Lecture 11
Introduction to Nonparametric Regression: Density Estimation

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Non Parametric Regression: Introduction

• The goal of a regression analysis is to produce a reasonable analysis to the unknown response function f, where for N data points (X_i,Y_i), the relationship can be modeled as

$$y_i = m(x_i) + \varepsilon_i, \qquad i = 1, \cdots, N$$

- Note: $m(.) = E[y|x]$ if $E[\varepsilon|x]=0$ –i.e., $\varepsilon \perp x$

• We have different ways to model the conditional expectation function (CEF), $m(.)$:

- Parametric approach
- Nonparametric approach
- Semi-parametric approach.

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Non Parametric Regression: Introduction

• Parametric approach: $m(.)$ is known and smooth. It is fully described by a finite set of parameters, to be estimated. Easy interpretation. For example, a linear model:

$$y_i = x_i'\beta + \varepsilon_i, \qquad i = 1, \cdots, N$$

• Nonparametric approach: $m(.)$ is smooth, flexible, but unknown. Let the data determine the shape of $m(.)$. Difficult interpretation.

$$y_i = m(x_i) + \varepsilon_i, \qquad i = 1, \cdots, N$$

• Semi-parametric approach: $m(.)$ have some parameters -to be estimated-, but some parts are determined by the data.

$$y_i = x_i'\beta + m_z(z_i) + \varepsilon_i, \qquad i = 1, \cdots, N$$

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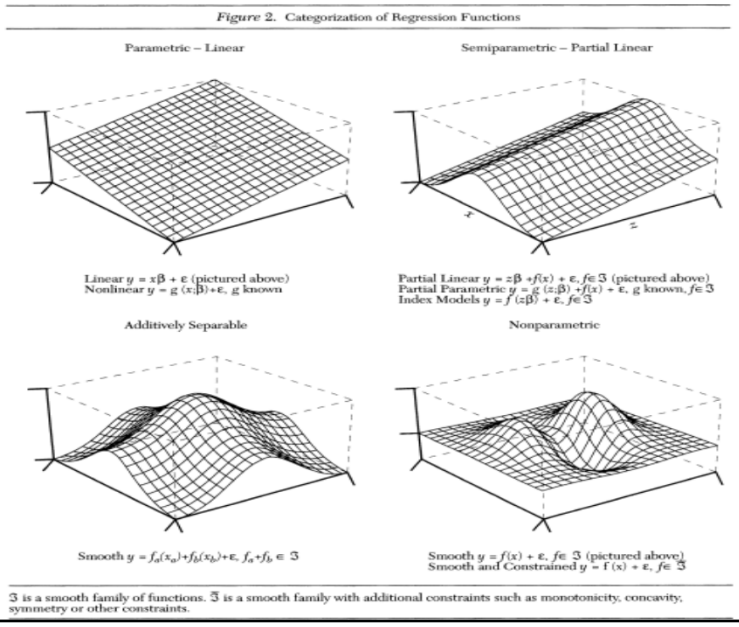
Non Parametric Regression: Introduction



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Non Parametric Regression: Introduction

• Parametric and non-parametric approaches use a weighted sum of the *y's* to obtain the fitted values, $\hat{y}$. That is,

$$\hat{y}_i = \Sigma_i \, \omega_i \, y_i$$

• Instead of using equal weights as in OLS or weights proportional to the inverse of variance as often in GLS, a different rationale determines the choice of weights in nonparametric regression.

• In the single regressor case, the observations with the most information about $f(x_0)$ should be those at locations x_i closest to x_0.

• Thus, a decreasing function of the distances of their locations x_i from x_0 determine the weights assigned to y_i's.

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Non Parametric Regression: Introduction

• A decreasing function of the distances of their locations x_i from x_0 determine the weights assigned to y_i's.

• The points closest to x_0 receive more weight than those more remote from x_0. Often, points remote from x_0 receive little or no weight.

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Density Estimation: Univariate Case

• We have a large number of observations on a RV X. We would like to "draw" the pdf of X.

• Simplest method: Use a *histogram*. That is, divide the range of X into a small number of intervals (*bins*), h, and count the number of times X, n_i, is observed in each interval:

$$p_i = \frac{n_i(h)}{N}$$

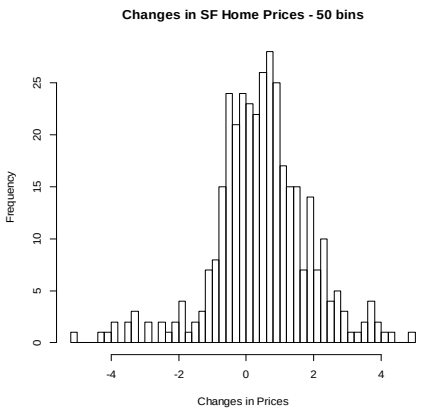
• Q: How wide should the bins be? Too small (too many bins) distribution looks jerky, too large (few bins), shape is not easy to visualize.

• Two questions: - Do we want the same bin-width everywhere?

- Do we believe the density is zero for empty bins? 7

Density Estimation – Bins: Example

• We use two histograms to fit percentage changes in monthly San Francisco home prices (r_sf, with N=359), with two h (large h, 10 bins; small h, 50 bins). =>Smaller h, more resolution.



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Density Estimation: Problems with Histograms

• The histogram is close to, but not truly density estimation. It does not estimate $f(x)$ at every x. Rather, it partitions the sample space into bins, and only approximate the density at the center of each bin.

• Two problems with histograms:

(1) For a given number of bins, moving their exact location (boundary points) can change the graph.

(2) The density function produced is a step function and the derivative either equals zero or is not defined (when at the cutoff point for two bins).

- This is a problem if we are trying to maximize a likelihood function that is defined in terms of the densities of the distributions.

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Density Estimation: Definition of Histogram

• First, define the density function for a variable x. For a particular value of x, call it x_0, the density function is:

$$f(x_0) = \lim_{h\to 0} \frac{F(x_0+h) - F(x_0-h)}{2h} = \lim_{h\to 0} \frac{\Pr ob[x_0 - h < x < x_0 + h]}{2h}$$

• For a sample of data on $\boldsymbol{X}$ of size N, a histogram with a column width of $2h$, centering the column around x_0 can be approximated by:

$$\hat{f}_{Hist}(x_0) = \frac{1}{N}\sum_{i=1}^{N} \frac{I[x_0 - h < x_i < x_0 + h])}{2h} = \frac{1}{Nh}\sum_{i=1}^{N} I(\frac{|\, x_i - x_0\,|}{h} < 1)$$

• This function equals the fraction of the sample that lies within h of x_0, divided by the column width ($2h$).We call this the *naive estimator*.

