Nonparametric Methods

Michael R. Roberts

Department of Finance
The Wharton School
University of Pennsylvania

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Overview

- Great for data analysis and robustness tests.
- Also used extensively in program evaluation
  1. Estimation of propensity scores
  2. Estimation of conditional regression functions
- Goal here is to introduce and operationalize nonparametric
  1. density estimation, and
  2. regression

Probability Density Functions (PDF)

- Basic characteristics of a random variable X is its PDF, f or CDF, F
- Given a sample of observations $X_i : i = 1, ..., N$, goal is to estimate the PDF
- Options
  1. Parametric: Assume a functional form for f and estimate the parameters of the function. E.g., $N(\mu, \sigma^2)$
  2. Nonparametric: Estimate the full function, f, without assuming a particular functional form for f.
- Nonparametric "let the data speak."
- We're going to follow Silverman (1986) closely.

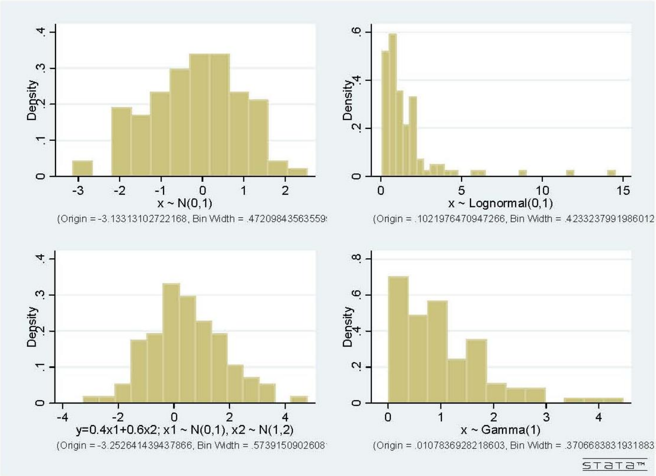
Histogram

- **Origin**: x_0
- **Bin Width**: h (a.k.a. **window width**)
- **Bins**: $[x_0 + mh, x_0 + (m+1)h)$ for $m \in \mathbb{Z}$
- **Histogram**:

$$\hat{f}(x) = \frac{1}{nh} (\# \text{ of } X_i \text{ in the same bin as } x)$$

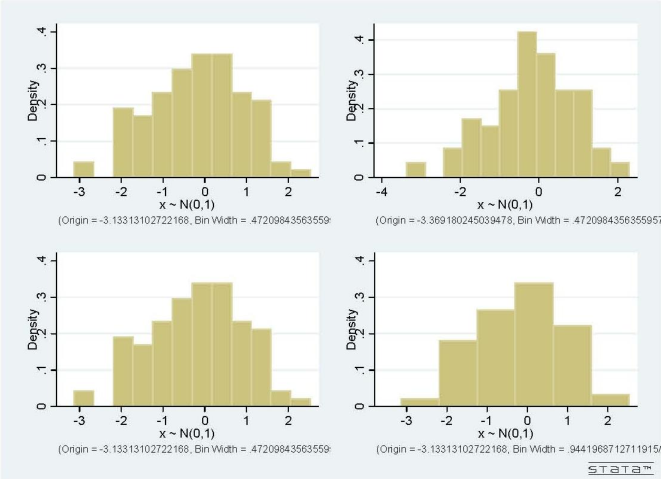
Sample Histograms

- $N = 100$, Origin $= Min(X_i)$, Bin Width $= 0.79 \times IQR \times N^{1/5}$



Sensitivity of Histograms

- Histogram estimate is sensitive to choice of origin and bin width



Naive Estimator

- The density, f, of rv X can be written

$$f(x) = \lim_{h \to 0} \frac{1}{2h} Pr(x - h < X < x + h)$$

- Given h, we can estimate $Pr(x - h < X < x + h)$ by the proportion of observations falling in the interval (bin)

$$\hat{f}(x) = \frac{1}{2nh}[\# \text{ of } X_i \text{ falling in } (x - h, x + h)]$$

