Advanced statistics and modelling

2023 spring

MODELS, INFERENCE, LEARNING

The basis statistical inference problem

- The basic statistical inference problem is the following:
  - We observe $X_1, X_2, \ldots, X_n \sim F$.
  - Based on the observations we would like to **infer** (or estimate or learn) F or some feature of F (such as e.g., its mean or variance).
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where θ is an unknown parameter (or a vector of parameters) that can take values in the parameter space Θ.

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E.g., if the data comes from a Normal distribution, then

$$\mathfrak{F} = \left\{\rho(x \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}},\ \ \mu \in \mathbb{R}, \sigma > 0\right\}$$

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- If θ is a vector, but we are interested in only a part of the parameters, then the remaining parameters are called **nuisance parameters.**
- A **non-parametric model** is a set $\mathfrak{F}$ that cannot be parametrised by a finite number of parameters. E.g., the set of all possible CDF-s, $\mathfrak{F} = \{$ all CDF's $\}$ is a non-parametric model.

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thus, the subscript θ indicates that the given probability or expectation is depending on θ and was taken with respect to $\rho(x \mid \theta)$, and it does NOT indicate that we were averaging over θ!

Regression, prediction, classification

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- The variables X and Y are called

$$X : \begin{cases} \text{predictor}, \\ \text{regressor}, \\ \text{feature variable}, \\ \text{independent variable} \end{cases} \qquad Y : \begin{cases} \text{outcome}, \\ \text{response variable}, \\ \text{dependent variable} \end{cases}$$

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- The **regression function** is given by the conditional expectation of Y given X, written as

$$r(x) = \mathbb{E}(Y \mid X = x).$$

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- If the goal is to estimate the curve $r(x)$, then this is called **curve estimation** or **regression**.

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Proof:
Since $\epsilon = Y - r(x) = Y - \mathbb{E}(Y \mid X)$ we can write

$$\mathbb{E}(\epsilon) = \mathbb{E}\left[Y - \mathbb{E}(Y \mid X)\right] = \mathbb{E}(Y) - \mathbb{E}\left[\mathbb{E}(Y \mid X)\right] = \mathbb{E}(Y) - \mathbb{E}(Y) = 0.$$

Point estimation and bias

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- Formally, if $X_1, X_2, \ldots, X_n$ are IID data points from some distribution F, then a **point estimator** $\widehat{\theta}$ of a parameter θ is some function of $X_1, X_2, \ldots, X_n$:

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- The **bias** corresponds to the difference between the mean of $\widehat{\theta}$ and the true value of the parameter,

$$\text{bias}(\widehat{\theta}) = \mathbb{E}_\theta(\widehat{\theta}) - \theta.$$

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- Often, it is not possible to compute $\text{se}(\widehat{\theta})$. However, usually we can estimate it, and the estimated standard error is denoted by $\widehat{\text{se}}(\widehat{\theta})$.

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  - $\rightarrow$ $\widehat{p} = \overline{X_n} = \frac{1}{n}\sum_{i=1}^{n} x_i$.
  - $\rightarrow$ Since $\mathbb{E}(\widehat{p}) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}(X_i) = p$, the $\widehat{p}$ is unbiased.

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  - $\rightarrow$ The standard error: $\text{se}(\widehat{p}) = \sqrt{\mathbb{V}(\widehat{p})} = \sqrt{p(1-p)/n}$.

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  - $\rightarrow$ The standard error: $\text{se}(\widehat{p}) = \sqrt{\mathbb{V}(\widehat{p})} = \sqrt{p(1-p)/n}$.
  - $\rightarrow$ The estimated standard error: $\widehat{\text{se}}(\widehat{p}) = \sqrt{\widehat{p}(1-\widehat{p})/n}$.

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Note that $\mathbb{E}_\theta(\cdot)$ refers to the expectation with respect to

$$\rho(x_1, x_2, \ldots, x_n \mid \theta) = \prod_{i=1}^{n} \rho(x_i \mid \theta)$$

that generated the data, and it does NOT mean that we are averaging with respect to some density of θ.