• x_0 is any value of $\boldsymbol{X}$, not necessarily equal to any x_i's in the sample.

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Density Estimation: Problems Revisited

• Dealing with the two problems:

(1) Arbitrary location of the bin cutoff points

Solution: Define a "moving" bin that is defined for every possible value of x. Then, count how many actual x_i's are within $h/2$ of the hypothetical point, and "normalizes" this count by the number of total observations *(N)* and the "bandwidth," *h*.

(2) Discontinuity in the function.

Solution: *Kernel density estimation (KDE)*. It avoids the discontinuities in the estimated (*empirical*) density function. In terms of histogram formula, the *kernel* is everything to the right of the summation sign. The general formula for the *kernel estimator* (*Parzen window*):

$$\hat{f}_{Hist}(x_0) = \frac{1}{Nh}\sum_{i=1}^{N} K\left(\frac{x_i - x_0}{h}\right)$$

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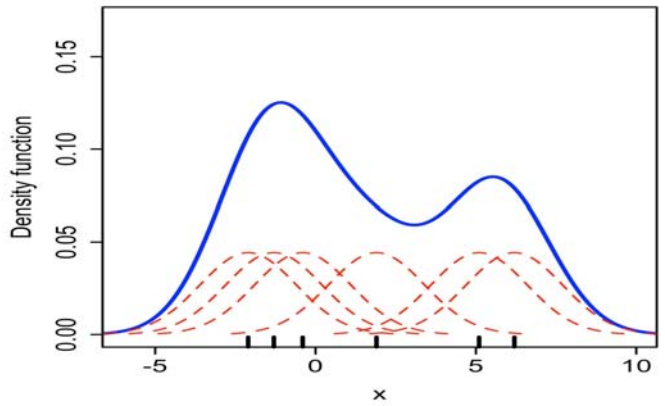
Kernel Density Estimation (KDE)

• The *kernel estimator* is given by: $\hat{f}_{Hist}(x_0) = \frac{1}{Nh}\sum_{i=1}^{N} K\left(\frac{x_i - x_0}{h}\right)$



• That is, $\hat{f}_{Hist}(x)$ is a superposition of N density functions.

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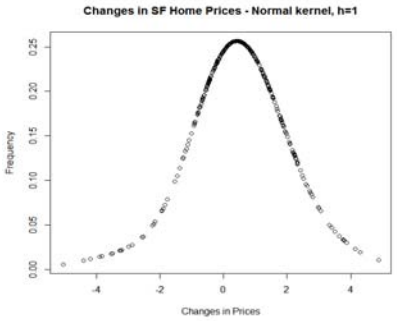
KDE: SF Prices Example With Normal Kernel

• Assume K(.)~N(0,1). Then, $\hat{f}_{Hist}(x_0) = \frac{1}{Nh}\sum_{i=1}^{N} dnorm(\frac{x_i - x_0}{h})$

```
d_h <- matrix(0, N, 2)          # N=359
h <- 1                          # bandwidth
for (j in 1:N){
 d_h[j,1] <- r_sf[j]
for (i in 1:N){
 d_h[j,2] <- d_h[j,2] + dnorm((r_sf[i]-d_h[j,1])/h)
}
d_h[j,2] <- d_h[j,2]/(N*h)
}
```




```
plot(d_h, xlab="Changes in Prices", ylab="Frequency",main = "Changes in SF Home Prices - Normal kernel, h=1")
```

• A lot of calculations: N^2=128,881 => Not practical for large N.

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KDE: Properties

• KDE: $\hat{f}_{Hist}(x_0) = \frac{1}{Nh}\sum_{i=1}^{N} K(\frac{x_i - x_0}{h})$

• Q: Is $\hat{f}_{Hist}(x)$ a legitimate density function? It needs to satisfy:

(1) nonnegative

(2) integrate to one.

=> Easy to do: Require the Kernel function, $K(.)$ to satisfy:

(1) $K(x) \geq 0$

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

Define the function: $\delta_n(x) = \frac{1}{h}K(\frac{x}{h})$

The $\hat{f}_{Hist}(x)$ can be written as $\hat{f}_{Hist}(x) = \frac{1}{N}\sum_{i=1}^{N} \delta(x_i - x_0)$

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KDE: Properties

• Check the properties of $\hat{f}_{Hist}(x)$ and $\delta_n(x)$:

$$\int \delta_n(x - x_i)dx = \int \frac{1}{h} K\left(\frac{x - x_i}{h}\right)dx = \int K(u)du = 1$$

$$\int \hat{f}_{Hist}(x) = \int \frac{1}{N}\sum_i \delta_n(x - x_i)dx = \frac{1}{N}\sum_i \int \delta_n(x - x_i)dx = 1$$

• The kernel function can be generalized.

Note: Any density function satisfies our requirements. For example, $K(.)$ can be a normal density.

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KDE: Kernels

• The *kernel* function $K(.)$ is a continuous and bounded (usually symmetric around zero) real function which integrates to 1.

• h is a smoothing parameter (*bandwidth*). $2h$ is called the *window width*.

• The order of a kernel, ν, is defined as the order of the first non-zero moment, $\varkappa_k$. For example, if $\kappa_1(K) = 0$ and $\varkappa_2(K) > 0$ then K is a 2nd order kernel. The order of a symmetric kernel is always even.

• Symmetric non-negative kernels are second-order kernels. We will emphasize these kernels (ν=2).

• Higher-order kernels are obtained by multiplying a second-order kernel by an $(2\nu\text{-}1)$-*th* order polynomial in z^2. See Hansen (2009).