- Mathematically, this is just

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

where

$$W(x) = \begin{cases} 1/2 & \text{if} \quad |x| < 1 \\ 0 & \text{otherwise} \end{cases}$$

Naive Estimator - An Example

- Consider a sample $\{X_i\}_{i=1}^{10}$

$$1, 2, 3, 4, 5, 6, 7, 8, 9, 10$$

- Let the bin width $= 2$, then

$$\begin{aligned}
\hat{f}(4) &= \frac{1}{10}\left\{\frac{1}{2}W\left(\frac{4-1}{2}\right)+\frac{1}{2}W\left(\frac{4-2}{2}\right)+\ldots+\frac{1}{2}W\left(\frac{4-10}{2}\right)\right\} \\
&= \frac{1}{10}\left\{0+0+\left(\frac{1}{2}\frac{1}{2}\right)+\left(\frac{1}{2}\frac{1}{2}\right)+\left(\frac{1}{2}\frac{1}{2}\right)+0+\ldots+0\right\} \\
&= \frac{3}{40}
\end{aligned}$$

Naive Estimator - An Example from Silverman

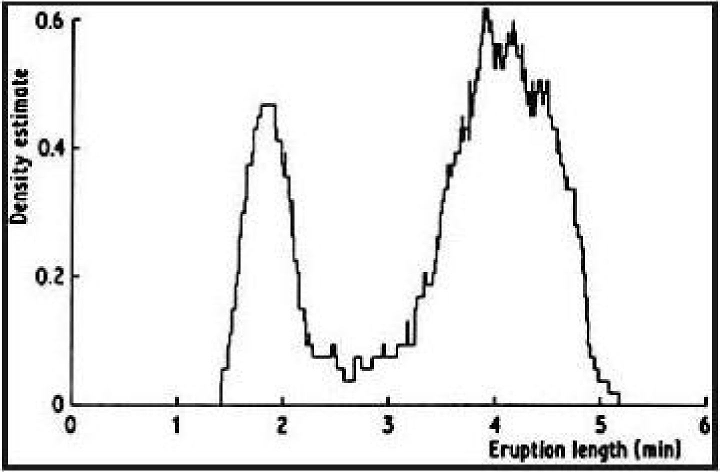


Fig. 2.3 Naive estimate constructed from Old Faithful geyser data, $h = 0.25$.

Naive Estimator - Discussion

- From def of $W(x)$, estimate of f is constructed by placing box of width $2h$ and height $(2nh)^{-1}$ on each observation and summing.
- Attempt to construct histogram where every point, x, is the center of a sampling interval $(x + h, x - h)$
- We don't need a choice of origin, x_0, anymore
- Choice of bin width, h, remains and is crucial for controlling degree of smoothing
  - Large h produce smoother estimates
  - Small h produce more jagged estimates
- Drawbacks: $\hat{f}$ is discontinuous, jumps at points $X + i \pm h$ and zero derivative everywhere else

Definition & Intuition

- Replace weight fxn W in naive estimator by a **Kernel Function K**:

$$\int_{-infty}^{\infty} K(x)dx = 1$$

- Kernel estimator is:

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

where h is **window width** or **smoothing parameter** or **bandwidth**

- Intuition:
  - Naive estimator is a sum of boxes centered at observations
  - Kernel estimator is a sum of bumps centered at observations

