# Nonparametric Density Estimation

Sections 17.1-17.8 of Hansen (2022)

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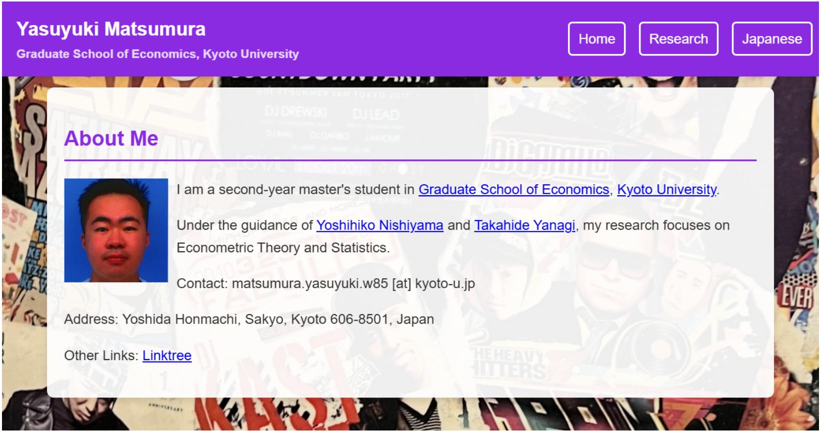



This slide is available on
`https://yasu0704xx.github.io/research.html`.

# Introduction

- As a general rule, density functions can take any shape. They are inherently nonparametric and cannot be described by a finite set of parameters.
- That is, functional and/or distributional specifications relied on when estimating density functions may be incorrect.
- If we assume that such specifications are "true," we might obtain incorrect empirical conclusions.
- Thus, it would be disirable if we develop estimation procedures without requiring functional and/or distributional specifications.
- Nonparametric kernel methods achieve such a goal.

## Setup

- Here we review Sections 17.1-17.8 of Hansen (2022) [3].
- We proceed with a discussion of how to estimate the probability density function $f(x)$ of a real-valued random variable $X$ for which we have $n$ IID observations $X_1, \cdots X_n$.
- We assume that $f(x)$ is continuous.
- The goal is to estimate $f(x)$ either at a single point $x$ or a set of points in the interior of the support of $X$.

## Literature

- Excellent textbooks on nonparametric density estimation include Silverman (1986) [11] and Scott (1992) [10].
- The following textbooks are often refered:
  - Silverman (1986) [11],
  - Scott (1992) [10],
  - van der Vaart (2000, Chapter 24) [12],
  - Pagan and Ullah (1999, Chapter 2) [7], and
  - Li and Racine (2007, Chapter 1) [6].
- 日本語の文献：
  - 西山・人見 (2023，第 1 章) [16]
  - 末石 (2015，第 9 章) [15]
  - 清水 (2023，第 5 章) [14]

# Contents

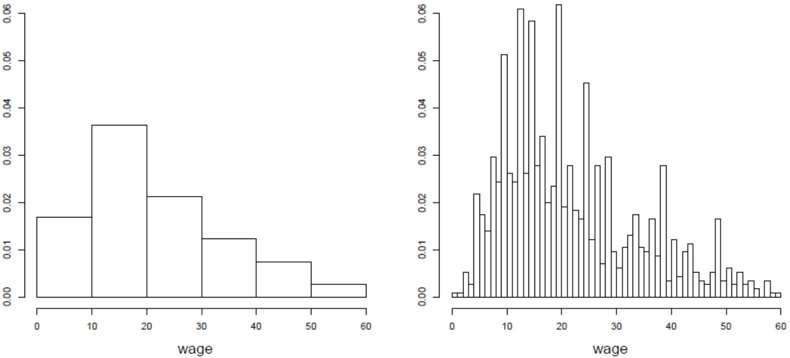
# Idea behind Kernel Density Estimation

# Histogram

- A simple and familiar estimator of $f(x)$ is a histogram.
- Devide the range of $f(x)$ into $B$ bins of width $w$.
- Counting the number of observations $n_j$ in each bin $j$, we obtain the histogram estimator of $f(x)$ for $x$ in the $j$-th bin:

$$\hat{f}(x) = \frac{n_j}{nw}. \tag{1}$$

- The histogram is the plot of these heights, displayed as rectangles.




