

french

1 TD : rappels

Exercice 1 On considère le modèle de régression de dimension N

$$x_k = \theta_k + \epsilon_k, \quad k = 1, \dots, N,$$

où $\mathbf{x} = (x_k)_{k=1, \dots, N}$ est l'observation dans \mathbb{R}^N , $\boldsymbol{\theta} = (\theta_k)_{k=1, \dots, N}$ le paramètre de \mathbb{R}^N et les ϵ_k sont des variables i.i.d. centrées de variance connue σ^2 .

1. On cherche un estimateur de $\boldsymbol{\theta}$ de la forme $\tilde{\boldsymbol{\theta}}(\lambda) = \lambda \mathbf{x}$ avec $\lambda \in [0, 1]$. Calculer son biais $\mathbb{E}[\tilde{\boldsymbol{\theta}}(\lambda)] - \boldsymbol{\theta}$ et sa variance sommée $\sum_{k=1}^N \text{Var}(\tilde{\theta}_k(\lambda))$. Quel est l'effet de λ sur le biais et la variance ?
2. Calculer $\lambda^* \in [0, 1]$ qui minimise le risque d'oracle de cet estimateur :

$$R(\lambda) = \mathbb{E} \left[\sum_{k=1}^N (\theta_k - \lambda x_k)^2 \right].$$

3. Proposer un estimateur sans biais de θ_k^2 à partir de x_k et σ^2 .
4. En déduire un estimateur sans biais $\mathcal{C}(\lambda)$ de $R(\lambda) - \sum_{k=1}^N \theta_k^2$.
5. Quel est l'estimateur $\hat{\boldsymbol{\theta}} = \lambda(\mathbf{x}) \mathbf{x}$, avec $\lambda : \mathbb{R}^N \rightarrow [0, 1]$, obtenu par minimisation du critère \mathcal{C} sur $[0, 1]$?

Exercice 2 Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be an unknown function. Suppose we observe noisy values of f :

$$Y_i = f(X_i) + \epsilon_i,$$

where $(X, \epsilon), (X_i, \epsilon_i)_{i=1, \dots, n} \subset \mathbb{R} \times \mathbb{R}$ is an i.i.d. collection of random variables such that $\epsilon \perp X$, $\mathbb{E}[\epsilon] = 0$, $\mathbb{E}[\epsilon^2] = \sigma^2$ and $\mathbb{E}[f(X)^2] < \infty$. To estimate the function f , we shall use a sequence of functions $(h_k)_{k \geq 1}$ where each $h_k : \mathbb{R} \rightarrow \mathbb{R}$ and $G = \mathbb{E}[h(X)h(X)^T]$ is invertible. . The procedure is as follows. We choose K , we set $h(x) = (h_1(x), \dots, h_K(x))^T$ and then compute

$$\theta_{K,n} \in \underset{\theta \in \mathbb{R}^K}{\operatorname{argmin}} \sum_{i=1}^n (Y_i - h(X_i)^T \theta)^2.$$

The estimate of f is given by $f_{K,n}(x) = h(x)^T \theta_{K,n}$. Define the risk $R(\theta) = \mathbb{E}[(f(X) - h(X)^T \theta)^2]$. The aim is to study the $R(\theta_{n,K})$.

1. Let $\theta_K^* \in \underset{\theta \in \mathbb{R}^K}{\operatorname{argmin}} R(\theta)$. Give the normal equations satisfied by θ_K^* and deduce an expression for θ_K^* .
2. Give the expression for $\theta_{K,n}$.
3. Show that the estimated function $f_{K,n}$ is invariant by any linear invertible transform on the set of functions h , i.e. h is replaced by Ah where $A \in \mathbb{R}^{K \times K}$ is invertible. In the following we shall assume that $G = I_K$.
4. Show that for any $\theta \in \mathbb{R}^K$, $R(\theta) = R(\theta_K^*) + \|\theta - \theta_K^*\|^2$ where the norm $\|\cdot\|$ should be specified.

5. From now on, we suppose that the smallest eigenvalue of $n^{-1} \sum_{i=1}^n h(X_i)h(X_i)^T$ is lower bounded by $\lambda > 0$. Show that $\|\theta_{K,n} - \theta_K^*\| \leq \lambda^{-1/2} \|n^{-1} \sum_{i=1}^n \xi_i h(X_i)\|$ where $\xi_i \neq \epsilon_i$ should be specified.
6. Show that $n^{-1} \sum_{i=1}^n \xi_i h(X_i) \rightarrow 0$ almost surely (hint : use the Cauchy-Schwarz inequality).
7. Suppose that $f \in \text{span}((h_k)_{k \geq 1})$. Conclude that choosing K large enough, $\limsup_n R(\theta_{K,n})$ can be made arbitrarily small.

