

Nonparametric Inference

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1 Recall

Parametric Inference

- Suppose we observe independent data $\{x_i\}_{i=1}^n$, the distribution of these data can be obtained through a large number of observations (prior information) (e.g. $N(\mu, \sigma^2)$, $\text{Uin}(0, \theta)$, $\text{Ber}(p)$), parameter information is inferred from the data (e.g. $\theta = (\mu, \sigma^2) \dots$).

$$MLE \Rightarrow \hat{\theta} \Rightarrow F_{\theta}.$$

- Suppose we observe pairs of data $\{(x_i, y_i)\}_{i=1}^n$.

$$r : x \in X \rightarrow y \in Y, \quad MSE : \min_r \mathbb{E}[y - r(x)]^2.$$

In order to find the regression function $r(x) = \mathbb{E}(Y|X = x)$, suppose:

$$r_{\beta}(x) = \beta_0 + \beta_1 x \quad \text{or} \quad r_{\beta}(x) = X^T \beta.$$

then apply MLE, LS to infer parameters $(r_{\hat{\beta}(x)})$.

All of the above are **generative models**.

2 Nonparametric Inference

Definition 1 *Nonparametric inference refers to statistical techniques that use data to infer unknown quantities of interest while making as few assumptions as possible.*

$$\{X_i\}_{i=1}^n \Rightarrow F_X(x),$$

the specific distribution function is unknown.

Empirical Distribution Function (EDF)

Definition 2 *For i.i.d. samples $\{X_i\}_{i=1}^n$, the EDF is:*

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

where $\mathbb{I}(X_i \leq x) = \begin{cases} 1 & \text{if } X_i \leq x, \\ 0 & \text{otherwise.} \end{cases}$

Derivation 1

$$F_X(x) = \mathbb{P}(X \leq x) = \mathbb{P}(\mathbb{I}(X \leq x) = 1) = \mathbb{E}[\mathbb{I}(X \leq x)],$$

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

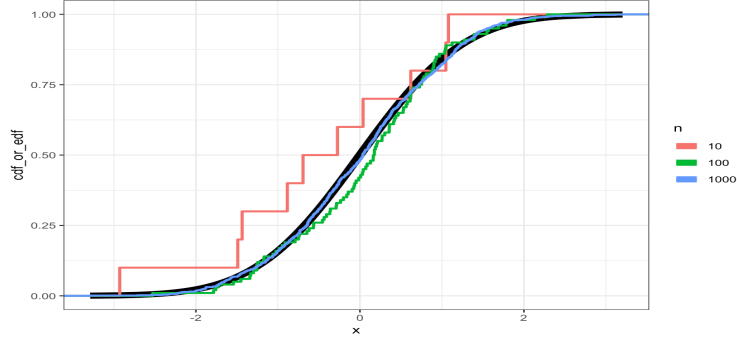


Figure 1. EDF

Theorem & Proof

1. **Unbiasedness:** $\mathbb{E}[F_n(x)] = F_X(x)$.

proof:

$$\mathbb{E}[F_n(x)] = \frac{1}{n} \sum_{i=1}^n \mathbb{E}[\mathbb{I}(X_i \leq x)] = \mathbb{P}(X \leq x) = F_X(x).$$

2. **Variance:** $\mathbb{V}(F_n(x)) = \frac{F_X(x)[1-F_X(x)]}{n}$.

proof:

$$\mathbb{V}(F_n(x)) = \frac{1}{n^2} \sum_{i=1}^n \mathbb{V}(\mathbb{I}(X_i \leq x)) = \frac{1}{n} \mathbb{V}(\mathbb{I}(X \leq x)),$$

$$\begin{aligned} \mathbb{V}(\mathbb{I}(X \leq x)) &= \mathbb{E}[\mathbb{I}^2(X \leq x)] - \mathbb{E}[\mathbb{I}(X \leq x)]^2 \\ &= \mathbb{P}(X \leq x) - (\mathbb{P}(X \leq x))^2 \\ &= F_X(x) - F_X^2(x) \\ &= F_X(x)[1 - F_X(x)]. \end{aligned}$$

3. **Consistency:** By Glivenko-Cantelli theorem, $F_n(x) \xrightarrow{P} F_X(x)$ as $n \rightarrow \infty$.

proof: For any $\epsilon > 0$:

$$\mathbb{P}(|F_n(x) - F_X(x)| \geq \epsilon) \leq \frac{\text{Var}(F_n(x))}{\epsilon^2} = \frac{F_X(x)(1 - F_X(x))}{n\epsilon^2} \xrightarrow{n \rightarrow \infty} 0.$$

3 Density Estimation

Histogram Density Estimation

Steps For i.i.d. samples $\{X_i\}_{i=1}^n$, the PDF is f , domain is $[0,1]$.

