\}_{j=1}^{p}$
- approximate $m(x) \approx \sum_{j=1}^{p} \gamma_j e_j(x)$

Then estimate m by least-squares:

$$\arg\min_{\gamma \in \mathbb{R}^p} \sum_{i=1}^{n} \left\{ Y_i - \gamma_1 e_1(X_i) - \ldots - \gamma_p e_p(X_i) \right\}^2$$

- just a single linear regression
- no penalty term, simplicity achieved via truncation
  - bias-variance trade-off controlled by the choice of p
  - can be related to smoothness when e_j's get more wiggly with increasing j (which is typical for most bases)
  - choice of location of knots is critical but tricky too (not needed with smoothing splines)

Assignment 3 [5 %]

Go to Assignment 3 for details.