KDE: Kernels

• Most common kernel functions (2nd order):

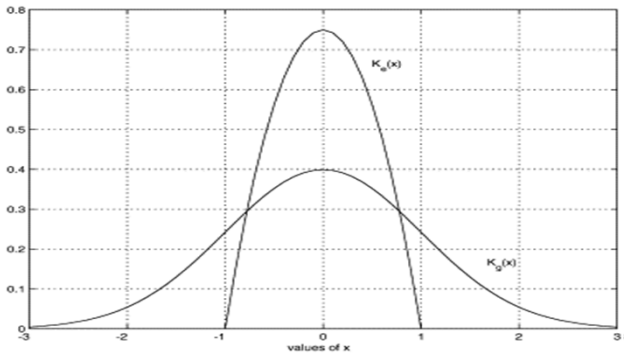
- Uniform kernel: $K(z) = 0.5$ for $|z| \leq 1$; $= 0$ for $|z| > 1$
- Epanechnikov kernel: $K(z) = 0.75(1-z^2)$ for $|z| \leq 1$; $= 0$ for $|z| > 1$
- Quartic (biweight) kernel: $K(z) = 15/16\ (1-z^2)^2$ for $|z| \leq 1$; $= 0$ for $|z| > 1$
- Triweight kernel: $K(z) = 35/32\ (1-z^2)^3$ for $|z| \leq 1$; $= 0$ for $|z| > 1$
- Gaussian (normal) kernel: $K(z) = 1/\text{sqrt}(2\pi)\ \exp(-z^2/2)$

• Density graph: Plot $\hat{f}_{Hist}(x)$ against x_0 and connect points.

KDE: Kernels - Examples

• Two kernels: - Epanechnikov kernel $K_e(z) = 0.75(1-z^2)\ \ I(|z| \leq 1)$

- Gaussian kernel $K_g(z) = 1/\text{sqrt}(2\pi)\ \exp(-z^2/2)$.

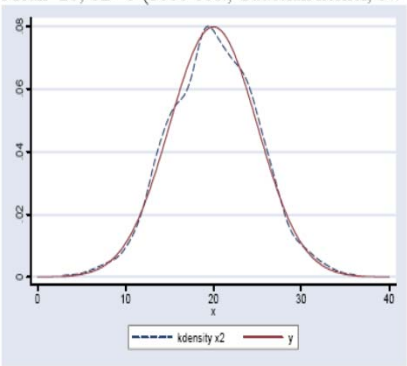


• A drawback of the Gaussian kernel is that its support is R; in many situation, we want to restrict the support, like in the Epanechnikov kernel --at the cost of being not differentiable at ± 1.

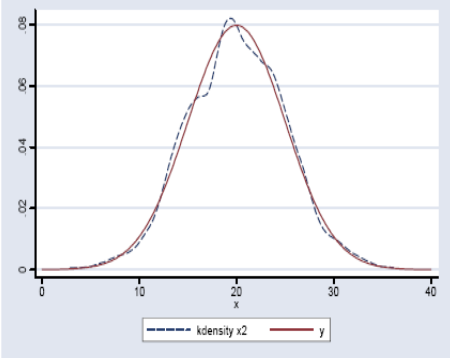
KDE: Kernels - Examples

• In practice, the choice of the kernel does not matter very much in terms of getting a good approximation to the true density function. Below, we show two estimations (gaussian and quartic) to simulated data.

Graph 5: Density of a Normally Distributed Variable, Mean=20, SD=5 (1000 obs., Gaussian kernel, bw=1)

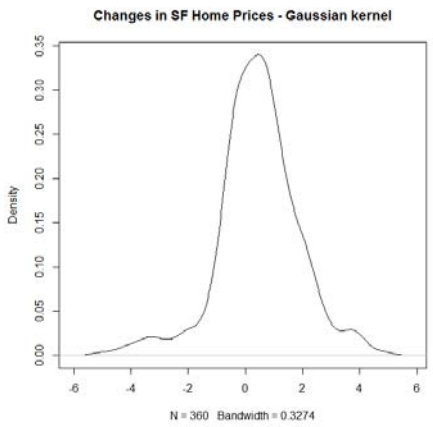


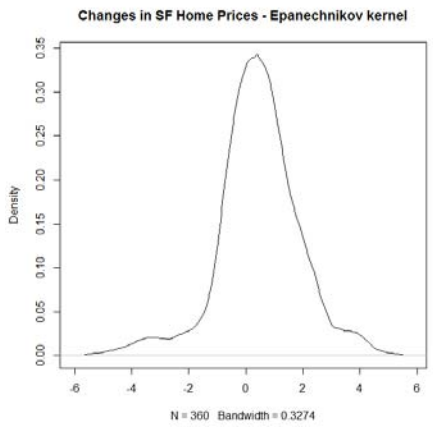
Graph 6: Density of a Normally Distributed Variable, Mean=20, SD=5 (1000 obs., Quartic kernel, bw=2)



KDE: Kernels - Examples

• We use a Gaussian and Epanechnikov kernels to fit percentage changes in monthly San Francisco home prices, with same *h*. Very similar results!





KDE: Statistical Inference

• *Expectation*

$$E[\hat{f}(x_0)] = \frac{1}{Nh}\sum_{i=1}^{N} E[K(\frac{x_i - x_0}{h})]$$

$$= \frac{1}{N}\sum_{i=1}^{N} \int_{-\infty}^{\infty} K(u) f(u) du = \int_{-\infty}^{\infty} K(u) f(x_0 + hu) du$$

where we use a change of variables $u = (x_i - x_0)/h$. We approximate the integral using a Taylor expansion of $f(x_0+hu)$ in hu (as $h \longrightarrow 0$):

$$f(x_0 + hu) = f(x_0) + f'(x_0)hu + \frac{1}{2} f''(x_0)h^2u^2 + ... + \frac{1}{v!} f^v(x_0)h^v u^v + o(h^v)$$

Then, for a *v-th* order $K(.)$ (then, $\kappa_j = 0$, *for* $j<v$):

$$\int_{-\infty}^{\infty} K(u) f(x_0 + hu) = f(x_0) + f'(x_0)h\kappa_1 + \frac{1}{2} f''(x_0)h^2\kappa_2 + ...$$

$$= f(x_0) + \frac{1}{v!} f^v(x_0)h^v\kappa_v + o(h^v)$$

KDE: Statistical Inference

• Then, the expectation is:

$$E[\hat{f}(x_0)] = f(x_0) + \frac{1}{v!} f^v(x_0)h^v\kappa_v + o(h^v)$$

It is a biased! The bias depends on h, the curvature of $f(.)$, and $K(.)$.

• For a 2nd-order kernel, the bias is:

$$E[\hat{f}(x_0)] - f(x_0) = \frac{1}{2} f^2(x_0)h^2\kappa_2 + o(h^2)$$

Note: When higher-order kernels are used, the bias is portional to h^v; which is of lower order than h^2. Then, higher-order kernels are *bias-reducing* kernels.