(a) Bin Width = 10

(b) Bin Width = 1

Figure 17.1: Histogram Estimate of Wage Density for Asian Women

# Empirical Distribution Function

- Let us generalize the concept of histogram estimator.
- The empirical distribution function is defined as

$$F_n(x) = \frac{1}{n} \sum_{i=1}^{n} 1(X_i \leq x).$$

- Let $F(x) = \int_{-\infty}^{x} f(x)dx$ denote the (cumulative) distribution function.
- By L.L.N. and C.L.T.,[1] we obtain

$$F_n(x) \xrightarrow{p} F(x),$$
$$\sqrt{n}(F_n(x) - F(x)) \xrightarrow{d} \text{Normal}(0, F(x)(1 - F(x))).$$

[1] We discuss these convergences in Chapter 18 of Hansen (2022) [3].

# Naive Estimator

- Since $F_n(x)$ includes an indicator function, the empirical distribution function is not differentiable.
- Instead, let us consider approximate the "derivative" of $F_n(x)$.
- Note that, for $h \to 0$, it holds that

$$f(x) \approx \frac{F(x+h) - F(x-h)}{2h}.$$

- Replacing $F$ with $F_n$, we obtain the naive estimator[2] of $f(x)$:

$$f_n(x) = \frac{F_n(x+h) - F_n(x-h)}{2h}.$$

- Under certain conditions, it can be shown that $f_n(x) \xrightarrow{p} f(x)$.

[2] The Rosenblatt estimator (Rosenblatt, 1956) [9]

- The naive estimator of $\phi(x)$ using IID observations $X_1, \cdots X_{100} \sim \text{Normal}(0,1)$: [3]

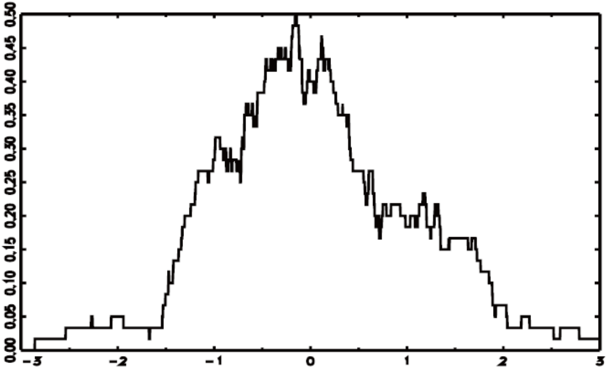



図 1: ナイーブ推定量 $(h = 0.3)$

[3] Cited from the lecture note 01 by N. Sueishi.

# Idea behind Kernel Density Estimation

- The naive estimator can be rewritten as

$$\begin{aligned} f_n(x) &= \frac{1}{2nh}\sum_{i=1}^{n} 1(x-h \le X_i \le x+h) \\ &= \frac{1}{nh}\sum_{i=1}^{n} k_0\left(\frac{X_i - x}{h}\right), \end{aligned}$$

where $k_0(\cdot)$ is given by

$$k_0(u) = \frac{1}{2}\cdot 1(-1 \le u \le 1).$$

- Replacing $k_0(\cdot)$ with some smooth function, we can obtain a differentiable, smooth estimator of $f(x)$ ...?

# Kernel Density Estimator

# Kernel Density Estimator

- The kernel density estimator[4] of $f(x)$ is given by

$$\hat{f}(x) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right). \tag{2}$$

- $K(u)$ is a weighting function known as a kernel function. The kernel $K(u)$ weights observations based on the distance between $X_i$ and $x$.
- $h > 0$ is a scalar known as a bandwidth. The bandwidth $h$ determines what is meant by "close."
- The kernel density estimator (2) critically depends on the bandwidth rather than the kernel function.

[4] The Parzen-Rosenblatt estimator (Parzen, 1962) [8]

# Kernel Function

**Definition 17.1**

- A kernel function $K(u)$ satisfies

$$1. \quad 0 \leq K(u) \leq \bar{K} < \infty, \tag{3}$$

$$2. \quad K(u) = K(-u), \tag{4}$$

$$3. \quad \int_{-\infty}^{\infty} K(u)du = 1, \text{ and} \tag{5}$$

$$4. \quad \int_{-\infty}^{\infty} |u|^r K(u)du < \infty \text{ for all positive integers } r. \tag{6}$$

- Essentially, a kernel function is a bounded PDF which is symmetric about zero.
- Assumption (6) is not essential for most results but is a convenient simplification and does not exclude any kernel functions used in standard empirical practice.