Kernel choice determines shape of bumps

Kernel Estimator - Example

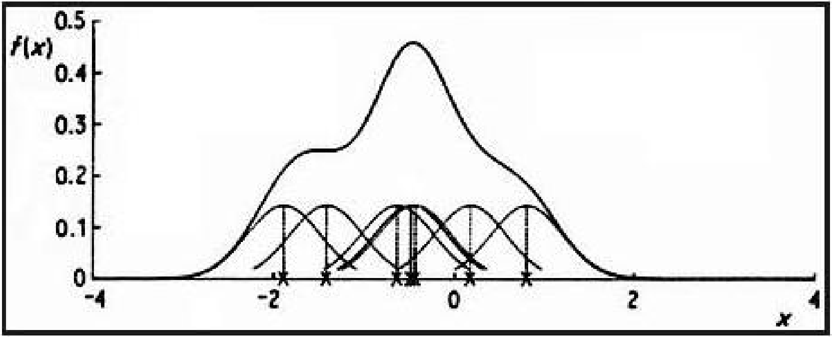


Fig. 2.4 Kernel estimate showing individual kernels. Window width 0.4.

Varying the Window Width

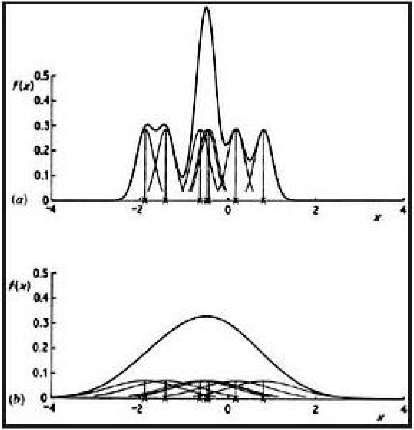


Fig. 2.5 Kernel estimates showing individual kernels. Window widths: (a) 0.2; (b) 0.8.

Example Discussion

- X's correspond to data points (the sample: $N = 7$)
- Centered over each data point, is a little curve — bump — $1/(nh)K[(x - X_i)/h]$
- The estimated density, $\hat{f}$, constructed by adding up each bump at each data point is also shown
- As $h \to 0$ we get a sum of Dirac delta function spikes at the observations
- If K is a PDF, then so is $\hat{f}$
- $\hat{f}$ inherits the continuity and differentiability properties of K
- For data with long-tails, get spurious noise to appear in the tails since window width is fixed across entire sample dynamic based on bootstrapped std
  - If window width widened to smooth away tail detail, detail in main part of dist is lost
  - adaptive methods address this problem

Long Tail Data

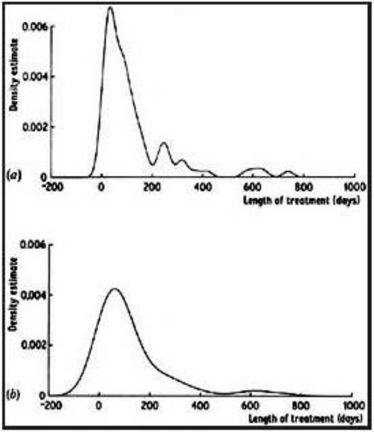


Fig. 2.9 Kernel estimates for suicide study data. Window widths: (a) 20; (b) 60.

Sample Kernels: Definitions

$$\text{Rectangular (Uniform)} : K(t) = \begin{cases} \frac{1}{2} & |t| < 1 \\ 0 & \text{otherwise} \end{cases}$$

$$\text{Triangular} : K(t) = \begin{cases} 1 - |t| & |t| < 1 \\ 0 & \text{otherwise} \end{cases}$$

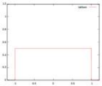
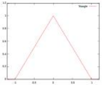
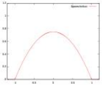
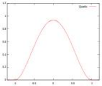
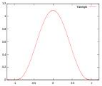
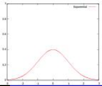
$$\text{Epanechnikov} : K(t) = \begin{cases} \frac{3}{4}\left(1 - \frac{1}{5}t^2\right) / \sqrt{5} & |t| < \sqrt{5} \\ 0 & \text{otherwise} \end{cases}$$

$$\text{Biweight (Quartic)} : K(t) = \begin{cases} \frac{15}{16}\left(1 - t^2\right)^2 & |t| < 1 \\ 0 & \text{otherwise} \end{cases}$$