KDE: Statistical Inference

• *Variance*

$$Var[\hat{f}(x_0)] = \frac{1}{(Nh)^2}\sum_{i=1}^{N} Var[K(\frac{x_i - x_0}{h})] = \frac{1}{Nh^2} Var[K(\frac{x_i - x_0}{h})]$$

$$= \frac{1}{Nh^2} E[K(\frac{x_i - x_0}{h})^2] - \frac{1}{N}(\frac{1}{h} E[K(\frac{x_i - x_0}{h})])^2$$

- From the analysis of bias we know the 2nd term is O(1/*N*). Recall,

$$E[\hat{f}(x_0)] = f(x_0) + o(1)$$

- For the 1st term, we make a change of variables and use a 1st-order Taylor expansion:

$$\frac{1}{h} E[K(\frac{x_i - x_0}{h})^2] = \int_{-\infty}^{\infty} K(u)^2 f(x_0 + hu) du = \int_{-\infty}^{\infty} K(u)^2 f(x_0 + O(h)) du$$

$$= f(x_0) R(K) + O(h)$$

KDE: Statistical Inference

• Then, the variance is:

$$Var[\hat{f}(x_0)] = \frac{f(x_0) R(K)}{Nh} + O(\frac{1}{N})$$

$\Longrightarrow$ The variance depends on the *N*, *h*, *f*(.) and *K*(.). It will go to 0 as $Nh \to \infty$.

Note: We can combine the previous results (bias and variance) to measure precision of $\hat{f}(x_0)$ as the MSE:

$$MSE\ [\hat{f}(x_0)] = (Bias\ )^2 + Variance$$

$$= \frac{(\kappa_v)^2}{(v!)^2} (f^v(x_0))^2 h^{2v} + \frac{f(x_0) R(K)}{Nh}$$

which is called *Asymptotic* MSE (AMSE). It depends on *N*, *h*, *f*(.) and *K*(.). The bias is increasing in *h,* the variance decreasing in *Nh*.

KDE: Statistical Inference

• *Consistency*

For an *i.i.d.* sample of the RV $\boldsymbol{X}$, for any value x_0 and a fixed h, $\hat{f}(x_0)$ is a *biased* estimate of $f(x_0)$. Yet the bias goes to zero if $h \to 0$ as $N \to \infty$.

• For a 2nd-order $K(.)$ the bias is given by:

$$bias(\hat{f}(x_0)) = E[\hat{f}(x_0)] - f(x_0) = \frac{1}{2} h^2 f''(x_0) \int_{-\infty}^{\infty} u^2 K(u) du$$

$\Longrightarrow$ The "size" of this bias is $O(h^2)$.

• Assuming that $h \to 0$ as $N \to \infty$, the variance of $\hat{f}(x_0)$ is:

$$\text{Var}[\hat{f}(x_0)] = [1/(Nh)] f(x_0) \int (K(z))^2 dz + o(1/Nh)$$

$\Longrightarrow$ The variance will go to 0 as $Nh \to \infty$, so h must converge to 0 at a *slower* rate than N goes to ∞.

KDE: Statistical Inference

• The previous results are approximations. They were derived by approximating integrals by a Taylor expansion of $f(x+hu)$ in the argument $hu \to 0$.

• The kernel estimator $\hat{f}(x_0)$ is *pointwise consistent* at any point x_0 if both the variance and bias disappear as $N \to \infty$ (check AMSE formula), which requires that $h \to 0$ and $Nh \to \infty$.

• The *uniform convergence* (stronger) property holds if $Nh/\ln(h) \to \infty$.

• See Cameron and Trivedi's (CT) textbook for formal details.

KDE: Statistical Inference

• *Asymptotic normality*

The kernel estimator is the sample average. A CLT can be applied. Using previous results:

- Given the order of the variance, the rate of convergence is sqrt(Nh), not sqrt(N) as in standard regression estimates.

- The estimator is biased, so we center $\hat{f}(x_0)$ around its expectation.

That is, by the CLT we get:

$$\text{sqrt}(Nh)\,(\hat{f}(x_0) - E[\hat{f}(x_0)]) \rightarrow^{d} N(0, f(x_0)\int(K(z))^2 dz)$$

Note: Given the bias, $[\hat{f}(x_0) - E[\hat{f}(x_0)]]$, is also asymptotically normally distributed, but with a non-zero mean.

KDE: Bandwidth

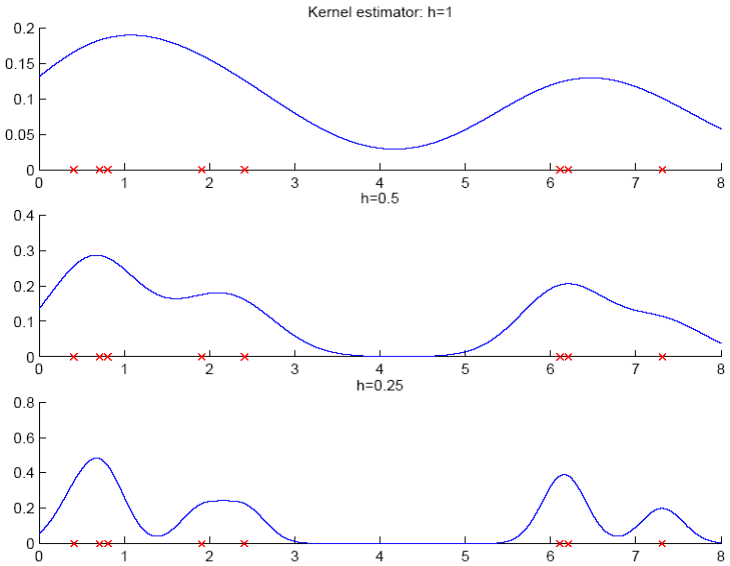
• As the previous formulas show, there is a genuine trade-off between avoiding bias and reducing the variance of the estimate at any given point x.

• In general, large h reduce the variance by smoothing over a large number of points, but this is likely to lead to bias because the points are "averaged" in a mechanical way that does not account for the particular shape of the distribution.

• In contrast, small h give higher variance but have less bias. In the limit, $h \rightarrow 0$, the kernel reproduced the data.

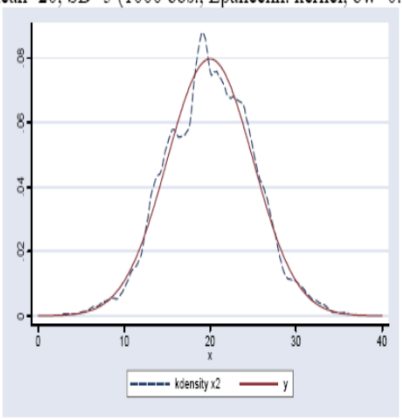
• We can play with different h's, but we would like a data-driven bandwidth ("*automatic*") selection process.