2 TD : histogramme

Exercice 3 On souhaite estimer “globalement” une densité de probabilité inconnue sur un intervalle donné, disons $[0, 1]$ pour simplifier, à partir de l’observation de la réalisation d’un n -échantillon (X_1, \dots, X_n) . Cela signifie que les variables aléatoires réelles X_1, X_2, \dots, X_n sont indépendantes et identiquement distribuées. Dans toute la suite, on notera $x \mapsto f(x)$ leur densité de probabilité commune définie sur $[0, 1]$. Le but est d’estimer les valeurs $(f(x), x \in [0, 1])$ simultanément.

Soit $m \geq 1$ un entier. On définit les boîtes B_1, B_2, \dots, B_m en posant :

$$B_1 = [0, \frac{1}{m}), \quad B_2 = [\frac{1}{m}, \frac{2}{m}), \dots, \quad B_m = [\frac{(m-1)}{m}, 1] .$$

On appelle *largeur de bande* associée aux boîtes B_j le nombre $h = 1/m$. Pour $j = 1, \dots, m$, on définit

$$\hat{p}_j = \frac{1}{n} \# \{X_i \in B_j, i = 1, \dots, n\} = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{B_j}(X_i) .$$

1. Montrer que \hat{p}_j est un estimateur sans biais de $p_j = \int_{B_j} f(u) du$. Quelle est sa variance ?

L’estimateur par histogramme de la densité est alors défini par la formule

$$\hat{f}_n(x) = \sum_{j=1}^m \frac{\hat{p}_j}{h} \mathbb{1}_{B_j}(x) \quad \text{pour } x \in [0, 1] .$$

2. Soit j l’indice de la boîte contenant x . Montrer que

$$\mathbb{E}[\hat{f}_n(x)] = \frac{p_j}{h} \quad \text{et} \quad \text{Var} [\hat{f}_n(x)] = \frac{p_j(1-p_j)}{nh^2} .$$

3. Supposons que f est continue en x . Que dire du biais de $\hat{f}_n(x)$ pour estimer $f(x)$ quand h tend vers 0 ?

On définit l’*erreur quadratique moyenne intégrée* de l’estimateur \hat{f}_n de f en posant

$$\mathcal{R}(\hat{f}_n, f) = \mathbb{E} \left[\int_0^1 (\hat{f}_n(u) - f(u))^2 du \right] .$$

On suppose désormais que f est 2 fois continûment dérivable sur $[0, 1]$.

On note $b(x) = \mathbb{E}[\hat{f}_n(x)] - f(x)$ le biais de l’estimateur $\hat{f}_n(x)$ et $v(x) = \text{Var} [\hat{f}_n(x)]$ sa variance.

4. Montrer que

$$b(x) = f'(x)(h(j - \frac{1}{2}) - x) + O(h^2) ,$$

où $x \in B_j$.

5. Montrer que

$$\int_0^1 b(x)^2 dx = \frac{h^2}{12} \int_0^1 (f'(x))^2 dx + o(h^2) .$$

On pourra utiliser que $f'(x) = f'(x_j) + O(h)$ pour $x \in B_j$, où x_j désigne le centre de la boîte B_j .

6. Comment varie le biais en fonction de h ?
 7. En reproduisant les arguments précédents, montrer que

$$v(x) = \frac{f(x) + O(h)}{nh} ,$$

puis que

$$\int_0^1 v(x) dx = \frac{1}{nh} + O(1/n) .$$

8. Comment varie la variance en fonction de h ?
 9. Dédurre des questions précédentes que

$$\mathcal{R}(\widehat{f}_n, f) = \frac{h^2}{12} \int_0^1 f'(u)^2 du + \frac{1}{nh} + o(h^2) + o(1/(nh)) . \quad (1)$$

10. On note $\widehat{f}_n = \widehat{f}_{n,h}$ pour mettre en évidence la dépendance en h de l'estimateur. Montrer que

$$\lim_{n \rightarrow \infty} n^{2/3} \inf_h \mathcal{R}^0(\widehat{f}_{n,h}, f) = (3/4)^{2/3} \left(\int_0^1 f'(u)^2 du \right)^{1/3} ,$$

où \mathcal{R}^0 est l'approximation du risque obtenue en négligeant les termes en $o(\dots)$ dans (1).