$$\text{Triweight} : K(t) = \begin{cases} \frac{35}{32}\left(1 - t^2\right)^3 & |t| < 1 \\ 0 & \text{otherwise} \end{cases}$$

$$\text{Gaussian} : K(t) = \frac{1}{\sqrt{2\pi}} e^{(-1/2)t^2}$$

Sample Kernels - Figures

Kernel Functions, $K(u)$			$\int u^2K(u)du$	$\int K^2(u)du$
Uniform	$K(u) = \frac{1}{2}\mathbf{1}_{\{\lvert u\rvert\leq 1\}}$		$\frac{1}{3}$	$\frac{1}{2}$
Triangular	$K(u) = (1-\lvert u\rvert)\,\mathbf{1}_{\{\lvert u\rvert\leq 1\}}$		$\frac{1}{6}$	$\frac{2}{3}$
Epanechnikov	$K(u) = \frac{3}{4}(1-u^2)\,\mathbf{1}_{\{\lvert u\rvert\leq 1\}}$		$\frac{1}{5}$	$\frac{3}{5}$
Quartic	$K(u) = \frac{15}{16}(1-u^2)^2\,\mathbf{1}_{\{\lvert u\rvert\leq 1\}}$		$\frac{1}{7}$	$\frac{5}{7}$
Triweight	$K(u) = \frac{35}{32}(1-u^2)^3\,\mathbf{1}_{\{\lvert u\rvert\leq 1\}}$		$\frac{1}{9}$	$\frac{350}{429}$
Gaussian	$K(u) = \frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}u^2}$		1	$\frac{1}{2\sqrt{\pi}}$

Measures of Discrepancy

- Mean Square Error (Pointwise Accuracy)

$$\begin{aligned} MSE_x(\hat{f}) &= E[\hat{f}(x) - f(x)]^2 \\ &= \underbrace{[E\hat{f}(x) - f(x)]^2}_{Bias} + \underbrace{Var\hat{f}(x)}_{Variance} \end{aligned}$$

- Tradeoff: Bias can be reduced at expense of increased variance by adjusting the amount of smoothing
- Mean Integrated Square Error (Global Accuracy)

$$\begin{aligned} MISE_x(\hat{f}) &= E\int [\hat{f}(x) - f(x)]^2 dx \\ &= \underbrace{\int [E\hat{f}(x) - f(x)]^2 dx}_{\text{Integrated Bias}} + \underbrace{\int Var\hat{f}(x)dx}_{\text{Integrated Variance}} \end{aligned}$$

Useful Facts

- The bias is *not* a fxn of sample size

$\Longrightarrow$ Increasing sample size will not reduce bias

$\therefore$ Need to adjust the weight fxn (i.e., Kernel)

- Bias is a fxn of window width (and Kernel)

$\Longrightarrow$ Decreasing window width reduces bias

  - If window width fxn of sample size, then bias

Choosing the Smoothing Parameter

- Optimal window width derived as minimizer of (approximate) MISE is a fxn of the unknown density f
- Appropriate choice of smooth parameter depends on the goal of the density estimation
  1. If goal is data exploration to guide models and hypotheses, subjective criteria probably ok (see below)
  2. When drawing conclusions from estimated density, undersmoothing is probably good idea (easier to smooth than unsmooth a picture)

Reference to a Standard Distribution

- Use a standard family of distributions to assign a value to unknown density in optimal window width computation.
- E.g., assume f normal with $Var = \sigma^2$ and Gaussian kernel $\Longrightarrow$

$$h^* = 1.06\sigma n^{-1/5}$$

- Can estimate σ from the data using SD
- If pop dist is multimodal or heavily skewed, h^* will oversmooth