**Definition 17.2**

- A normalized kernel function $K(u)$ satisfies

$$\int_{-\infty}^{\infty} u^2 K(u) du = 1.$$

- The $j$-th moment of a kernel is defined as

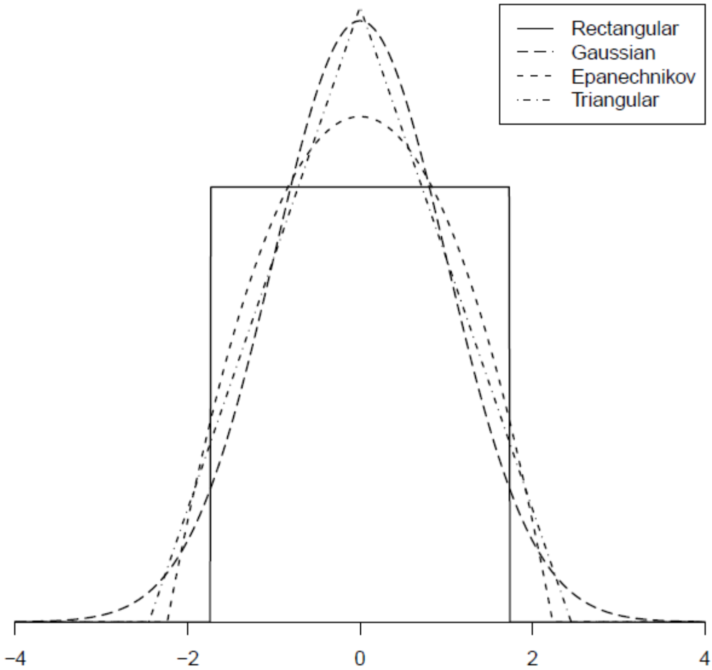
$$\kappa_j(K) = \int_{-\infty}^{\infty} u^j K(u) du.$$

- The order of a kernel $\nu$ is defined as the order of the first non-zero moment.

# Examples of Second-Order Kernel

- Rectangular kernel: $K(u) = \frac{1}{2\sqrt{3}} 1(|u| \leq \sqrt{3})$
- Gaussian kernel: $K(u) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right)$
- Epanechnikov kernel:[5] $K(u) = \frac{3}{4\sqrt{5}} \left(1 - \frac{u^2}{5}\right) 1(|u| \leq \sqrt{5})$
- Triangular kernel: $K(u) = \frac{1}{\sqrt{6}} \left(1 - \frac{|u|}{\sqrt{6}}\right) 1(|u| \leq \sqrt{6})$
- Quartic (Biweight) kernel: $K(u) = \frac{15}{16}(1 - u^2)^2 1(|u| \leq 1)$
- Triweight kernel: $K(u) = \frac{35}{32}(1 - u^2)^3 1(|u| \leq 1)$

[5] Epanechnikov (1969) [1]


Rectangular
Gaussian
Epanechnikov
Triangular
−4
−2
0
2
4

# Higher-Order Kernel

- Higher-order kernels can be used. See Section 1.11 of Li and Racine (2007) [6] for details.

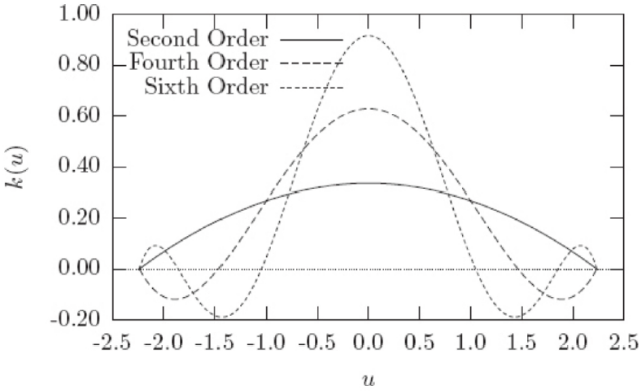



Figure 1.2: Epanechnikov kernels of varying order.

# Bandwidth

**Definition 17.3**

- A bandwidth or tuning parameter $h > 0$ is a real number used to control the degree of smoothing of a nonparametric estimator.

- Larger values of $h$ result in smoother estimators.
- Smaller values $h$ result in less smooth estimators.