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$$\begin{aligned}
\mathrm{MSE}_\theta(\widehat{\theta}) &= \mathbb{E}_\theta\left[(\widehat{\theta}-\theta)^2\right] = \mathbb{E}_\theta\left[(\widehat{\theta}-\bar{\theta}+\bar{\theta}-\theta)^2\right] = \\
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&\mathbb{V}_\theta(\widehat{\theta}) + (\bar{\theta}-\theta)^2 = \mathbb{V}_\theta(\widehat{\theta}) + \left[\mathrm{bias}(\widehat{\theta})\right]^2.
\end{aligned}$$

Consequence:
If $\widehat{\theta}$ is unbiased, the MSE is simply the variance of $\widehat{\theta}$.

Asymptotically normal estimator

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The estimator $\widehat{\theta}$ is asymptotically normal if

$$\frac{\widehat{\theta} - \theta}{\text{se}} \xrightarrow{\text{d}} N(0,1).$$

Confidence interval

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A $1-\alpha$ **confidence interval** for a parameter θ is an interval $C = [a, b]$ where $a = a(X_1, X_2, \ldots, X_n)$ and $b = b(X_1, X_2, \ldots, X_n)$ are functions of the data such that

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- Note: θ is fixed, and C_n is random.

Confidence interval

Example:

- Assume a coin tossing experiment, where $\widehat{p} = \overline{X_n} = \frac{1}{n}\sum_{i=1}^{n} x_i$, and let the confidence interval be $[\widehat{p} - \epsilon, \widehat{p} + \epsilon]$. How should we choose ϵ for a given value of α?

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→ According to Hoeffding's inequality:
If $X_1, X_2, \ldots, X_n \sim$ Bernoulli(p), then for the sample mean $\overline{X_n}$ we can write

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$$P(|\widehat{p} - p| > \epsilon) \leq 2e^{-2n\epsilon^2} = \alpha.$$

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$$C = [\widehat{\theta} - z_{\alpha/2}\widehat{\text{se}}, \widehat{\theta} + z_{\alpha/2}\widehat{\text{se}}],$$

where $z_{\alpha/2} = \Phi^{-1}(1 - \alpha/2)$ with $\Phi(z)$ denoting the CDF of the standard Normal distribution.

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Proof:
Let us define $Z = (\widehat{\theta} - \theta)/\widehat{\text{se}}$. Assuming $Z \xrightarrow{\text{d}} N(0, 1)$, we have

$$P_\theta(\theta \in C) = P_\theta\left(\widehat{\theta} - z_{\alpha/2}\widehat{\text{se}} < \theta < \widehat{\theta} + z_{\alpha/2}\widehat{\text{se}}\right) =$$

$$P_\theta\left(-z_{\alpha/2} < \frac{\widehat{\theta} - \theta}{\widehat{\text{se}}} < z_{\alpha/2}\right) \longrightarrow P(-z_{\alpha/2} < Z < z_{\alpha/2}) = 1 - \alpha$$

Confidence interval

Example:

- Assuming $X_1, X_2, \ldots, X_n \sim \text{Bernoulli}(p)$ we have

$$\widehat{p} = \frac{1}{n}\sum_{i=1}^{n} x_i, \qquad \mathbb{V}(\widehat{p}) = \frac{1}{n^2}\sum_{i=1}^{n}\mathbb{V}(X_i) = \frac{1}{n^2}\sum_{i=1}^{n} p(1-p) = \frac{p(1-p)}{n}.$$

$$\text{se} = \sqrt{\frac{p(1-p)}{n}} \qquad \widehat{\text{se}} = \sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}.$$

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- This interval is shorter compared to the one given based on Hoeffding's inequality.
- However, this is only an **approximate** confidence interval, whereas in case of Hoeffding's inequality we have guarantee for smaller sample sizes as well.

Empirical CDF

Empirical CDF

Empirical CDF

Based on IID variables $X_1, X_2, \ldots, X_n$, the empirical distribution function $\widehat{F}_n(x)$ is defined as the fraction of observed data points falling below x, which can be formulated e.g., as

$$\widehat{F}(x) = \frac{1}{n} \left| \{ x_i \mid x_i < x \} \right| = \frac{1}{n} \sum_{i=1}^{n} I(X_i < x),$$

where $I(X_i < x) = 1$ if $x_i > x$ and $I(X_i < x) = 0$ otherwise.