KDE: Bandwidth - Examples

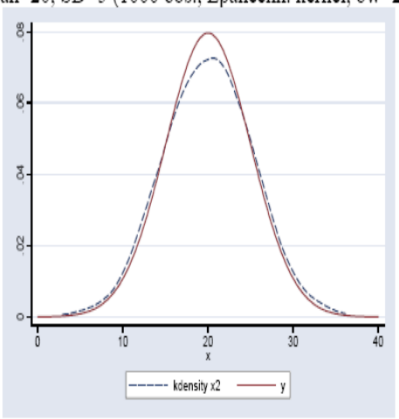


KDE: Bandwidth - Examples

Graph 8: Density of a Normally Distributed Variable, Mean=20, SD=5 (1000 obs., Epanechn. kernel, bw=0.5)

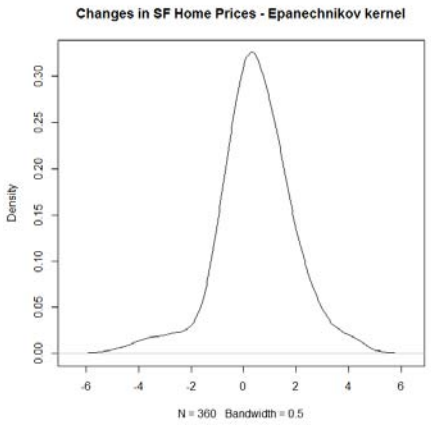


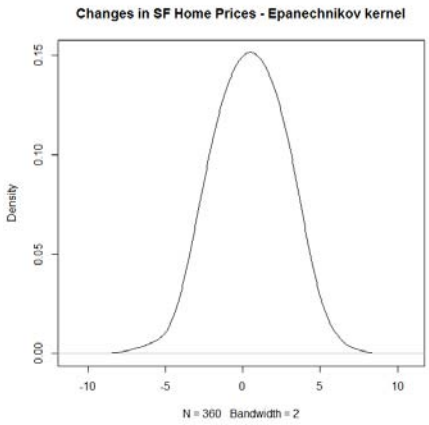
Graph 9: Density of a Normally Distributed Variable, Mean=20, SD=5 (1000 obs., Epanechn. kernel, bw=2)



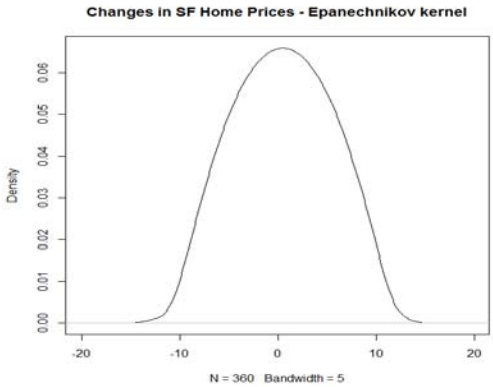
KDE: Bandwidth - Examples

• We use an Epanechnikov kernels to fit percentage changes in monthly San Francisco home prices, with two h = .5, 2 & 5. Different results.





KDE: Bandwidth - Examples



• Q: How do we deal with the trade-off between bias and variance?
A: A "natural" approach is to minimize the MSE:

$$\text{MSE}(\hat{f}(x_0)) = \text{Var}[\hat{f}(x_0)] + [\text{bias}(\hat{f}(x_0))]^2$$

=> *optimal bandwith*

KDE: Bandwidth - Selection

• A "natural" approach is to minimize the MSE:

$$MSE(\hat{f}(x_0)) = Var[\hat{f}(x_0)] + [bias(\hat{f}(x_0))]^2$$

• As shown in previous formulas, the bias is $O(h^2)$ and the variance is $O(1/Nh)$. Intuitively, h should be chosen to that the $(bias)^2$ and the variance are of the same order.

• The square of the bias is $O(h^4)$ $\quad \Rightarrow h^4 = 1/Nh$,
$\quad \Rightarrow h = (1/N)^{1/5}$.

That is, $h = O(N^{-0.2})$ and $sqrt(Nh) = O(N^{0.4})$.

• A more formal derivation is given on C&T.

• Note: Recall that the MSE is approximated using asymptotic expansion. We called it AMSE (asymptotic MSE).

KDE: Bandwith and MISE

• Rosenblatt (1956) developed a global measure of accuracy for $\hat{f}(x_0)$: Minimizing the SSE at a large number of hypothetical points. As this number goes to infinity, this amounts to minimizing the *mean of the integrated squared error* (MISE). If the previous asymptotic approximations are used, the MISE becomes *AMISE*.

• That is, an optimal bandwidth minimizes

$$MISE(h) = E[\int(\hat{f}(x_0)-f(x_0))^2\, dx_0] = E[\int MSE(\hat{f}(x_0))\, dx_0]$$

• Differentiating AMISE(h) w.r.t. h yields the optimal bandwidth:

$$h^* = \delta\, [\int (f''(x_0)^2\, dx_0]^{-0.2} N^{-0.2},$$

where δ depends on the kernel function used:

$$\delta = [\int (K(z))^2\, dz]^{0.2}\, [\int z^2 K(z)\, dz]^{-0.4}.$$

• Note: $\int (K(z))^2\, dz$ is called the *roughness* of $K(.)$.

KDE: Optimal Bandwith

• The optimal bandwidth, h^*:

$$h^* = \delta \left[\int (f''(x_0)^2 \, dx_0 \right]^{-0.2} N^{-0.2}.$$

• The optimal bandwidth decreases (very slowly) as N increases. Then, $h^* \to 0$ as $N \to \infty$ (as required for consistency).

• h^* depends on δ, which is a function of the kernel $K(\,)$. For example, if $K(.)$ is Gaussian,

$$\delta = \left[\int (K(z))^2 \, dz\right]^{0.2} \left[\int z^2 K(z) \, dz\right]^{-0.4} = [1/(2*\text{sqrt}(\pi))]^{0.2} [\sigma^2=1]^{-0.4}$$
$$= [1/(2*\text{sqrt}(\pi))]^{0.2} \; (=.776388)$$

• Values for δ are given in Table 9.1 in C&T.

• This result also shows that if the true density function has a lot of curvature ($f''(x)$ is large), the bandwidth should be smaller.

