

Project: Cross-validation for model selection (notes on papers)

Diego Urdapilleta de la Parra

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1 Introduction

The goal of this project is to study the asymptotic properties of cross-validation (CV) methods for model selection in a variety of scenarios. [...] *motivation, brief description of CV methods, outline of the project.*

Throughout the paper, we consider the usual regression setup: Let n, p_n be positive integers and $\mathcal{D}_n := \{(y_i, \mathbf{x}_i) : i \in [n]\}$ be a set of independent data points drawn from a distribution $\mathbb{P}_{y, \mathbf{x}}$ for $(y, \mathbf{x}) \in \mathbb{R} \times \mathcal{X}$. We treat the \mathbf{x}_i 's as predictors of the outcome y_i , and we assume a model

$$y_i = f(\mathbf{x}_i) + e_i, \quad i \in [n], \quad (1)$$

where f is an unknown Borel-measurable function $f : \mathcal{X} \rightarrow \mathbb{R}$ with $f(x_i) \stackrel{\text{a.s.}}{=} \mathbb{E}[y_i | \mathbf{x}_i]$ and the e_i 's are zero-mean random variables.

2 CV for Linear Model Selection

2.1 Setup and preliminary results

In this section, the regression function f in (1) is assumed to be linear, so that the data is generated from a linear model of the form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$$

where $\mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_n]^\top \in \mathbb{R}^{n \times p_n}$ is the design matrix, $\mathbf{y} = [y_1 \ y_2 \ \cdots \ y_n]^\top$, and \mathbf{e} is a mean-zero random vector with $\text{Cov}(\mathbf{e}) = \sigma^2 \mathbf{I}_n$.

In the context of linear models, the model selection procedure reduces to selecting a subset of covariates from a set of candidate covariates of size p_n . This is also known as *variable selection*. We remark that the number p_n may depend on n , and some assumptions on the growth of p_n will be established later.

We let $\mathcal{A}_n \subset 2^{[p_n]}$ be a family of index sets representing candidate models. For $\alpha \in \mathcal{A}_n$, we denote by $p_n(\alpha)$ the cardinality of α and consider the model given by

$$f_\alpha(\mathbf{X}) = \mathbf{X}_\alpha \boldsymbol{\beta}_\alpha,$$

where \mathbf{X}_α is the sub-matrix of \mathbf{X} containing only the columns indexed by α , and $\boldsymbol{\beta}_\alpha$ is the coefficient vector containing only the entries indexed by α in $\boldsymbol{\beta}$.

1. We say $\alpha \in \mathcal{A}_n$ is *correct* if $\mathbb{E}[\mathbf{y} | \mathbf{X}] \stackrel{\text{a.s.}}{=} f_\alpha(\mathbf{X})$, and we denote by \mathcal{T}_n the set of correct models in \mathcal{A}_n
2. We say $\alpha \in \mathcal{A}_n$ is *wrong* if it is not correct, and we denote by \mathcal{T}_n^c the set of wrong models in \mathcal{A}_n
3. We say \mathcal{A}_n is *embedded* if there exists an enumeration $\alpha_1, \alpha_2, \dots, \alpha_k$ of all elements in \mathcal{A}_n such that

$$\alpha_1 \subset \alpha_2 \subset \cdots \subset \alpha_k.$$

Definition 2.1. For $\alpha \in \mathcal{A}_n$, let $\hat{\beta}_\alpha$ be the OLS estimator of β_α and $\hat{f}_\alpha(\mathbf{X}) := \mathbf{X}_\alpha \hat{\beta}_\alpha$. We denote the average squared error of \hat{f}_α by

$$L_n(\alpha) := \frac{1}{n} \|f(\mathbf{X}) - \hat{f}_\alpha(\mathbf{X})\|^2.$$

Additionally, we write

$$R_n(\alpha) := \mathbb{E}[L_n(\alpha) \mid \mathbf{X}].$$

The following conditions will be used throughout out treatment of linear models:

- H1 :** $\liminf_{n \rightarrow \infty} \frac{1}{n} \|M_\alpha \mathbf{X} \beta\|^2 > 0$ for all $\alpha \in \mathcal{A}_n$.
- H2 :** $\mathbf{X}^\top \mathbf{X} = O(n)$ and $(\mathbf{X}^\top \mathbf{X})^{-1} = O(n^{-1})$.
- H3 :** $\lim_{n \rightarrow \infty} \max_{i \leq n} h_{ii, \alpha} = 0$ for all $\alpha \in \mathcal{A}_n$.
- H4 :** $\sum_{\alpha \in \mathcal{T}_n^c} \frac{1}{(n R_n(\alpha))^m} \rightarrow_{\mathbb{P}} 0$ for some $m \geq 1$.