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Glivenko-Cantelli theorem

Let $X_1, X_2, \ldots, X_n \sim F$ be IID variables. Then

$$\sup_x \left| \widehat{F}_n(x) - F(x) \right| \xrightarrow{\text{a.s.}} 0.$$

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Note that for any fixed x, the sequence of $\widehat{F}_n(x)$ is a sequence of random variables that is converging to $F(x)$ according to the law of large numbers. The theorem above strengthens this to the uniform convergence of $\widehat{F}_n$ to F.

Empirical CDF

Dvoretzky-Kiefer-Wolfowitz inequality

Let $X_1, X_2, \ldots, X_n \sim F$ be IID variables. Then for any $\epsilon > 0$

$$P\left(\sup_x \left|\widehat{F}_n(x) - F(x)\right| > \epsilon\right) \leq 2e^{-2n\epsilon^2}.$$

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Note that for any fixed x, the sequence of $\widehat{F}_n(x)$ is a sequence of bounded random variables for which we can apply Hoeffding's inequality. The above theorem strengthens this by providing a uniform bound.

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Application:
We can use the DKW inequality for providing a **confidence band** for the empirical CDF.

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We can use the DKW inequality for providing a **confidence band** for the empirical CDF.

- Let us choose first an α value, and the goal is to give a confidence band (confidence set) C_n such that

$$P(F \in C_n) \geq 1 - \alpha.$$

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We can use the DKW inequality for providing a **confidence band** for the empirical CDF.

- Let us choose first an α value, and the goal is to give a confidence band (confidence set) C_n such that

$$P(F \in C_n) \geq 1 - \alpha.$$

- According to the above theorem, for any x the lower bound can be given as $L(x) = \widehat{F}_n(x) - \epsilon_n$ and the upper bound can be given as $U(x) = \widehat{F}_n(x) + \epsilon_n$ where

$$\epsilon_n = \sqrt{\frac{1}{2n} \ln\left(\frac{2}{\alpha}\right)}.$$

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Given $X_1, X_2, \ldots, X_n \sim F$ IID variables the **empirical PDF** $\widehat{\rho}_n(x)$ provides a simple estimate for the PDF $\rho(x)$.

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- Let's assume altogether m bins of equal bin width h.
- If the number of observations in bin B_i is ν_i, then the estimate for the probability of this bin is $\widehat{p}_i = \nu_i/n$, (whereas the true probability is $p_i = \int_{B_i} \rho(x)dx$).

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- Based on that, the empirical PDF can be given as

$$\widehat{\rho}_n(x) = \sum_{i=1}^{m} \frac{\widehat{p}_i}{h} I(x \in B_i),$$

where $I(x \in B_i)$ is the indicator function of B_i, (i.e., $I(x \in B_i) = 1$ if $x \in B_i$ and $I(x \in B_i) = 0$ otherwise.)

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Risk (MISE)

For a statistical estimate $\widehat{\rho}_n(x)$ of the PDF $\rho(x)$ we can define the integrated squared error simply as

$$L(\widehat{\rho}_n, \rho) = \int \left(\widehat{\rho}_n(x) - \rho(x)\right)^2 dx.$$

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The expected value of this is the **mean integrated squared error** (MISE) or **risk**:

$$R(\widehat{\rho}_n, \rho) = \mathbb{E}\left(L(\widehat{\rho}_n, \rho)\right).$$

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→ The MISE (or risk) can be written as

$$\begin{aligned} R(\widehat{\rho}_n, \rho) &= \mathbb{E}\left(\int \left(\mathbb{E}(\widehat{\rho}_n(x)) - \rho(x)\right)^2\right) = \dots \\ &= \int b^2(x)dx + \int v(x)dx. \end{aligned}$$

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Thus, in other words,

RISK = BIAS^2 + VARIANCE.