KDE: Optimality

• The optimal h^* is unknown –we do not know $f(x_0)$ or $f''(x_0)$. Approximations methods are required.

• In practice, a normal density is commonly used instead of $f(x_0)$. *Silverman's (1986) rule of thumb* assumes $f \sim N(\mu,\sigma^2)$, then:

$$h^* = (4\hat{\sigma}^5/3N)^{0.2} \approx 1.059 \, \hat{\sigma} \, N^{-0.2}$$

• As seen in the graphs, the choice of the kernel matters very little. More formally, MISE(h^*) varies little across the different kernels.

• Technically speaking we can select the *best* kernel. The one that minimizes the AMISE. It is a calculus of variation problem

• The Epanechnikov (1969) kernel is "*optimal,*" but the advantage is small. It is often used to judge the efficiency of a kernel.

KDE: Confidence Intervals

• We can obtain confidence intervals for estimates of $f(x_0)$ for any point x_0. Use the variance formula above to get the conventional C.I.:

$$f(x_0) \in \hat{f}(x_0) - \text{bias}(x_0) \pm z_{\alpha/2} \text{ sqrt}\{(1/Nh)\, \hat{f}(x_0) [\int (K(z))^2 dz]\}$$

where $\text{bias}(x_0)$ is given above and we have assumed that $\hat{f}(x_0)$ is asymptotically normal.

• Problem: It can contain negative values.
Solution: Consider constructing the C.I. by inverting a test statistic.

$$C(x) = \{f: |\hat{f}(x_0) - \text{bias}(x_0)| / [\text{sqrt}\{(1/Nh)\, \hat{f}(x_0) \int (K(z))^2 dz]\} \leq z_{\alpha/2}\}$$

This set must be found numerically.

• In practice, it is hard to calculate the bias, and, there may not be a reason to calculate the C.I. for $\hat{f}(x_0)$.

KDE in Practice: Bandwidth Selection

• As mentioned above to calculate h^* we need the unknown $f''(x_0)$. Approximations methods are required. In practice, a normal density is commonly used instead of $f(x_0)$.

1. If $X \sim$Normal, then we get $[\int (f''(x_0))^2 dx_0]^{-0.2} = 1.3643$

$$h^* = \delta [\int (f''(x_0))^2 dx_0]^{-0.2} N^{-0.2} = 1.3643\, \delta\, N^{-0.2}\, \hat{\sigma}, \qquad \hat{\sigma} = \text{SD}(x).$$

If in addition, $K(.)$ is normal (δ=.776388) $\Rightarrow h^* = 1.059\, N^{-0.2}\, \hat{\sigma}$.
If in addition, $K(.)$ is the Epanechnikov $\Rightarrow h^* = 2.34\, N^{-0.2}\, \hat{\sigma}$.

2. A refinement of the formula in (1), to account for outliers, is

$$h^* = 1.3643\, \delta\, N^{-0.2} \min[\hat{\sigma}, \text{iqr}/1.349],$$

where "iqr" is the (sample) interquartile range.

• These rules for selecting h^* are generally called *rules of thumb*.

KDE in Practice: Boundary Effects

• So far, we have not paid much attention to the boundaries of the data, implicitly assuming that the density is supported on the entire R.

• In many situations, this is not the case. Then, the estimator can behave quite poorly due to what are called *boundary effects*.

• At the boundaries, $\hat{f}(x_0)$ usually underestimates $f(x_0)$. Suppose the data is positive, then $\hat{f}(x_0=0)$ penalizes $x_0=0$ for lack of data. At $x_0=0$, $\hat{f}(x_0)$ is inconsistent.

• Many proposed techniques to deal with boundary effects:
– Reflection of data ("reflect" data at $x_0=0$, $-x_1$, $-x_2$,...,$-x_Q$).
– Transformation of data (use a function g(x); estimate $\hat{f}(x_0)$ instead).
– Pseudo-Data Methods ("add" reasonable data, say by interpolation).
– Boundary Kernel Methods (use a non-symmetric K(.) at $x_0=0$).

KDE in Practice: Computational Issues

• To get $\hat{f}_{Hist}(x)$ exactly, we must calculate for all x's (x_1, ..., x_N):

$$\hat{f}_{Hist}(x_j) = \frac{1}{Nh}\sum_{i=1}^{N} K\left(\frac{x_i - x_j}{h}\right), \qquad j = 1,..., N$$

• Then, the number of evaluations of K(.) is proportional to N^2 (for a bounded Kernel, like the Epanechnikov, we have $h\,N^2$ evaluations). This increases the computation time if the N is large.

• For graphing the density, we do not need to evaluate K(.) at all x's. Instead, $\hat{f}_{Hist}(x)$ can be computed at using some points, for example using an equidistant grid $z_1, z_2, ..., z_M$:

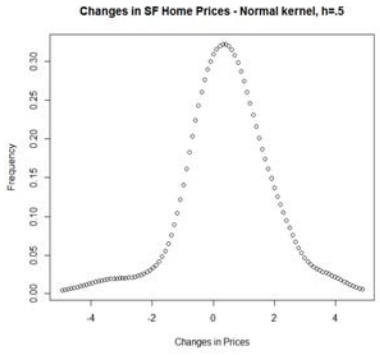
$$z_k = x_{min} + (k/M)(x_{max} - x_{min}), \qquad k = 1, 2, ..., M << N$$

• Now, we only need $M*h*N$ K(.) evaluations. But, we can do better by "binning" the data –i.e., using a *"binned estimator."*

KDE in Practie: Computational Issues -

• For the SF changes in home prices data, we do KDE, with M=100.

```
M <- 100
d_h <- matrix(0, M, 2)
h <- .5
dist <- (max(r_sf)- min(r_sf))/1
for (j in 1:M){
 d_h[j,1] <- min(r_sf) + j/M*dist
for (i in 1:N){
 d_h[j,2] <- d_h[j,2] + dnorm((r_sf[i] - d_h[j,1])/h)
}
d_h[j,2] <- d_h[j,2]/(N*h)
}
plot(d_h, xlab="Changes in Prices", ylab="Frequency",main = "Changes in SF Home Prices - Normal kernel, h=.5")
```



• Still a lot of calculations: $M*N$=35,900 (better than N^2 = 128,881)[41]

KDE in Practice: Computational Issues

• Binning or WARPing (Weighted Average of Rounded Points) "bins" the data in bins of length d starting at the origin x_1. Each x_i is replaced by the bincenter of the corresponding bin.