# Properties of Kernel Density Estimator

- Invariance to rescaling the kernel function and bandwidth: The estimator (2) using $K(u)$ and $h$ is equal for any $b > 0$ to the one using $K\left(\frac{u}{b}\right)$ and $\frac{h}{b}$.
- Invariance to data scaling: Suppose that $Y = cX$ for some $c > 0$, which means the (true) density of $Y$ is

$$f_Y(y) = \frac{f_X(\frac{y}{c})}{c}.$$

Letting $\hat{f}_X(x)$ and $\hat{f}_Y(x)$ be the estimator (2) using $\{X_i\}_{i=1}^n$ and $h$ and the one using $\{Y_i\}_{i=1}^n = \{cX_i\}_{i=1}^n$ and $ch$, respectively, Then, it hold that

$$\hat{f}_Y(y) = \frac{\hat{f}_X(\frac{y}{c})}{c}.$$

- The kernel density estimator (2) is non-negative, and integrates to 1: Letting $u = \dfrac{(X_i - x)}{h}$, we obtain

$$\int_{-\infty}^{\infty} \hat{f}(x)dx = \frac{1}{nh} \sum_{i=1}^{n} \int_{-\infty}^{\infty} K\left(\frac{X_i - h}{h}\right) dx$$
$$= \frac{1}{n} \sum_{i=1}^{n} \int_{-\infty}^{\infty} K(u)du = 1.$$

# Bias, Variance, MSE

# Bias, Variance, MSE

- The mean squared error (MSE) of a generic estimator $\hat{f}(x)$ can be decomposed as follows:

$$
\begin{aligned}
\text{MSE}\left(\hat{f}(x)\right) &\equiv \mathbb{E}\left[\{\hat{f}(x) - f(x)\}^2\right] \\
&= \mathbb{E}\left[\{\hat{f}(x) - \mathbb{E}[\hat{f}(x)] + \mathbb{E}[\hat{f}(x)] - f(x)\}^2\right] \\
&= \mathbb{E}\left[\{\hat{f}(x) - \mathbb{E}[\hat{f}(x)]\}^2\right] + \left[\mathbb{E}[\hat{f}(x)] - f(x)\right]^2 \\
&\equiv \text{var}\left(\hat{f}(x)\right) + \left[\text{bias}\left(\hat{f}(x)\right)\right]^2.
\end{aligned}
$$

# Bias Evaluation

- Since $\{X_i\}_{i=1}^n$ is an IID sample, it holds that

$$\begin{aligned}\mathbb{E}[\hat{f}(x)] &= \mathbb{E}\left[\frac{1}{nh}\sum_{i=1}^n K\left(\frac{X_i - x}{h}\right)\right] \\ &= \mathbb{E}\left[\frac{1}{h}K\left(\frac{X - x}{h}\right)\right].\end{aligned}$$

- By definition,

$$\mathbb{E}\left[\frac{1}{h}K\left(\frac{X - x}{h}\right)\right] = \int_{-\infty}^{\infty}\frac{1}{h}K\left(\frac{v - x}{h}\right)f(v)dv.$$

- Let $u = \dfrac{v-x}{h}$. Under certain conditions, we obtain

$$\int_{-\infty}^{\infty} \frac{1}{h} K\left(\frac{v-x}{h}\right) f(v)dv = \int_{-\infty}^{\infty} K(u) f(x+hu) du$$
$$= \int_{-\infty}^{\infty} K(u) \left\{ f(x) + f'(x)hu + \frac{1}{2} f''(x) h^2 u^2 + o(h^2) \right\} du$$
$$= f(x) \int_{-\infty}^{\infty} K(u)du + f'(x)h \int_{-\infty}^{\infty} uK(u)du$$
$$+ \frac{h^2}{2} f''(x) \int_{-\infty}^{\infty} u^2 K(u)du + o(h^2)$$
$$= f(x) + 0 + \frac{h^2}{2} f''(x)\kappa_2 + o(h^2)$$

- Thus, the bias of the kernel density estimator (2) is described as

$$\text{bias}\left(\hat{f}(x)\right) \equiv \mathbb{E}[\hat{f}(x)] - f(x) = \frac{h^2}{2} f''(x)\kappa_2 + o(h^2).$$

## Theorem 17.1

- Letting $\mathcal{N}$ denote the neighborhood of $x$, assume that $f(x)$ is continuous in $\mathcal{N}$. Then, as $h \to 0$,

$$\mathbb{E}[\hat{f}(x)] \to f(x).$$

- Assume additionally that $f''(x)$ is continuous in $\mathcal{N}$. Then, as $h \to 0$,

$$\text{bias}\left(\hat{f}(x)\right) \equiv \mathbb{E}[\hat{f}(x)] - f(x) = \frac{h^2}{2} f''(x)\kappa_2 + o(h^2).$$

# Variance Evaluation

**Theorem 17.2**

- Assume that $f(x)$ is continuous in $\mathcal{N}$. Then, as $h \to 0$ and $nh \to \infty$,

$$\text{var}\left(\hat{f}(x)\right) = \frac{R_K f(x)}{nh} + o\left(\frac{1}{nh}\right)$$

  where $R_K = \int K^2(u)du$ denotes the roughness of $K(u)$.