1. **Bin Construction:** Partition the domain into m bins of width $h = \frac{1}{m}$.
 $B_1 = [0, \frac{1}{m}), B_2 = [\frac{1}{m}, \frac{2}{m}), \dots, B_m = [\frac{m-1}{m}, 1]$.

2. **Count Observations:** Let n_j be the number of samples in the j -th bin.

3. **Probabilistic estimation :**

$$\hat{p}_j = \frac{n_j}{n}.$$

4. **Density Estimate:**

$$\hat{f}_n(x) = \frac{\hat{p}_j}{h} \quad \text{if } x \in B_j.$$

$$\hat{f}_n(x) = \frac{1}{h} \sum_{j=1}^m \hat{p}_j \mathbb{I}(x \in B_j).$$

Motivation

1. $p_j = \int_{B_j} f(x)dx = f(x^*)h, x^* \in B_j$ (mean value theorem).
2. $\mathbb{E}[\hat{p}_j] = \frac{\mathbb{E}(n_j)}{n} = \frac{[\sum_{i=1}^n \mathbb{I}(x_i \in B_j)]}{n} = \frac{\sum_{i=1}^n \mathbb{E}[\mathbb{I}(x_i \in B_j)]}{n} = \frac{np_j}{n} = p_j$.
3. $\mathbb{E}[\hat{f}_n(x)] = \frac{1}{h} \mathbb{E}(\hat{p}_j) = \frac{p_j}{h} = f(x^*)$ (as $m \rightarrow \infty, x \sim x^*$).

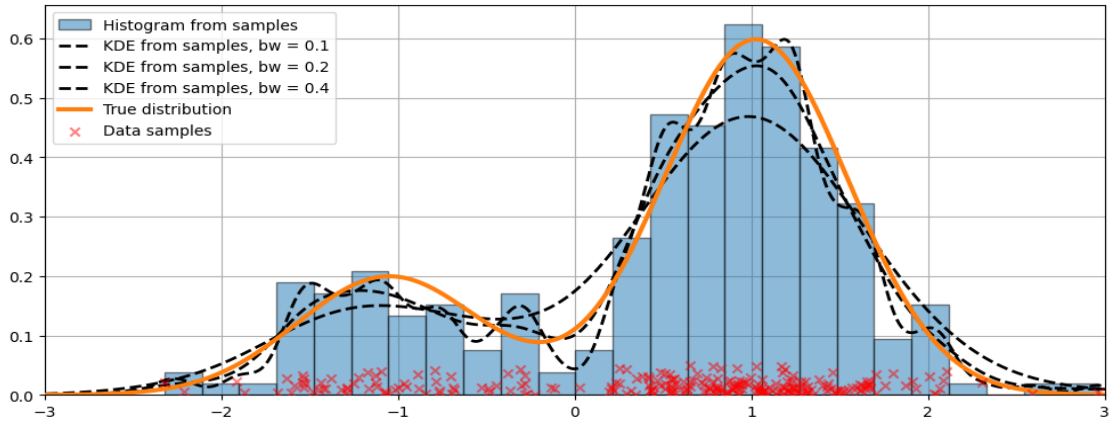


Figure 2. Density Estimation

Kernel Density Estimation (KDE)

Derivation 2 According to histogram:

$$\begin{aligned}
 \hat{f}_n(x) &= \frac{1}{h} \sum_{j=1}^m \hat{p}_j \mathbb{I}(x \in B_j) \\
 &= \frac{1}{h} \sum_{j=1}^m \frac{n_j}{n} \mathbb{I}(x \in B_j) \\
 &= \frac{1}{nh} \sum_{j=1}^m \sum_{i=1}^n [\mathbb{I}(x_i \in B_j) \mathbb{I}(x \in B_j)] \\
 &= \frac{1}{nh} \sum_{i=1}^n [\sum_{j=1}^m \mathbb{I}(x_i \in B_j) \mathbb{I}(x \in B_j)] \\
 \hat{f}_n(x) &= \frac{1}{nh} \sum_{i=1}^n K\left(\frac{x - X_i}{h}\right),
 \end{aligned}$$

where K is a kernel function.

Different Kernel Functions

$$\text{Kernel Functions} = \begin{cases} (1) \text{Gaussian} & k(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right); \\ (2) \text{Uniform} & k(x) = \frac{1}{2} \mathbb{I}[-1, 1]; \\ (3) \text{Epanechnikov} & k(x) = \frac{3}{4} \max\{1 - x^2, 0\}; \\ \dots & \end{cases}$$