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- For a given x, let's assume that x is in bin B_j. Then

$$\begin{aligned}\mathbb{E}(\widehat{\rho}_n(x)) &= \frac{p_j}{h} = \frac{1}{h}\int_{B_j}\rho(x)dx,\\ \mathbb{V}(\widehat{\rho}_n(x)) &= \frac{p_j(1-p_j)}{nh^2},\end{aligned}$$

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  Based on that, the probability p_j can be approximated as

$$p_j = \int_{x_{B_j}}^{x_{B_j}+h}\rho(u)du \approx \int_{x_{B_j}}^{x_{B_j}+h}\left(\rho(x)+(u-x)\rho'(x)\right)du =$$

$$h\rho(x) - hx\rho'(x) + \rho'(x)\left[u^2/2\right]_{x_{B_j}}^{x_{B_j}+h} = h\rho(x) + h\rho'(x)\left[\frac{h}{2} + x_{B_j} - x\right]$$

Empirical PDF

- Based on that, bias can be given as

$$b(x) = \mathbb{E}(\widehat{\rho}_n(x)) - \rho(x) = \frac{p_j}{h} - \rho(x) \approx \frac{h\rho(x) + h\rho'(x)\left[\frac{h}{2} + x_{B_j} - x\right]}{h} - \rho(x) = \rho'(x)\left[\frac{h}{2} + x_{B_j} - x\right]$$

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- The integral of $b^2(x)$ over the bin can be approximated as

$$\int_{x_{B_j}}^{x_{B_j}+h} b^2(x)dx \approx \int_{x_{B_j}}^{x_{B_j}+h} \left[\rho'(x)\right]^2 \left(\frac{h}{2} + x_{B_j} - x\right)^2 dx = \ldots = \left[\rho'(x)\right]^2 \frac{h^3}{12}.$$

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- Thus, the total contribution to the MISE from bias^2 is

$$\int b^2(x)dx \approx \sum_{j=1}^{m} \left[\rho'(x_{B_j} + h/2)\right]^2 \frac{h^3}{12} = \frac{h^2}{12} \sum_{j=1}^{m} h\left[\rho'(x_{B_j} + h/2)\right]^2 \approx \frac{h^2}{12} \int \left[\rho'(x)\right]^2 dx.$$

Empirical PDF

- In case of the variance, let's assume that h is small, and thus, p_j is close to 0, and therefore, $1 - p_j \approx 1$. Based on that, at a given x falling into bin B_j, the $v(x)$ can be written as

$$v(x) = \frac{p_j(1-p_j)}{nh^2} \approx \frac{p_j}{nh^2} \approx \frac{h\rho(x) + h\rho'(x)\left[\frac{h}{2} + x_j - x\right]}{nh^2}.$$

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Empirical PDF

MISE of the histogram estimator

- According to the previous calculations, given a PDF $\rho(x)$ where $\int \left[\rho'(x)\right]^2 dx < \infty$, the risk of the corresponding histogram estimator $\widehat{\rho}_n(x)$ with uniform bin width h can be written as

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$$h^* = \left(\frac{1}{6n} \int \left[\rho'(x)\right]^2 dx\right)^{\frac{1}{3}},$$

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and with this choice

$$R(\widehat{\rho}_n, \rho) \approx \frac{C}{n^{2/3}}, \qquad C = \left(\frac{3}{4}\right)^{\frac{2}{3}} \left(\int \left[\rho'(x)\right]^2 dx\right)^{\frac{1}{3}}$$

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- Although the decay of $R(\widehat{\rho}_n, \rho)$ as $n^{-2/3}$ is nice from a theoretical point of view, the formula for the optimal bin width h^* is "useless" from a practical point of view, since we have to know the true $\rho(x)$ in order to calculate it...

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→ Let's write the loss function which we want to minimise as

$$R(\widehat{\rho}_n, \rho) = \int (\widehat{\rho}_n(x) - \rho(x))^2 \, dx =$$
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The last term does not depend on the estimator, so we have to minimise only

$$J(h) = \int \widehat{\rho}_n^2(x)dx - 2\int \widehat{\rho}_n(x)\rho(x)dx,$$

(where the h dependence is implicit in this form through $\widehat{\rho}_n(x)$).