• A usual choice for d is to use $h/5$ or $(x_{min} - x_{max})/100$. In the latter case, the effective sample size (or number of grid points) R for the computation (the number of nonempty bins) can be at most 101.

• Now, K(.) needs to be evaluated only at $l\,d/h$, where $l=1,..., s$, where s is the number of bins which contains the support of K(.):

$$\hat{f}_{Hist}(w_j) = \frac{N_j}{Nh}\sum_{i=1}^{R} N_i K\left(\frac{(i-j)d_j}{h}\right), \qquad j = 1,..., R$$

computed on the grid $w_j = (j+0.5)\,d$ (j integer) with N_i and N_j denoting the number of observations in the i-th and j-th bins, respectively.

KDE in Practice: Computational Issues

• The WARPing approximation requires $(h*R/d)$ evaluations of K(.) and $N + (h*R/d)$ steps in total.

• Much faster than the exact computation, when N is large.

• The accuracy of binned estimators has been studied by Hall (1982), and Hall and Wand (1996), among others. The accuracy depends on the number of grid points R and can be made arbitrarily good by increasing R, at the cost of increasing the number of computations.

• Hall and Wand (1996) proposed that using R between 100 and 500 should give a reasonably good approximation.

KDE in Practice: Computational Issues

• For all but very small N, direct computation of K(.) is inefficient. By noticing that the KDE is based on a convolution of the data with the K(.), fast Fourier transformations (FFT) speed up computations:

$$\tilde{f}(x) = (2\pi)^{-1/2} \int \exp(ixt)\, f(t)\, dt \qquad \textit{(Fourier transform)}$$

• Recall the convolution theorem:

If $g(x)$ and $k(x)$ are integrable functions with Fourier transforms $\tilde{g}(\xi)$ and $\tilde{k}(\xi)$ respectively, then the Fourier transform of the convolution is given by the product of the Fourier transforms $\tilde{g}(\xi)$ and $\tilde{k}(\xi)$. That is,

if $\quad f(x) = \int g(y)\, k(x-y)\, dy,$

then, $\quad \tilde{f}(\xi) = \tilde{g}(\xi)\ \tilde{k}(\xi).$ $\qquad$ => invert $\tilde{f}(\xi)$ to get $f(\xi)$!

• Another approach: Fast Gaussian transformations (FGT).

KDE in R

• Kernel density estimates are available in R via the *density* function:

```
d <- density(r_sf, kernel=c("epanechnikov"), bw = .5)
plot(d, main = "Changes in SF Home Prices - Epanechnikov kernel")
```

which reproduces a previous density plot for SF home price changes, using the Epanechnikov kernel, with h=.5 (or bw =.5).

• By default, density uses a Gaussian kernel, but a large variety of other kernels are available by specifying the kernel option, like above with kernel=c("epanechnikov"),

• By default, density selects the bandwidth based on Silverman's (1986) rule of thumb. Other inputs (and manual inputs) can be used.

Estimating the Derivative of a Density

• Sometimes we need to estimate $f'(x)$ or even $f''(x)$ –like in a C.I.

• One approach for estimating f '(x) is straightforward:

$$f'(x) = [\hat{f}(x_0+\Delta) - \hat{f}(x_0-\Delta)]/2\Delta,$$

for some small Δ.

• Alternatively, differentiate the expression $\hat{f}(x_0) = \frac{1}{Nh}\sum_{i=1}^{N} K(\frac{x_i - x_0}{h})$ with respect to x_0:

$$\hat{f}'(x_0) = \frac{1}{Nh^2}\sum_{i=1}^{N} K'(\frac{x_i - x_0}{h})$$

• We can extend this approach to get the *r-th* derivative:

$$\hat{f}^{(r)}(x_0) = \frac{1}{Nh^{r+1}}\sum_{i=1}^{N} K^{(r)}(\frac{x_i - x_0}{h})$$

Estimating the Derivative of a Density

• Since the Gaussian kernel has derivatives of all orders this is a common choice for derivative estimation.

• The estimator of $f^{(r)}(x)$ is biased –same order as for estimation of $f(x)$. But the variance is of a much larger order.

• We can derive an optimal bandwidth, we can optimize MISE(h), as before.

• In practice, for either method, you should use a larger bandwidth than you use for estimating $\hat{f}(x_0)$.

• We can also ask the question of which kernel function is optimal. Muller (1984) found that the Biweight class is the optimal for the first derivative and for a second derivative the Triweight class.

Density Estimation: Adaptive Kernels

• So far, h has been fixed. But, this may not be optimal: what works fine in areas of high density may not necessarily be appropriate in a low-density regions.

• A possibility is to vary h, to use adaptive bandwidth kernel estimators, in which the bandwidth changes as a function of x_0.

• Idea: Where there is a lot of data, we use a small neighborhood around x_0; but in areas with few data points, we expand the neighborhood. That is, $h_i=h(x_i)$

• But, note that these estimators introduce added bias in regions with little data in order to reduce variance there. The bias-variance trade-off is still there.

Density Estimation: *k*-Nearest Neighbor

• In K-Nearest Neighbor (*k-NN)*, instead of fixing bin width *h* and counting the number of instances, we fix the instances (neighbors) *k* and check bin width.

• The neighborhood is defined through those *X*–variables which are among the *k*-nearest neighbors of x.

• The observations ranked by the distances, or "*nearest neighbors,*" are $(x_{(1)}, ..., x_{(N)})$: The k-th nearest neighbor (or k-NN of x is $x_{(k)}$):

• The *k-NN* estimator is given by: $\hat{f}_{Hist,k-NN}(x_0) = \frac{k}{2Nd_k(x_0)}$

where $d_k(x)$ is the ordered distance to *k*-th closest instance to x. $d_k(x)$ is usually the Euclidian distance (others, OK: Minkowski, Manhattan).

Density Estimation: *k*-Nearest Neighbor

• The *k-NN* estimator is given by: $\hat{f}_{Hist,k-NN}(x_0) = \frac{k}{2Nd_k(x_0)}$

a function of $d_k(x)$. If we use the Euclidian distance, $d_k(x) = \|x - x_{(k)}\|$.