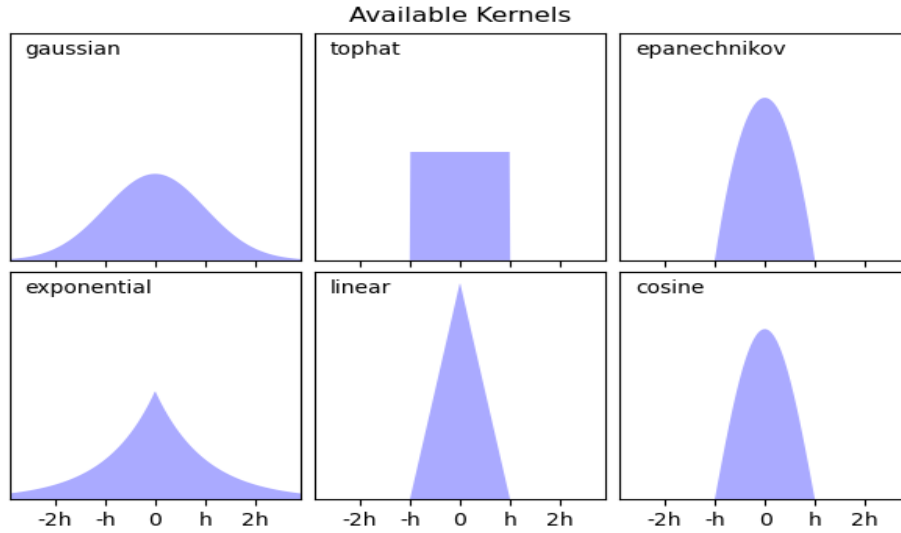


Figure 3. Different Kernel Function

Property of Kernel Functions

1. $\int_{\mathbb{R}} k(x)dx = 1.$
2. $\int_{\mathbb{R}} xk(x)dx = 0 \Rightarrow k(x) = k(-x).$
3. $\lim_{x \rightarrow +\infty} k(x) = \lim_{x \rightarrow -\infty} k(x) = 0.$

4 Mean Integrated Squared Error (MISE)

Definition 3

$$MISE = \mathbb{E} \left[\int (\hat{f}_n(x) - f(x))^2 dx \right] = \int Bias^2(\hat{f}_n(x))dx + \int \mathbb{V}(\hat{f}_n(x))dx,$$

$$Bias(x) = \mathbb{E}[\hat{f}_n(x)] - f(x), \quad \mathbb{V}(x) = \mathbb{E}[(\hat{f}_n(x) - \mathbb{E}(\hat{f}_n(x)))^2].$$

Derivation 3

$$\begin{aligned} D(\hat{f}_n(x), f(x)) &= \int_{\mathbb{R}} (\hat{f}_n(x) - f(x))^2 dx, \\ MISE &= R(\hat{f}_n(x), f(x)) = \mathbb{E}[D(\hat{f}_n(x), f(x))] = \int_{\mathbb{R}^n} \int_{\mathbb{R}} (\hat{f}_n(x) - f(x))^2 dx dF(x), \\ R(\hat{f}_n(x), f(x)) &= \int_{\mathbb{R}} Bias^2(\hat{f}_n(x))dx + \int_{\mathbb{R}} \mathbb{V}(\hat{f}_n(x))dx. \end{aligned}$$

MISE for Density Estimation

MISE for Histogram Density Estimation

Theorem 1 *If f is an L -Lipschitz function, $\max_{x \in [0,1]} f(x) \leq M$, then*

$$bias(\hat{f}_n(x)) \leq Lh, \quad \mathbb{V}(\hat{f}_n(x)) \leq \frac{M}{nh} + \frac{M^2}{n},$$

where $\hat{f}_n(x)$ is the histogram density estimation of f .

$$\begin{aligned} MISE &= \int_{\mathbb{R}} Bias^2(\hat{f}_n(x))dx + \int_{\mathbb{R}} \mathbb{V}(\hat{f}_n(x)) \\ &= L^2 h^2 + \frac{M}{nh} + \frac{M^2}{n}, \end{aligned}$$

Find minimizing MISE $MISE \Rightarrow h_{opt} = O(n^{-1/3})$, leading to $MISE = O(n^{-2/3})$.

MISE for KDE

Theorem 2 *If f is an L -Lipschitz function,*

then

$$\mu_k^2 = \int x^2 k(x) dx, \quad \sigma_k^2 = \int h^2(x) dx,$$

$$\text{bias}(\hat{f}_n(x)) = \frac{1}{2} h^2 f''(x) \mu_k^2 + O(h^2), \quad \mathbb{V}(\hat{f}_n(x)) = \frac{1}{nh} f(x_0) \sigma_k^2 + O\left(\frac{1}{nh}\right),$$

where $\hat{f}_n(x)$ is the kernel density estimation of f .

$$\text{MISE} \approx \frac{1}{4} h^4 \int (f''(x))^2 dx + \frac{1}{nh} \int K^2(u) du.$$

Find minimizing MISE $\text{MISE} = 0 \Rightarrow h_{\text{opt}} = O(n^{-1/5})$, leading to $\text{MISE} = O(n^{-4/5})$.

Density Estimation	Convergence speed
Histogram	$O(n^{-2/3})$
Kernel	$O(n^{-4/5})$