Robust Measures of Spread

- Can use robust measure of spread ($R =$IQR) to get different optimal smoothing parameter

$$h^* = 0.79Rn^{-1/5}$$

  but this exacerbates problems from multimodality/skew because it oversmooths

- Can try

$$h^* = 1.06An^{-1/5} \text{ or } h^* = 0.9An^{-1/5} \text{ or}$$

  where

$$A = min(SD, IQR/1.34)$$

Setup

- The basic problem is to estimate a function m:

$$y_i = m(x_i) + \varepsilon_i$$

where x_i is scalar rv (for ease), $E(\varepsilon_i | x) = 0$

- This is just a generalization of the linear model:

$$m(x_i) = x_i' \beta$$

- The goal is to estimate m

First Stab

- $$y_i = m(x_i) + \varepsilon_i$$

  where x_i is k-vector of rv's, $E(\varepsilon_i|x) = 0$
- This is just a generalization of the linear model:

  $$m(x_i) = x_i'\beta$$

- The goal is to estimate m

Local Regression

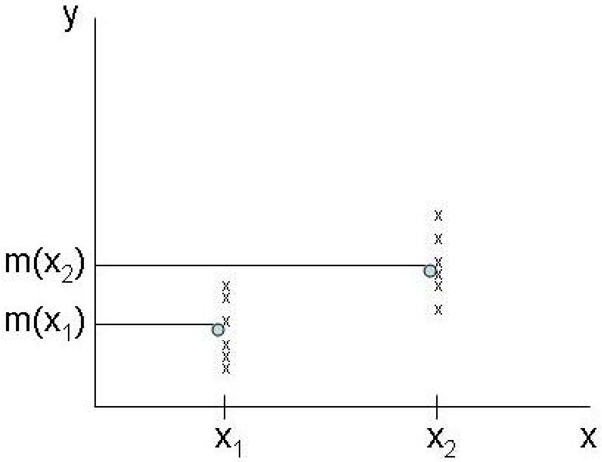
- Imagine x_i is a discrete rv.
- For each value that x_i can take, such as x, we can just average all of the y_i at that point to estimate m.

$$\hat{m} = \frac{1}{N_x} \sum_{i:x_i=x} y_i$$

where N_x is the number of observations where $x_i = x$

- This estimator is consistent (and a lot like OLS)

Local Regression - An Illustration



More Generally

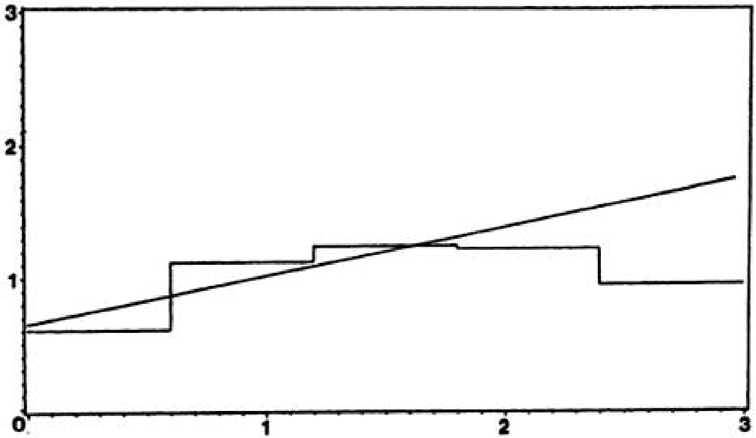
- This local averaging procedure can be defined by

$$\hat{m} = \frac{1}{N} \sum_{i=1}^{N} W_{ni}(x) Y_i \tag{1}$$

  where $\{W_{ni}(x)\}_{i=1}^{N}$ is a sequence of **weights** which may depend on the whole vector $\{X_i\}_{i=1}^{N}$
- Same bias versus variance tradeoff:
  - Large window width $\Longrightarrow$ a lot of smoothing $\Longrightarrow$ a lot of bias but small variance
  - Small window width $\Longrightarrow$ a lot of smoothing $\Longrightarrow$ little bias but a lot of variance