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→ As a side track, let us quickly have an overview of Jackknife, and then return to the problem of estimating $J(h)$.

Jackknife

- Based on our original data $\{x_1, x_2, \ldots, x_n\}$ we can define n Jackknife samples by always **leaving out one data point**, thus, the i^{th} Jackknife sample is $X_{[i]} = \{x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n\}$.

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- Any statistics or estimator can be evaluated on these samples as if we would on the whole data; let us denote the result of the estimator $s(\cdot)$ of interest on the i^{th} Jackknife sample as

$$\theta_{(i)} = s\left(X_{[i]}\right).$$

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→ Where does the factor $(n-1)/n$ come from?

Jackknife

To illustrate that $(n-1)/n$ is the correct prefactor, let us consider the case where $s(\cdot)$ is the sample mean, $s(\cdot) = \overline{X}_n = \frac{1}{n}\sum_{i=1}^{n} x_i$.

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- We know actually, that the variation of $\overline{X}_n$ is simply σ^2/n.
- Let's consider the inner term in $\mathbb{V}_{\text{jack}}(\theta)$:

$$\theta_{(i)} - \overline{\theta} = \frac{n\overline{X}_n - x_i}{n-1} - \frac{1}{n}\sum_{i=1}^{n}\overline{X}_{(i)},$$

where $\overline{X}_{(i)}$ denotes the sample mean calculated based on $X_{(i)}$ (leaving out x_i).

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where $\overline{X}_{(i)}$ denotes the sample mean calculated based on $X_{(i)}$ (leaving out x_i). The above expression can be also written as

$$\begin{aligned}
\theta_{(i)} - \overline{\theta} &= \frac{1}{n-1}\left(n\overline{X}_n - x_i\right) - \frac{1}{n}\sum_{i=1}^{n}\frac{1}{n-1}\sum_{j=1,j\neq i}^{n} x_j = \\
&\frac{1}{n-1}\left(n\overline{X}_n - x_i\right) - \frac{1}{n}\sum_{i=1}^{n}\frac{1}{n-1}\left(n\overline{X}_n - x_i\right) = \\
&\frac{1}{n-1}\left(n\overline{X}_n - x_i - \frac{1}{n}\sum_{i=1}^{n}\left(n\overline{X}_n - x_i\right)\right) = \frac{1}{n-1}\left(\overline{X}_n - x_i\right).
\end{aligned}$$

Jackknife

- By squaring, summing and applying the prefactor $(n-1)/n$ we obtain

$$\frac{n-1}{n}\sum_{i=1}^{n}(\theta_{(i)}-\overline{\theta})^2 = \frac{1}{n(n-1)}\sum_{i=1}^{n}(x_i-\overline{X}_n)^2,$$

  which is an unbiased estimator of the variance of the sample mean.

Jackknife

- The bias of a general statistic $s(\cdot)$ can be estimated based on Jackknife as

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- Consequently, the expected value of the average over the Jackknife replicas is

$$\mathbb{E}(\overline{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}(\theta_{(i)}) = \theta + \frac{b_1}{n-1}$$

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$$\mathbb{E}(s(\cdot) - \overline{\theta}) = \theta + \frac{b_1}{n} - \theta - \frac{b_1}{n-1} = \frac{b_1}{n(n-1)}.$$

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- By multiplying with $(n-1)$ we obtain that the expected value of $\text{bias}_{\text{jack}}$ is equal to b_1/n, which is the bias of $s(\cdot)$.

Empirical PDF

Let us now return to the problem of the empirical PDF, where we would like to obtain an estimate for the loss function

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- In the spirit of Jackknife replicas, we can consider the following estimator:

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where $\widehat{\rho}_{(i)}(x = x_i)$ is the histogram estimator obtained by excluding data point i from the sample evaluated at $x = x_i$.