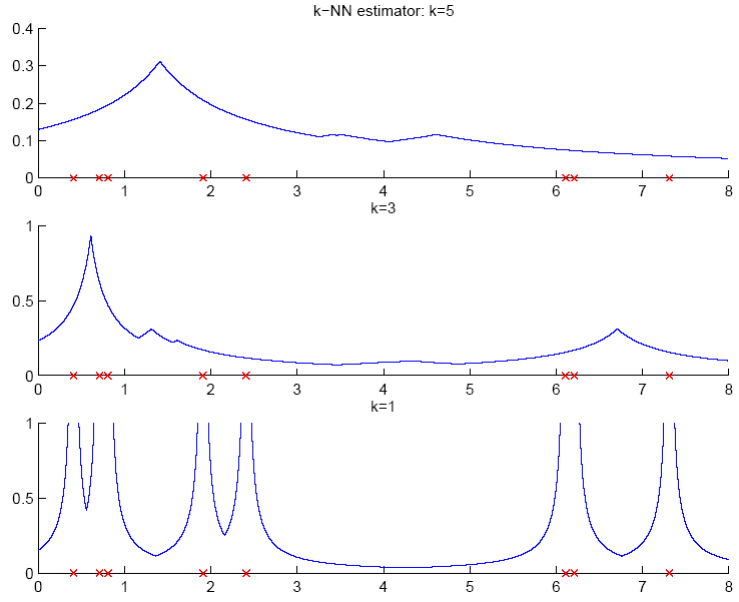
• Intuitively, we allow the bandwidth to vary depending on the density of the function. At areas of low density, we use a higher bandwidth to average over a larger number of (dispersed) points.

• While the traditional *k-NN* estimator uses a uniform kernel, smooth kernels can also be used. For example:

$$\hat{f}_{k-NN}(x_j) = \frac{1}{Nd_k(x_j)} \sum_{i=1}^{N} K\left(\frac{x_i - x_j}{d_k(x_j)}\right), \qquad j = 1,..., N$$

In this case, the estimator is not just a function of $d_k(x)$.

Density Estimation: *k*-Nearest Neighbor



Density Estimation: *k*-Nearest Neighbor

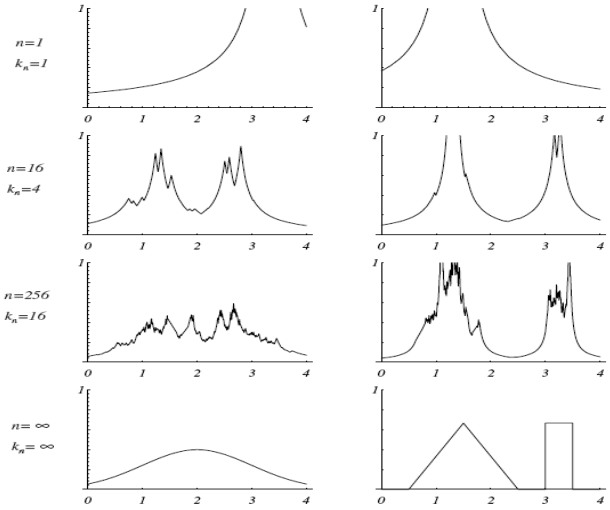


FIGURE 4.12. Several *k*-nearest-neighbor estimates of two unidimensional densities: a Gaussian and a bimodal distribution. Notice how the finite *n* estimates can be quite "spiky." From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

Density Estimation: Observations

• *k-NN* density estimation has a lot of discontinuities (very spiky, not differentiable). For small *N,* it is not even a density!

• Even for large regions with no observed data the estimated density is far from zero (tails are too heavy).

• Same trade-off as in selecting *h*: A smaller *k* allows only nearby data points to be considered (reduce bias); but a larger *k* allows for smoothness (reduce variance). Not easy to balance both issues.

• Given the variance-bias trade-off, selecting *k i*s similar to selecting *h* (though *k* is an integer). There is no clear rule of thumb or optimality rule. Some proposals exist, but practictioners insist on "*know your data"* to select *k*.

Density Estimation: Kernel or *k*-NN?

• The asymptotic analysis of the *k-NN* estimator are complicated by the fact that $d_k(x)$ is random. The solution is to condition on $d_k(x)$, which is similar to treating it as fixed.

• Then, the conditional bias and variance are identical to those of the standard kernel estimator.

• For the unconditional bias, we need moments of $d_k(x)$, under Euclidian distance, given by the k-th order statistics. It turns out that the MSE behaves similarly to the kernel estimator's MSE.

• Q: Which one is better?

Not clear. In the tails, the Kernel estimator has smaller bias, but larger variance (the *k-NN* tends to be smoother in the tails).

Density Estimation: Multivariate Case

• Now suppose that $\boldsymbol{X}$ is a d-vector and we want to estimate its density $f(\mathbf{x}) = f(x_1;...; x_d)$. Easy to extend the idea to this multivariate cases. Computations and interpretation get complicated once we move beyond 3 dimensions.

• Multivariate Kernel density estimator

$$\hat{f}(\mathbf{x}) = \frac{1}{Nh^d} \sum_{t=1}^{N} K\left(\frac{\mathbf{x} - \mathbf{x}^t}{h} \right)$$

• Multivariate Gaussian kernel

- spheric $K(\boldsymbol{u}) = \left(\frac{1}{\sqrt{2\pi}} \right)^d \exp\left[-\frac{\|\boldsymbol{u}\|^2}{2} \right]$

- ellipsoid $K(\boldsymbol{u}) = \frac{1}{(2\pi)^{d/2} |\mathbf{S}|^{1/2}} \exp\left[-\frac{1}{2} \boldsymbol{u}^T \mathbf{S}^{-1} \boldsymbol{u} \right]$

Density Estimation: Multivariate Case

• We can estimate an optimal bandwith, as before, by minimizing MISE(h). The optimal bandwith for the j-th variable is:

$$h_j^* = \delta \left[\int (f''(x_0))^2 \, dx_0 \right]^{-0.2} N^{-0.2} = C_v(K,d) \, N^{-1/(2v+d)} \, s,$$

• The optimal bandwidths will all be of order $N^{-1/(2v+d)}$ and the optimal MISE of order $N^{-2v/(2v+d)}$. This rates are slower than the univariate ($d = 1$) case.

• The fact that dimension has an adverse effect on convergence rates is called the *curse of dimensionality*.

• Rules of thumb can be derived for the constant $C_v(K,d)$.

For example, for the Epanechnikov kernel, $C_{v=2}(K,d)$, is for d=2, 2.20, for d=3, 2.12; for d=3, 2.07.

Readings

• Cameron, A. and P. Trivedi (2003), **Microeconometrics: Methods and Applications**, Cambridge University Press.

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• Silverman, B. W. (1986), **Density Estimation for Statistics and Data Analysis**.