Nous avons vu que la taille de fenêtre optimale $h_n^* = h_n^*(f)$ dépend de f , qui est inconnu. On s'intéresse maintenant au problème du choix automatique de la fenêtre pour l'estimation de la densité par histogramme. Nous allons donc chercher un choix de h dicté par l'observation X_1, \dots, X_n uniquement, et dont l'erreur imite le mieux possible l'erreur idéale fournie par le choix de h_n^* . Nous considérons la méthode de **validation croisée** de type *leave one out*. Nous écrivons désormais $\widehat{f}_n(x) = \widehat{f}_{n,h}(x)$ et définissons

$$L_n(h) = \int_0^1 (\widehat{f}_{n,h}(u) - f(u))^2 du = \int_0^1 (\widehat{f}_{n,h}(u))^2 du - 2 \int_0^1 \widehat{f}_{n,h}(u) f(u) du + \int_0^1 f(u)^2 du .$$

Définition 1

L'estimateur du risque par validation croisée est

$$\widehat{J}_n(h) = \int_0^1 (\widehat{f}_{n,h}(u))^2 du - \frac{2}{n} \sum_{i=1}^n \widehat{f}_{n,h,i}(X_i) ,$$

où $\widehat{f}_{n,h,i}(x)$ est l'estimateur de f au point x obtenu en ignorant la donnée X_i .

Exercice 4 1. Montrer que minimiser $\mathcal{R}(\widehat{f}_{n,h}, f)$ est équivalent à minimiser l'espérance de

$$J_n(h) = \int_0^1 (\widehat{f}_{n,h}(u))^2 du - 2 \int_0^1 \widehat{f}_{n,h}(u) f(u) du .$$

2. Comparer $\mathbb{E}[\widehat{J}_n(h)]$ et $\mathbb{E}[J_n(h)]$.

En principe, pour minimiser $h \mapsto \widehat{J}_n(h)$, on doit reconstruire n histogrammes pour chaque valeur de h . Heureusement, on dispose du raccourci suivant.

3. Montrer que :

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

Solution de l'exercice 1

1. For all $1 \leq k \leq N$, $\mathbb{E}[x_k] = \mathbb{E}[\theta_k + \epsilon_k] = \theta_k$ so $\mathbb{E}[\mathbf{x}] = \boldsymbol{\theta}$ and the bias is equal to

$$\text{Bias}(\lambda) = \mathbb{E}[\tilde{\boldsymbol{\theta}}(\lambda)] - \boldsymbol{\theta} = \lambda \mathbb{E}[\mathbf{x}] - \boldsymbol{\theta} = (\lambda - 1)\boldsymbol{\theta}.$$

For the variance, we have $\text{Var}(\tilde{\theta}_k(\lambda)) = \lambda^2 \text{Var}(x_k) = \lambda^2 \sigma^2$ and $\sum_{k=1}^N \text{Var}(\tilde{\theta}_k(\lambda)) = N\lambda^2 \sigma^2$. We recover the well-known bias/variance trade-off

- $\text{Bias}(\lambda) \xrightarrow{\lambda \rightarrow 1} 0$, $\text{Var}(\lambda) \xrightarrow{\lambda \rightarrow 1} N\sigma^2$.
- $\text{Bias}(\lambda) \xrightarrow{\lambda \rightarrow 0} -\boldsymbol{\theta}$, $\text{Var}(\lambda) \xrightarrow{\lambda \rightarrow 0} 0$.