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- The expected value of the second term is

$$\mathbb{E}\left(\frac{2}{n}\sum_{i=1}^{n}\widehat{\rho}_{(i)}(x_i)\right) = \frac{2}{n}\sum_{i=1}^{n}\mathbb{E}\left(\widehat{\rho}_{(i)}(x_i)\right) \approx 2\int \widehat{\rho}_n(x)\rho(x)dx,$$

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  thus, we obtained a nearly unbiased estimator of the loss function,

$$\mathbb{E}(\widehat{J}(h)) \approx \mathbb{E}(J(h)).$$

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Calculation of $\widehat{J}(h)$:

Empirical PDF

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- At first sight, searching for the optimal h by minimising $\widehat{J}(h)$ seems painful, since at every examined value of h, we have to prepare n Jackknife replicas, calculate $\widehat{\rho}_{(i)}$ for every replica, and then evaluate the sum defining $J(h)$ as

$$\widehat{J}(h) = \int \widehat{\rho}_n^2(x)dx - \frac{2}{n}\sum_{i=1}^{n}\widehat{\rho}_{(i)}(x = x_i) = \sum_{j=1}^{m}\widehat{\rho}_n^2(x_j)h - \frac{2}{n}\sum_{i=1}^{n}\widehat{\rho}_{(i)}(x = x_i),$$

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→ Let us first express the first term in $\widehat{J}(h)$ based on $\widehat{p}_j$:

$$\sum_{j=1}^{m}\widehat{\rho}_n^2(x_j)h = \sum_{j=1}^{m}\frac{\widehat{p}_j^2}{h^2}h = \sum_{j=1}^{m}\frac{\widehat{p}_j^2}{h}.$$

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- However, according to the above $\widehat{\rho}_{(i)}(x)$ is taken at $x = x_i$, corresponding to the actual bin where x_i is missing from. Thus,

$$\widehat{\rho}_{(i)}(x = x_i) = \frac{1}{h}\frac{\nu_j - 1}{n-1} = \frac{1}{h}\frac{n\widehat{p}_j - 1}{n-1},$$

where we denoted the bin of x_i as j, and expressed the number of elements in the original data in this bin as $\nu_j = n\widehat{p}_j$.

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- We can also regroup the summation over the individual data points i to summation over the bins j, taking into account that the number of data point falling into bin j is again $\nu_j = n\widehat{p}_j$:

$$-\frac{2}{n}\sum_{i=1}^{n}\widehat{\rho}_{(i)}(x = x_i) = -\frac{2}{n}\sum_{j=1}^{m}\frac{1}{h}\frac{n\widehat{p}_j - 1}{n-1}n\widehat{p}_j = -\frac{2}{hn}\sum_{j=1}^{m}\frac{n^2\widehat{p}_j^2}{n-1} + \frac{2}{hn}\sum_{j=1}^{m}\frac{n\widehat{p}_j}{n-1} =$$

$$-\frac{2n}{h(n-1)}\sum_{j=1}^{m}\widehat{p}_j^2 + \frac{2}{h(n-1)}\underbrace{\sum_{j=1}^{m}\widehat{p}_j}_{1}.$$

Empirical PDF

- Putting it all together we obtain

$$\widehat{J}(h) = \sum_{j=1}^{m} \frac{\widehat{p}_j^2}{h} - \frac{2n}{h(n-1)} \sum_{j=1}^{m} \widehat{p}_j^2 + \frac{2}{h(n-1)} =$$

$$\frac{1}{h} \underbrace{\left[1 - \frac{2n}{n-1}\right]}_{\frac{-n-1}{n-1}} \sum_{j=1}^{m} \widehat{p}_j^2 + \frac{2}{h(n-1)} =$$

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→ Thus, we do not have to actually generate/evaluate anything related to the individual Jackknife replicas, we can calculate $\widehat{J}(h)$ for a given h straight away based on simply the original $\widehat{p}_j$ values.