Nonparametric Regression Example

- Assume constant weights $\Longrightarrow$ jagged discontinuous function



Least Squares

- Local averaging formula (1) is a least squares estimator
- Assume weights $\{W_{ni}(x)\}_{i=1}^{N}$ are > 0 & sum to 1 $\forall x$

$$N^{-1}\sum_{i=1}^{N} W_{ni}(x) = 1$$

- Then $\hat{m}$ is a least squares estimate at x since $\hat{m}$ is the solution to

$$min_{\theta} N^{-1}\sum_{i=1}^{N} W_{ni}(x)(Y_i - \theta)^2$$

$$= \quad N^{-1}\sum_{i=1}^{N} W_{ni}(x)(Y_i - \hat{m}(x))^2$$

- Local avg is like finding a local WLS estimate

The Kernel

- Kernel regression defines the weight fxn W by a continuous, bounded (often symmetric) real function — the kernel K — that integrates to one.
- The weight sequence is:

$$W_{Ni}(x) = K_{h_N}(x - X_i)/\hat{f}_{h_N}$$

  where

$$\begin{aligned} \hat{f}_{h_N} &= N^{-1} \sum_{i=1}^{N} K_{h_N}(x - X_i) \\ K_{h_N}(u) &= h_N^{-1} K(u/h_N) \end{aligned}$$

  is the kernel with scale factor h_N and N is still the sample size
- $\hat{f}_{h_N}$ is the *Rosenblatt-Parzen* kernel density estimator of the marginal density of X

Nadaraya-Watson Estimator

- The complete weighting sequence is:

$$W_{Ni}(x) = h_N^{-1} K(x - X_i/h_N) / N^{-1} \sum_{i=1}^{N} h_N^{-1} K(x - X_i/h_N)$$

- This form of weights was proposed by Nadaraya and Watson.
- Hence, the Nadaraya-Watson estimator is

$$\begin{aligned} \hat{m}_h(x) &= N^{-1} \sum_{i=1}^{N} W_{Ni}(x) Y_i \\ &= \frac{N^{-1} \sum_{i=1}^{N} K_{h_N}(x - X_i) Y_i}{N^{-1} \sum_{i=1}^{N} K_{h_N}(x - X_i)} \end{aligned}$$

- Shape of kernel weights determined by choice of K
- Size of the weights determined by h_N (bandwidth)
- For choice of Kernel, see earlier slide

Example

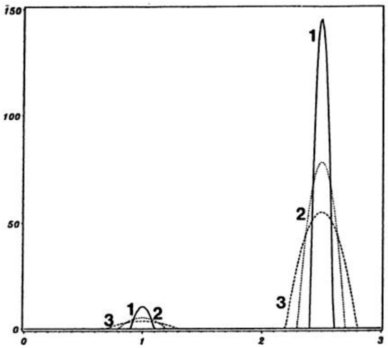


Figure 3.2. The effective kernel weights for the food versus net income data set. $K_h(x-\cdot)/\hat{f}_h(x)$ at $x = 1$ and $x = 2.5$ for $h = 0.1$ (label 1), $h = 0.2$ (label 2), $h = 0.3$ (label 3) with Epanechnikov kernel $K(u) = 0.75(1-u^2)I(|u| \le 1)$ and density estimate as in Figure 1.5, year = 1973, $n = 7125$. Family Expenditure Survey (1968–1983).

Choice of Kernel

1. Smaller bandwidth $\implies$ greater concentration of weights around x
2. In regions with sparse data where marginal density estimate $\hat{f}_h$ is small, sequence $\{W_{ni}(x)\}_{i=1}^{N}$ gives more weight to obs around x
   - There are a lot of X_i's concentrated around the value $X = 1$, not so many around $X = 2.5$

   $\implies$ the density of X, estimated by $\hat{f}_h$ is very large around $X = 1$ and very small around $X = 2.5$

   $\implies$ the weights, $W_N i$, are very small around $X = 1$ and very large around $X = 2.5$ since $\hat{f}_h$ is in the denominator of the weight fxn