2. Define $\mathcal{L}(\lambda) = \sum_{k=1}^N (\theta_k - \lambda x_k)^2$ and $R(\lambda) = \mathbb{E}[\mathcal{L}(\lambda)]$. For all $1 \leq k \leq N$,

$$\begin{aligned} (\theta_k - \lambda x_k) &= \theta_k - \lambda(\theta_k + \epsilon_k) = (1 - \lambda)\theta_k - \lambda\epsilon_k, \\ (\theta_k - \lambda x_k)^2 &= (1 - \lambda)^2 \theta_k^2 - 2\lambda(1 - \lambda)\theta_k \epsilon_k + \lambda^2 \epsilon_k^2. \end{aligned}$$

Taking the expectation leads to

$$\begin{aligned} \mathbb{E}[(\theta_k - \lambda x_k)^2] &= (1 - \lambda)^2 \theta_k^2 + \lambda^2 \sigma^2 \\ \mathbb{E}[(\theta_k - \lambda x_k)^2] &= \lambda^2 (\theta_k^2 + \sigma^2) - 2\lambda \theta_k^2 + \theta_k^2, \end{aligned}$$

and by sum we finally get a 2nd ordre polynomial in λ ,

$$R(\lambda) = \left(\sum_{k=1}^N (\theta_k^2 + \sigma^2) \right) \lambda^2 - \left(2 \sum_{k=1}^N \theta_k^2 \right) \lambda + \left(\sum_{k=1}^N \theta_k^2 \right).$$

The minimizer λ^* is given by

$$\lambda^* = \frac{\sum_{k=1}^N \theta_k^2}{\sum_{k=1}^N (\theta_k^2 + \sigma^2)}.$$

3. For all $1 \leq k \leq N$, $x_k^2 = \theta_k^2 + 2\theta_k \epsilon_k + \epsilon_k^2$ so $\mathbb{E}[x_k^2 - \sigma^2] = \theta_k^2$, and by sum

$$\mathbb{E} \left[\sum_{k=1}^N (x_k^2 - \sigma^2) \right] = \sum_{k=1}^N \theta_k^2.$$

4. Define $S_N = \sum_{k=1}^N \theta_k^2$, we want an estimate $\mathcal{C}(\lambda)$ such that $\mathbb{E}[\mathcal{C}(\lambda)] = R(\lambda) - S_N$. By the previous question, we have an estimate of S_N so that

$$\begin{aligned} \mathcal{C}(\lambda) &= \mathcal{L}(\lambda) - \sum_{k=1}^N (x_k^2 - \sigma^2) = \sum_{k=1}^N (\theta_k - \lambda x_k)^2 - \sum_{k=1}^N (x_k^2 - \sigma^2) \\ \mathcal{C}(\lambda) &= \left(\sum_{k=1}^N x_k^2 \right) \lambda^2 - \left(2 \sum_{k=1}^N \theta_k x_k \right) \lambda + \left(\sum_{k=1}^N \theta_k^2 - x_k^2 + \sigma^2 \right). \end{aligned}$$

5. Minimizing $\mathcal{C}(\lambda)$ w.r.t. λ yields an estimate $\hat{\boldsymbol{\theta}} = \lambda(\mathbf{x}) \mathbf{x}$, with $\lambda : \mathbb{R}^N \rightarrow [0, 1]$,

$$\lambda(x_1, \dots, x_N) = \frac{\left(\sum_{k=1}^N \theta_k x_k \right)_+}{\sum_{k=1}^N x_k^2}.$$

Solution de l'exercice 2

1. $\theta_K^* \in \operatorname{argmin}_{\theta \in \mathbb{R}^K} R(\theta)$ satisfies $\nabla R(\theta_K^*) = 0$ with $\nabla R(\theta) = -2\mathbb{E}[h(X)(f(X) - h(X)^T\theta)]$. Therefore we have the normal equation

$$\underbrace{\mathbb{E}[h(X)h(X)^T]}_{G=I_K} \theta_K^* = \mathbb{E}[h(X)f(X)].$$

We can recover this expression using Hilbert projection theorem since $\operatorname{Span}((h_k)_{k \geq 1})$ is a closed linear subspace of L^2 . Define $\hat{f}(X) = h(X)^T \theta_K^*$, it is unique and characterized by $f - \hat{f} \perp \operatorname{Span}((h_k)_{k \geq 1})$, i.e.,

$$\begin{aligned} \mathbb{E}[(f(X) - \hat{f}(X))h(X)] &= 0 \\ \mathbb{E}[(f(X) - h(X)^T \theta_K^*)h(X)] &= 0. \end{aligned}$$

2. Consider the empirical risk $R_n(\theta) = \sum_{i=1}^n (Y_i - h(X_i)^T \theta)^2$ along with its minimizer $\theta_{K,n} \in \operatorname{argmin}_{\theta \in \mathbb{R}^K} R_n(\theta)$ which is a stationnary point : $\nabla R_n(\theta_{K,n}) = 0$.