Proposition 2.1. Assuming a linear model $\mathbf{y} = \mathbf{X} \beta + \mathbf{e}$,

$$L_n(\alpha) = \frac{1}{n} \|H_\alpha \mathbf{e}\|^2 + \frac{1}{n} \|M_\alpha \mathbf{X} \beta\|^2 \quad \text{and} \quad R_n(\alpha) = \frac{1}{n} \sigma^2 p_n(\alpha) + \frac{1}{n} \|M_\alpha \mathbf{X} \beta\|^2$$

almost surely, where $H_\alpha = \mathbf{X}_\alpha (\mathbf{X}_\alpha^\top \mathbf{X}_\alpha)^{-1} \mathbf{X}_\alpha^\top$ and $M_\alpha = I_n - H_\alpha$.

Proof. First, we have that

$$\begin{aligned} \|f(\mathbf{X}) - \hat{f}_\alpha(\mathbf{X})\|^2 &= \|\mathbf{X} \beta - \mathbf{X}_\alpha \hat{\beta}_\alpha\|^2 \\ &= \|\mathbf{X} \beta - H_\alpha (\mathbf{X} \beta + \mathbf{e})\|^2 \\ &= \|M_\alpha \mathbf{X} \beta - H_\alpha \mathbf{e}\|^2. \end{aligned}$$

Notice that $M_\alpha \mathbf{X} \beta$ and $H_\alpha \mathbf{e}$ are orthogonal:

$$\mathbf{e}^\top H_\alpha M_\alpha \mathbf{X} \beta = \mathbf{e}^\top H_\alpha (I_n - H_\alpha) \mathbf{X} \beta = \mathbf{e}^\top H_\alpha \mathbf{X} \beta - \mathbf{e}^\top H_\alpha \mathbf{X} \beta = 0.$$

Hence, the first part follows from the Pythagorean theorem.

For the second part, we note that $\mathbb{E}[\|H_\alpha \mathbf{e}\|^2 \mid \mathbf{X}] \stackrel{\text{a.s.}}{=} \sigma^2 p_n(\alpha)$ by the “trace trick”, where $p_n(\alpha)$ denotes the size of model α . \square

Proposition 2.2. Suppose that that \mathcal{T}_n is non-empty, and let α_n^* be the smallest correct model in \mathcal{T}_n . Then, α_n^* minimizes $R_n(\alpha)$ (with probability 1?) over $\alpha \in \mathcal{A}_n$.

Proof. Let $\alpha \in \mathcal{A}_n$ be arbitrary and suppose that $\alpha \in \mathcal{T}_n$. Then, $\mathbf{X}_\alpha \beta_\alpha = \mathbf{X} \beta$ and $p_n(\alpha_n^*) \leq p_n(\alpha)$. Thus,

$$\begin{aligned} R_n(\alpha) &= \frac{1}{n} \sigma^2 p_n(\alpha) + \frac{1}{n} \|M_\alpha \mathbf{X} \beta\|^2 \\ &= \frac{1}{n} \sigma^2 p_n(\alpha) + \frac{1}{n} \underbrace{\|M_\alpha \mathbf{X}_\alpha \beta_\alpha\|^2}_0 \\ &= \frac{1}{n} \sigma^2 p_n(\alpha) \geq \frac{1}{n} \sigma^2 p_n(\alpha_n^*) = R_n(\alpha_n^*). \end{aligned}$$

Now suppose that $\alpha \in \mathcal{T}_n^c$. If $p_n(\alpha) \geq p_n(\alpha_n^*)$, the result follows immediately by assumption H1. On the other hand, if $p_n(\alpha) \leq p_n(\alpha_n^*)$, we must verify that

$$\|M_\alpha \mathbf{X} \boldsymbol{\beta}\|^2 \geq \sigma^2 (p_n(\alpha_n^*) - p_n(\alpha)). \quad (2)$$

To this end, we note that $\|M_\alpha \mathbf{X} \boldsymbol{\beta}\|^2 = \|M_\alpha \mathbf{X}_{\alpha_n^*} \boldsymbol{\beta}_{\alpha_n^*}\|^2$ and that

$$\mathbf{X}_{\alpha_n^*} \boldsymbol{\beta}_{\alpha_n^*} = \mathbf{X}_\alpha \boldsymbol{\beta}_\alpha + \mathbf{X}_{\alpha_n^* \setminus \alpha} \boldsymbol{\beta}_{\alpha_n^* \setminus \alpha}.$$