Empirical PDF

Optimal histogram based estimator

- For a given h bin width the empirical PDF is constructed the usual way,

$$\widehat{\rho}_n(x) = \sum_{j=1}^{m} \frac{\widehat{p}_j}{h} I(x \in B_j) = \sum_{j=1}^{m} \frac{\nu_j}{nh} I(x \in B_j).$$

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- The risk (up to an additive constant independent of h) can be estimated by

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- By changing the value of h from low to high we locate the optimal h, minimising the above function.
- Luckily, the cross-validation terms do not have to be evaluated individually, since $\widehat{J}(h)$ can equally be formulated as

$$\widehat{J}(h) = \frac{2}{h(n-1)} - \frac{n+1}{h(n-1)}\sum_{j=1}^{m}\widehat{p}_j^2 = \frac{2}{h(n-1)} - \frac{n+1}{h(n-1)n^2}\sum_{j=1}^{m}\nu_j^2$$

Kernel density estimation

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Kernel density estimation

- The basic idea of kernel density estimation is to "smudge" the data points, and obtain the estimation of the PDF based on the sum of these.
- A bit more precisely: we represent each data point by a unimodal decaying function (gven by the kernel) who's peak is centred on the data point, and the estimate of the PDF at a given x is the sum over these functions.

Kernel density estimation

Kernel density estimation

- Let the kernel $K(x)$ be a smooth function with the following properties:
  - $K(x) \geq 0$,
  - $\int K(x)dx = 1$,
  - $\int xK(x)dx = 0$, and $\int x^2K(x)dx > 0$.

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  (In other words, $K(x)$ can be viewed as the PDF of some probability distribution with 0 mean and a larger than 0 variance).
- Based on $K(x)$, the kernel density estimator of the PDF at a fixed bandwith h is given by

$$\widehat{\rho}_n(x) = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{h}K\left(\frac{x - x_i}{h}\right).$$

Kernel density estimation

Most widely used kernels:

- Gaussian kernel:

$$K(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}.$$

- Epanechnikov kernel:

$$K(x) = \begin{cases} \frac{3}{4\sqrt{5}}\left(1 - \frac{x^2}{5}\right) & \text{if } |x| < \sqrt{5}, \\ 0 & \text{if } |x| \geq \sqrt{5}. \end{cases}$$

Kernel density estimation

Risk for kernel density estimation

- Under weak assumptions on $\rho(x)$ and $K(x)$, the MISE can be given as

$$R(\widehat{\rho}_n, \rho) \approx \frac{\sigma_K^4 h^4}{4} \int \left[\rho''(x)\right]^2 dx + \frac{1}{nh} \int K^2(x) dx,$$

  where $\sigma_K^2 = \int x^2 K(x) dx$.

- The optimal bandwidth is

$$h^* = \frac{c_1^{-2/5} c_2^{1/5} c_3^{-1/5}}{n^{1/5}},$$

  where $c_1 = \int x^2 K(x) dx$, $c_2 = \int K^2(x) dx$ and $c_3 = \int \left[\rho''(x)\right]^2 dx$.

- With this choice of the bandwidth,

$$R(\widehat{\rho}_n, \rho) \approx \frac{c_4}{n^{4/5}},$$

  where c_4 is some further constant.

Kernel density estimation

- According to the above, the empirical PDF based on kernel density estimation is converging faster with n compared to the histogram estimator.
- However, similarly to the histogram estimator, the previous formulation is not usefuly in practise, because it needs the knowledge of the true PDF ρ.

→ Luckily, the cross validation approach works here as well.

→ The MISE (up to constant independent from the bin width h) can be estimated by

$$\widehat{J}(h) = \int \widehat{\rho}_n(x)dx - \frac{2}{n}\sum_{i=1}^{n}\widehat{\rho}_{(i)}(x = x_i),$$

where $\widehat{\rho}_{(i)}$ is the kernel density estimator obtained after removing x_i from the data set.

Kernel density estimation

- Finally, $\widehat{J}(h)$ based on cross validation can be evaluated at a given h simply as

$$\widehat{J}(h) \approx= \frac{1}{hn^2} \sum_{i=1}^{n} \sum_{j=1}^{n} K^* \left(\frac{x_i - x_j}{h} \right) + \frac{2}{nh} K(0),$$

  where $K^*(x) = \int K(x-y)K(y)dy - 2K(x)$.