Univariate Regression 1

- Same model

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

- We want to fit this model at a particular x-value, say x_0
- Ultimately, we fit the model at either a representative range of x-values or the N sample points, $x_i : i = 1, ..., N$
- Run a pth-order regression of Y on X around x_0

$$Y_i = \alpha + \beta_1(X_i - x_0) + \beta_1(X_i - x_0)^2 + ... + \beta_p(X_i - x_0)^p + \varepsilon_i$$

- Weight the observations according to proximity to x_0. E.g.,

$$\text{Tricube} : K(t) \;=\; \begin{cases} (1 - |t|^3)^3 & |t| < 1 \\ 0 & \text{otherwise} \end{cases}$$

where $t = (X_i - x_0)/h$, h is window width

Univariate Regression 2

- Fitted value at x_0 (i.e., height of estimated regression curve) is $\hat{y}_0 = \alpha$
- It's just the intercept because we centered the predictor x at x_0
- Sometimes we adjust h so that each local regression includes a fixed proportion s of the data
- s is the **span** of the local regression smoother
  - Larger span s, smoother the result
  - Larger the order of the local polynomial, more flexible the smooth

Example

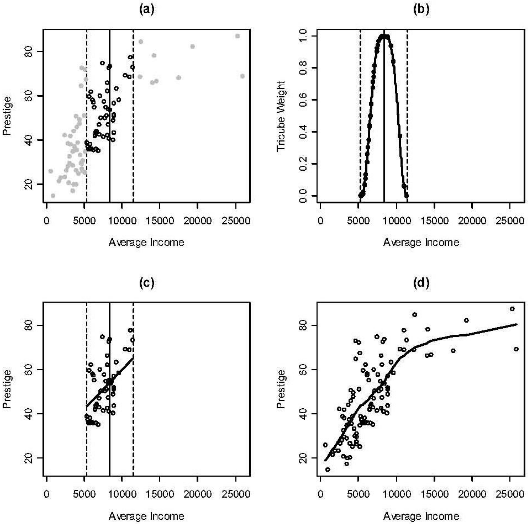

(a)
(b)
(c)
(d)
Prestige
Tricube Weight
Average Income
0
5000
10000
15000
20000
25000
20
40
60
80
0.0
0.2
0.4
0.6
0.8
1.0

Fig (a): Window Width & Span

- Focus on one point, $x_0 = x_{(80)}$ (i.e., the 80th largest x value)
- This point is denoted by the solid vertical line
- Fig (a) shows the window that includes the 50 nearest x-neighbors of $x_{(80)}$
  - This implies a span s of $\approx 50\%$ (50/102)

Fig (b): Kernel

- The tricube kernel provides the weights for all of the observations in the window
- Note the weights are declining in the distance from the reference point $x_{(80)}$
- Note that the tricube $K(t)$ is strictly positive only for $|t| < 1$
- But, the raw distances as measured along the x-axis are much greater than 1
- This is because the argument t is $(X_i - x_0)/h$. So, big h shrinks the argument t

Fig (c): Local Weighted Linear Regression

- The line is a:
    - locally (Just the 50 obs around $x_{(80)}$,
    - weighted (each observation is weighted by the Kernel $K((X_i - x_{(80)})/h)$,
    - linear (assume the polynomial is of order $p = 1$),
    - regression.
- The fitted value of y at $x_{(80)}$, $\hat{y}|x_{(80)}$ is presented as a large solid dot

Fig (d): The Curve

- Local regressions are estimated for a range of x-values (e.g., all the sample points)
- The fitted values are connected to form the curve
    - How are the points connected?

Other Smoothers

- Alternatives to kernel regression include:
  1. k Nearest Neighborhood smoothers
  2. Orthogonal series smoothers
  3. Spline smoothers
  4. Recursive smoothers
  5. Convolution smoothers
  6. Median smoothers

References

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- Hardle, Wolfgang 1990, *Applied Nonparametric Regression* Cambridge University Press, Cambridge, U.K.