Thus, if we let λ denote the smallest eigenvalue of $\mathbf{X}_{\alpha_n^*}^\top M_\alpha \mathbf{X}_{\alpha_n^*}$, we have that

$$\|M_\alpha \mathbf{X} \boldsymbol{\beta}\|^2 = \|M_\alpha \mathbf{X}_{\alpha_n^* \setminus \alpha} \boldsymbol{\beta}_{\alpha_n^* \setminus \alpha}\|^2 \geq \lambda \|\boldsymbol{\beta}_{\alpha_n^* \setminus \alpha}\|^2$$

(for a proof of the latter inequality, see [2]). This is as far as I got. I don't know how to show that $\lambda \|\boldsymbol{\beta}_{\alpha_n^* \setminus \alpha}\|^2 \geq \sigma^2 (p_n(\alpha_n^*) - p_n(\alpha))$, but it seems reasonable if the coefficients in $\boldsymbol{\beta}$ are not too small. \square

From Proposition 2.2, we see that R_n is a good choice of selection criterion. Unfortunately, R_n depends on the unknown regression function, and therefore cannot be used in practice. Instead, we may try to approximate it through other empirically feasible criteria.

Definition 2.2. Let $\hat{\alpha}_n$ be the model selected by minimizing some criterion \hat{R}_n over \mathcal{A}_n , and let α_n^* denote the model minimizing R_n over \mathcal{A}_n . We say \hat{R}_n is consistent if

$$\mathbb{P} \{ \hat{\alpha}_n = \alpha_n^* \} \rightarrow 1$$

as $n \rightarrow \infty$. We say that \hat{R}_n is asymptotically loss efficient if

$$\frac{L_n(\hat{\alpha}_n)}{L_n(\alpha_n^*)} \xrightarrow{\mathbb{P}} 1.$$

Lemma 2.3. If \hat{R}_n is consistent, then it is asymptotically loss efficient.

Proof. Suppose that \hat{R}_n is consistent. Clearly, if $\hat{\alpha}_n = \alpha_n^*$, then $L_n(\hat{\alpha}) = L_n(\alpha_n^*)$. Therefore,

$$\mathbb{P} \{ \hat{\alpha}_n = \alpha_n^* \} \leq \mathbb{P} \{ L_n(\hat{\alpha}) = L_n(\alpha_n^*) \}.$$

By consistency, the left-hand side converges to 1, so that the right-hand side must also converge to 1. \square

Proposition 2.4 (Shao, 1997 [3]). Suppose H1, $p_n/n \rightarrow 0$, and that \mathcal{T}_n is non-empty for all but finitely many n .

1. If $|\mathcal{T}_n| = 1$ for all but finitely many n , then consistency is equivalent to efficiency in the sense of Definition 2.2.
2. If $p_n(\alpha_n^*) \not\xrightarrow{\mathbb{P}} \infty$, then consistency is equivalent to efficiency in the sense of Definition 2.2.

Proof. From Lemma 2.3, it remains to show that, under the given conditions, asymptotic loss efficiency implies consistency. We show the contrapositive:

1. Suppose that \hat{R}_n is not consistent. By Proposition 2.2, α_n^* must be the correct model in \mathcal{T}_n minimizing R_n . Therefore, $L_n(\alpha_n^*) = (1/n)\|H_\alpha \mathbf{e}\|^2$, and

$$\mathbb{E}[L_n(\alpha_n^*)] = \frac{1}{n}\sigma^2 p_n(\alpha_n^*) \leq \frac{1}{n}\sigma^2 p_n \rightarrow 0 \quad \text{as } n \rightarrow \infty$$

by assumption. We have shown that $L_n(\alpha_n^*) \xrightarrow{L_1} 0$, which implies $L_n(\alpha_n^*) \xrightarrow{\mathbb{P}} 0$.

On the other hand, since \hat{R}_n is not consistent, there must exist $\tilde{\alpha}_n \neq \alpha^*$ for infinitely many n such that $\mathbb{P}\{\hat{\alpha}_n = \tilde{\alpha}_n\} \neq 0$. Notice that, since $\mathcal{T}_n = \{\alpha^*\}$, it must be the case that $\tilde{\alpha}_n \in \mathcal{T}_n^c$. We have the following:

$$L_n(\hat{\alpha}_n) \geq \mathbb{1}_{[\hat{\alpha}_n = \tilde{\alpha}_n]} L_n(\tilde{\alpha}_n) = \mathbb{1}_{[\hat{\alpha}_n = \tilde{\alpha}_n]} \left(\frac{1}{n} \|H_{\tilde{\alpha}_n} \mathbf{e}\|^2 + \frac{1}{n} \|M_\alpha \mathbf{X} \beta\|^2 \right).$$

By assumption **H1**, the latter expression cannot not converge to 0. We conclude that the ratio $L_n(\hat{\alpha}_n)/L_n(\alpha_n^*) \not\xrightarrow{\mathbb{P}} 1$.