$$\begin{aligned} \nabla R_n(\theta_{K,n}) &= -2 \sum_{i=1}^n h(X_i)(Y_i - h(X_i)^T \theta_{K,n}) = 0, \\ \left(\sum_{i=1}^n h(X_i)h(X_i)^T \right) \theta_{K,n} &= \left(\sum_{i=1}^n h(X_i)Y_i \right) = \left(\sum_{i=1}^n h(X_i)f(X_i) \right) + \left(\sum_{i=1}^n h(X_i)\epsilon_i \right). \end{aligned}$$

Define $\hat{G}_n = n^{-1} \left(\sum_{i=1}^n h(X_i)h(X_i)^T \right)$ the empirical Gram matrix, we have

$$\begin{aligned} \hat{G}_n \theta_{K,n} &= \frac{1}{n} \sum_{i=1}^n h(X_i)Y_i \\ &= \frac{1}{n} \sum_{i=1}^n h(X_i)(Y_i - h(X_i)^T \theta_K^*) + \frac{1}{n} \sum_{i=1}^n h(X_i)h(X_i)^T \theta_K^* \\ \hat{G}_n \theta_{K,n} &= \frac{1}{n} \sum_{i=1}^n h(X_i)(Y_i - h(X_i)^T \theta_K^*) + \hat{G}_n \theta_K^* \\ \hat{G}_n (\theta_{K,n} - \theta_K^*) &= \frac{1}{n} \sum_{i=1}^n h(X_i)(Y_i - h(X_i)^T \theta_K^*). \end{aligned}$$

3. Any linear invertible transform $A \in \mathbb{R}^{K \times K}$ on the set of functions changes \hat{G}_n into $\hat{G}_n A^{-1}$ and these two matrices both share the same column space. Indeed, consider $\tilde{h} = Ah$ so that $h = A^{-1}\tilde{h}$, we have

$$A^{-1} \left(\sum_{i=1}^n \tilde{h}(X_i)\tilde{h}(X_i)^T \right) (A^{-T} \theta_{K,n}) = A^{-1} \left(\sum_{i=1}^n \tilde{h}(X_i)Y_i \right),$$

meaning that $\tilde{\theta}_{K,n} = A^{-T} \theta_{K,n}$ and the invariance of the estimate

$$\tilde{f}_{K,n}(x) = \tilde{h}(x)^T \tilde{\theta}_{K,n} = h(x)^T A^T A^{-T} \theta_{K,n} = h(x)^T \theta_{K,n} = f_{K,n}(x).$$

4. For any $\theta \in \mathbb{R}^K$,

$$\begin{aligned}
R(\theta) &= \mathbb{E} [(f(X) - h(X)^T \theta)^2] \\
&= \mathbb{E} [(f(X) - h(X)^T \theta_K^* + h(X)^T (\theta_K^* - \theta))^2] \\
&= \mathbb{E} [(f(X) - h(X)^T \theta_K^*)^2 - 2(f(X) - h(X)^T \theta_K^*)h(X)^T (\theta_K^* - \theta) + (h(X)^T (\theta_K^* - \theta))^2] \\
&= \mathbb{E} [(f(X) - h(X)^T \theta_K^*)^2] - 2 \underbrace{\mathbb{E} [(f(X) - \hat{f}(X))h(X)^T]}_{=0} (\theta_K^* - \theta) + \mathbb{E} [(h(X)^T (\theta_K^* - \theta))^2] \\
R(\theta) &= R(\theta_K^*) + (\theta_K^* - \theta)^T \mathbb{E} [h(X)h(X)^T] (\theta_K^* - \theta) \\
R(\theta) &= R(\theta_K^*) + (\theta_K^* - \theta)^T G (\theta_K^* - \theta).
\end{aligned}$$

In the general case, we have the norm associated to the matrix G and in the particular case $G = I$ we have the euclidian norm,

$$R(\theta) = R(\theta_K^*) + \|\theta_K^* - \theta\|_2^2.$$

5. Define $\xi_i = Y_i - h(X_i)^T \theta_K^*$ and use the expression of question 2,

$$\hat{G}_n (\theta_{K,n} - \theta_K^*) = \frac{1}{n} \sum_{i=1}^n h(X_i) \xi_i.$$

Therefore

$$\|\theta_{K,n} - \theta_K^*\|^2 = \|\hat{G}_n^{-1} \left(\frac{1}{n} \sum_{i=1}^n h(X_i) \xi_i \right)\|^2.$$