- The variance of kernel density estimator can be estimated by the sample analogue of $\mathbb{E}\left[\{\hat{f}(x) - \mathbb{E}[\hat{f}(x)]\}^2\right]$, or by $\dfrac{\kappa \hat{f}(x)}{nh}$.

# MSE Evaluation

- Combining Theorems 17.1 and 17.2, we obtain the following result:

**Theorem 1.1 of Li and Racine (2007) [6]**

- Supppose that $f(x)$ is three-times differentiable.
- Assume that $K(\cdot)$ satisfies (3) and (4).
- As $n \to \infty$, $h \to 0$ and $nh \to \infty$,

$$\text{MSE}\left(\hat{f}(x)\right) = \frac{h^4}{4}\left[\kappa_2 f''(x)\right]^2 + \frac{\kappa f(x)}{nh} + o\left(h^4 + \frac{1}{nh}\right),$$

where $\kappa_2 = \int u^2 K(u) du$ and $\kappa = \int K^2(u) du$.

- This result implies that $\text{MSE}\left(\hat{f}(x)\right) \to 0$ and that $\hat{f}(x)$ is a consistent estimator of $f(x)$.

# Take Away

- バイアス，分散，MSE それぞれの漸近的な評価のために必要な仮定については，Li and Racine (2007, Chapter 1) [6] や西山・人見 (2023，第 1 章) [16] が詳しい．
- 漸近的な評価を導出するために必要な定理や補題については，Li and Racine (2007, Appendix A) [6]，清水 (2021，第 4 章) [13] や西山・人見 (2023，第 1 章) [16] が詳しい．

# IMSE, AIMSE

## IMSE, AIMSE

- The integrated mean squared error (IMSE) is a useful measure of precision of a kernel density estimator:

$$\text{IMSE} = \int_{-\infty}^{\infty} \text{MSE}\left(\hat{f}(x)\right) dx = \int_{-\infty}^{\infty} \mathbb{E}\left[\{\hat{f}(x) - f(x)\}^2\right] dx$$

- Suppose that $f''(x)$ is uniformly continuous. By similar arguments as we discuss MSE, it can be shown that as $n \to \infty$, $h \to 0$, and $nh \to \infty$,

$$\text{IMSE} = \frac{1}{4} R(f'') h^4 + \frac{\kappa}{nh} + o\left(h^4 + \frac{1}{nh}\right), \tag{7}$$

where $R(f'') = \int \{f''(x)\}^2 \, dx$ denotes the roughness of $f''(x)$.

- The leading term in (7) is called the asymptotic integrated mean squared error (AIMSE).

## Optimal Bandwidth

- Bias-Variance Trade-Off: The first term of AIMSE is increasing in $h$, while the second term is decreasing in $h$.
- For a fixed second-order $K(\cdot)$, we can obtain AIMSE optimal bandwidth $h_0$ by solving the FOC: [6]

$$h_0 = \left( \frac{R_K}{R(f'')} \right)^{\frac{1}{5}} n^{-\frac{1}{5}}. \tag{8}$$

- In reality, AIMSE optimal $h_0$ depends on the second derivative of unknown $f(x)$. Thus, researchers need to select a bandwidth $h$ by certain procedures. [7]

[6] Explanations on the estimation of $R(f'')$ can be found in Hall and Marron (1987) [2] and Jones and Sheather (1991) [4] among others.

[7] See Sections 17.9-17.11 and 17.15 of Hansen (2022) [3] for futher discussions on bandwidth selection.

# Optimal Kernel

**Theorem 17.4**

- Letting $h$ be the AIMSE optimal bandwidth $h_0$ given in (8), AIMSE is minimized by the Epanechnikov kernel:[a]

$$K(u) = \frac{3}{4\sqrt{5}}\left(1 - \frac{u^2}{5}\right)1(|u| \leq \sqrt{5})$$

[a] Epanechnikov (1969) [1]

- See Section 17.8 of Hansen (2022) [3] for the proof.
- Kanaya and Okamoto (2025) [5] suggest to use another kernel function for certain optimality.

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