Recall that for any matrix $A \in \mathbb{R}^{p \times p}$ and $u \in \mathbb{R}^p$, $\|Au\|^2 \leq \lambda_{\max}(A) \|u\|^2$. By assumption, we have $\lambda_{\min}(\hat{G}_n) \geq \lambda$ so the maximum eigenvalue of the inverse is such that $\lambda_{\max}(\hat{G}_n^{-1}) = 1/\lambda_{\min}(\hat{G}_n) \leq 1/\lambda$ and we get the following bound

$$\|\theta_{K,n} - \theta_K^*\| \leq \frac{1}{\sqrt{\lambda}} \left\| \frac{1}{n} \sum_{i=1}^n h(X_i) \xi_i \right\|.$$

6. We apply the strong law of large numbers to the random variables $h(X_i) \xi_i$. Notice that for all $k \in K$, $h_k \in L^2$ and since $\mathbb{E}[f(X)^2] < \infty$ and $\mathbb{E}[\epsilon_i^2] = \sigma^2 < \infty$, we have $Y_i \in L^2$ and $\xi_i \in L^2$. Using Cauchy-Schwarz inequality, we have

$$\mathbb{E} [|h_k(X_i) \xi_i|^2] \leq \mathbb{E} [|h_k(X_i)|^2] \mathbb{E} [|\xi_i|^2] < \infty.$$

Besides the expectation is given by

$$\begin{aligned}
\mathbb{E} [h(X_i) \xi_i] &= \mathbb{E} [h(X_i) (Y_i - h(X_i)^T \theta_K^*)] \\
&= \mathbb{E} [h(X_i) (f(X_i) + \epsilon_i - h(X_i)^T \theta_K^*)] \\
&= \mathbb{E} [h(X_i) (f(X_i) - h(X_i)^T \theta_K^*)] + \mathbb{E} [h(X_i) \epsilon_i] \\
\mathbb{E} [h(X_i) \xi_i] &= 0,
\end{aligned}$$

where we used the normal equation to treat the first term and the fact that the noise ϵ is centered for the second term.

7. Thanks to questions 4 and 5, we have

$$\begin{aligned} R(\theta_{K,n}) &= R(\theta_K^*) + \|\theta_{K,n} - \theta_K^*\| \\ &\leq R(\theta_K^*) + \frac{1}{\sqrt{\lambda}} \left\| \frac{1}{n} \sum_{i=1}^n h(X_i) \xi_i \right\|. \end{aligned}$$

Assume that $f \in \text{span}((h_k)_{k \geq 1})$ and set $\varepsilon > 0$. We can choose K large enough to have

$$\left\| f - \sum_{k=1}^K \alpha_k h_k \right\|_{L^2} \leq \varepsilon,$$

and the risk is such that $R(\theta_K^*) \leq \varepsilon$. Using the law of large numbers, the second term goes to 0 so we can take the limit sup and write

$$\limsup_{n \rightarrow \infty} R(\theta_{K,n}) \leq \varepsilon.$$

Solution de l'exercice 3

1. By linearity of the expectation, we have

$$\mathbb{E}[\hat{p}_j] = \frac{1}{n} \sum_{i=1}^n \mathbb{E}[\mathbb{1}_{B_j}(X_i)].$$

Using the fact that the sequence (X_1, \dots, X_n) is independently and identically distributed, we have

$$\mathbb{E}[\hat{p}_j] = \mathbb{E}[\mathbb{1}_{B_j}(X_1)] = \int_{B_j} f(u) du.$$

Because for any random variable Z and any constant a , $\text{Var}[Z-a] = \text{Var}[Z]$, the variance is given by

$$\begin{aligned} \text{Var}[\hat{p}_j] &= \text{var}[\hat{p}_j - p_j] \\ &= n^{-1} \text{var}(\mathbb{1}_{B_j}(X_1)) \\ &= n^{-1} p_j(1 - p_j). \end{aligned}$$

2. As x is lying in the box with index j , we have $\hat{f}(x) = \hat{p}_j/h$. Using again the linearity of the expectation, we get

$$\mathbb{E}[\hat{f}_n(x)] = h^{-1} \mathbb{E}[\hat{p}_j] = h^{-1} \int_{B_j} f(u) du.$$

The computation of the variance is as follows,

$$\text{Var}[\hat{f}_n(x)] = \text{Var}[\hat{p}_j/h] = (nh^2)^{-1} p_j(1 - p_j).$$

3. By definition, the bias is given by $b(x) = \mathbb{E}[\hat{f}_n(x)] - f(x)$. Because $\int_{B_j} du = h$, we have

$$b(x) = h^{-1} \int_{B_j} f(u) du - f(x) = h^{-1} \int_{B_j} (f(u) - f(x)) du. \quad (2)$$

It follows that

$$\begin{aligned}
|b(x)| &\leq h^{-1} \int_{B_j} |f(u) - f(x)| du \\
&\leq \sup_{u \in B_j} |f(u) - f(x)| h^{-1} \int_{B_j} du \\
&= \sup_{u \in B_j} |f(u) - f(x)| \\
&\leq \sup_{|u-x| < h} |f(u) - f(x)|.
\end{aligned}$$

The latter bound is independant on the block index j . Let $\epsilon > 0$. From the continuity of the function f , there exists $\tilde{h} > 0$ such that whenever $|u - x| < \tilde{h}$, it holds that $|f(u) - f(x)| < \epsilon$. As a consequence, for h sufficiently small ($h \leq \tilde{h}$), one has

$$|b(x)| \leq \epsilon.$$

Since ϵ is arbitrary, this means that $b(x) \rightarrow 0$ as $h \rightarrow 0$.

4. Using the identity $a^2 - b^2 = (a - b)(a + b)$, note that

$$\begin{aligned}
\int_{B_j} (u - x) du &= [(u - x)^2 / 2]_{(j-1)/m}^{j/m} \\
&= (1/m) \left(\frac{j - 1/2}{m} - x \right) \\
&= h \left(h(j - \frac{1}{2}) - x \right). \tag{3}
\end{aligned}$$

Denote by f' and f'' the first and second derivatives of f . Using the fact that f is 2 times continuously differentiable on $[0, 1]$, we have that (Taylor formula with integral remainder)

$$f(u) - f(x) - f'(x)(u - x) = \int_x^u f''(v)(u - v) dv.$$

It follows that, for every $(x, u) \in [0, 1]^2$,

$$|f(u) - f(x) - f'(x)(u - x)| \leq \frac{1}{2}(u - x)^2 \sup_{v \in [0, 1]} |f''(v)|.$$

As a consequence, using (2) and (3), we get

$$\begin{aligned}
b(x) - f'(x)(h(j - \frac{1}{2}) - x) &= h^{-1} \int_{B_j} (f(u) - f(x)) du - h^{-1} f'(x) \int_{B_j} (u - x) du \\
&= h^{-1} \int_{B_j} (f(u) - f(x)) - f'(x)(u - x) du.
\end{aligned}$$

It follows that

$$\begin{aligned}
|b(x) - f'(x)(h(j - \frac{1}{2}) - x)| &\leq \frac{1}{2} \sup_{v \in [0, 1]} |f''(v)| h^{-1} \int_{B_j} (u - x)^2 du \\
&\leq \frac{1}{2} \sup_{v \in [0, 1]} |f''(v)| h^{-1} h^2 \int_{B_j} du \\
&= \frac{1}{2} \sup_{v \in [0, 1]} |f''(v)| h^2.
\end{aligned}$$

5. First remark that

$$\int_{B_j} (h(j - \frac{1}{2}) - x)^2 dx = -\frac{1}{3} [(h(j - \frac{1}{2}) - x)^3]_{h(j-1)}^{hj} = \frac{h^3}{12} . \quad (4)$$

Using that f' is continuously differentiable on $[0, 1]$, we have that

$$\sup_{x \in B_j} |f'(x) - f'(x_j)| \leq h \sup_{x \in [0,1]} |f''(x)| ,$$

and that

$$\sup_{x \in B_j} |f'(x)^2 - f'(x_j)^2| \leq 2h \sup_{x \in [0,1]} |f'(x)| \sup_{x \in [0,1]} |f''(x)| .$$

Consequently, defining $\tilde{b}(x) = f'(x)^2 \sum_{j=1}^m (h(j - \frac{1}{2}) - x)^2 1_{\{x \in B_j\}}$,

$$\begin{aligned} \int \tilde{r}(x) dx &= \sum_{j=1}^m \int_{B_j} f'(x)^2 (h(j - \frac{1}{2}) - x)^2 dx \\ &= \sum_{j=1}^m f'(x_j)^2 \int_{B_j} (h(j - \frac{1}{2}) - x)^2 dx + r_1(h), \end{aligned}$$

where, using (4),

$$\begin{aligned} |r_1(h)| &= \left| \sum_{j=1}^m \int_{B_j} (f'(x)^2 - f'(x_j)^2) (h(j - \frac{1}{2}) - x)^2 dx \right| \\ &\leq 2h \sup_{x \in [0,1]} |f'(x)| \sup_{x \in [0,1]} |f''(x)| \sum_{j=1}^m \int_{B_j} (h(j - \frac{1}{2}) - x)^2 dx \\ &= O(h^3) . \end{aligned}$$

Finally, using (4) again,

$$\begin{aligned} \int f'(x)^2 (h(j - \frac{1}{2}) - x)^2 dx &= \frac{h^3}{12} \sum_{j=1}^m f'(x_j)^2 + r_1(h) \\ &= \frac{h^2}{12} \sum_{j=1}^m \int_{B_j} f'(x_j)^2 dx + r_1(h) \\ &= \frac{h^2}{12} \int_0^1 f'(x)^2 dx + r_1(h) + r_2(h) , \end{aligned}$$

with

$$r_2(h) = \frac{h^2}{12} \sum_{j=1}^m \int_{B_j} (f'(x_j)^2 - f'(x)^2) dx .$$

We conclude remarking that $|r_2(h)| \leq \frac{h^3}{6} \sup_{x \in [0,1]} |f'(x)| \sup_{x \in [0,1]} |f''(x)|$.

6. Let x be a point in the box B_j . From question 4., we have

$$|f'(x)(h(j - \frac{1}{2}) - x)| \leq |f'(x)| \sup_{x \in B_j} |h(j - \frac{1}{2}) - x| = |f'(x)|h/2 .$$

As a result, we have that $b(x) = O(h)$. For the previous question, we have also proved that the square integrated bias is of order h^2 .

7. For the first point, it is enough to show that there exists $C > 0$ such that for every $j \in \{1, \dots, m\}$,

$$\sup_{x \in B_j} |p_j(1 - p_j) - hf(x)| \leq C h^2 .$$

As we have, in virtue of the triangle inequality, that, for every $x \in B_j$,

$$|p_j(1 - p_j) - hf(x)| \leq |p_j(1 - p_j) - h^{-1} \int_{B_j} f(u) du| + | \int_{B_j} (f(u) - f(x)) du | ,$$

we can proceed in the two following steps. First,

$$|p_j(1 - p_j) - h^{-1} \int_{B_j} f(u) du| = p_j^2 \leq h^2 \sup_{x \in [0,1]} |f(x)|^2 .$$

Second,

$$| \int_{B_j} (f(u) - f(x)) du | \leq h^2 \sup_{x \in [0,1]} |f'(x)| .$$

8. For each $x \in [0, 1]$, the variance $v(x)$ goes to infinity as h goes to 0 and n remains fixed. We have shown in question 6. that the bias is going to 0 as h goes to 0. This two facts imply that we should define h as a sequence $h := h_n$ which satisfies

$$h_n \rightarrow 0 , \quad nh_n \rightarrow +\infty .$$

9. Start writing that

$$\mathcal{R}(\widehat{f}_n, f) = \mathbb{E} \left[\int_0^1 (\widehat{f}_n(u) - \mathbb{E}[\widehat{f}_n(u)])^2 du \right] + \int_0^1 b(u)^2 du .$$

Then use Tonelli's theorem to obtain that

$$\mathcal{R}(\widehat{f}_n, f) = \int_0^1 v(u) du + \int_0^1 b(u)^2 du .$$

Conclude by using question 7.

10. Neglecting the terms in the $o(\dots)$, we compute the infimum over h by minimizing the function $h \mapsto \frac{Ih^2}{12} + \frac{1}{nh}$. We find

$$h^{*3} = \frac{6}{I^2 n} \quad \text{with } I = \int_0^1 f'(u)^2 du .$$

Injecting the previous value gives that

$$\inf_h \mathcal{R}(\widehat{f}_{n,h}, f) = \frac{I^{1/3}}{n^{2/3}} \left(\frac{3}{4} \right)^{2/3} + o\left(\frac{1}{n^{2/3}} \right) .$$