2. Suppose again that \hat{R}_n is not consistent. Since \mathcal{T}_n contains at least two models, there must exist $\tilde{\alpha}_n \in \mathcal{T}_n$ such that $\tilde{\alpha}_n \neq \alpha^*$ and $\mathbb{P}\{\hat{\alpha}_n = \tilde{\alpha}_n\} \not\xrightarrow{\mathbb{P}} 0$. Hence,

$$\frac{L_n(\hat{\alpha}_n)}{L_n(\alpha_n^*)} - 1 \geq \left(\frac{L_n(\tilde{\alpha}_n)}{L_n(\alpha_n^*)} - 1 \right) \mathbb{1}_{[\hat{\alpha}_n = \tilde{\alpha}_n]} = \left(\frac{\|H_{\tilde{\alpha}_n}\|^2}{\|H_{\alpha_n^*}\|^2} - 1 \right) \mathbb{1}_{[\hat{\alpha}_n = \tilde{\alpha}_n]} \not\xrightarrow{\mathbb{P}} 0.$$

□

2.2 A Result on the Leave-one-out: Shao, 1993

[Brief introduction to LOOCV and motivation]

For this section, we will consider the case where the set $\mathcal{A}_n =: \mathcal{A}$ and all its elements are constant across all $n \geq 1$. That is, the candidate models are not changed by the number of observations.

Definition 2.3. *The Leave-one-out estimator of $R_n(\alpha)$ is defined as*

$$\hat{R}_n^{(1)}(\alpha) := \frac{1}{n} \sum_{i=1}^n \left(\frac{y_i - \mathbf{x}_{i\alpha}^\top \hat{\beta}_\alpha}{1 - h_{ii,\alpha}} \right)^2$$

Lemma 2.5 (Shao, 1993 [4]).

$$\hat{R}_n^{(1)}(\alpha) = \begin{cases} R_n(\alpha) + \sigma^2 + o_{\mathbb{P}}(1) & \text{if } \alpha \in \mathcal{T}^c \\ \frac{1}{n} \|M_\alpha \mathbf{e}\|^2 + \frac{2}{n} \sigma^2 p(\alpha) + o_{\mathbb{P}}(n^{-1}) & \text{if } \alpha \in \mathcal{T} \end{cases} \quad (3)$$

Proof. Using the Taylor expansion of $1/(1-x)^2 = 1 + 2x + O(x^2)$, we have

$$\frac{1}{(1 - h_{ii,\alpha})^2} = 1 + 2h_{ii,\alpha} + O_{\mathbb{P}}(h_{ii,\alpha}^2).$$

Thus,

$$\hat{R}_n^{(1)}(\alpha) = \underbrace{\frac{1}{n} \sum_{i=1}^n \left(y_i - \mathbf{x}_{i\alpha}^\top \hat{\boldsymbol{\beta}}_\alpha \right)^2}_{\xi_{\alpha,n}} + \underbrace{\frac{1}{n} \sum_{i=1}^n \left(2h_{ii,\alpha} + O_{\mathbb{P}}(h_{ii,\alpha}^2) \right) \left(y_i - \mathbf{x}_{i\alpha}^\top \hat{\boldsymbol{\beta}}_\alpha \right)^2}_{\zeta_{\alpha,n}} \quad (4)$$

Let $\xi_{\alpha,n}$ and $\zeta_{\alpha,n}$ denote the first and second terms in (4), respectively. Note that

$$\begin{aligned} \xi_{\alpha,n} &= \frac{1}{n} \|M_\alpha \mathbf{X} \boldsymbol{\beta} + M_\alpha \mathbf{e}\|^2 \\ &= \frac{1}{n} \left(\|M_\alpha \mathbf{e}\|^2 + \|M_\alpha \mathbf{X} \boldsymbol{\beta}\|^2 + 2\mathbf{e}^\top M_\alpha \mathbf{X} \boldsymbol{\beta} \right) \end{aligned} \quad (5)$$

$$= \frac{1}{n} \|\mathbf{e}\|^2 + \frac{1}{n} \|M_\alpha \mathbf{X} \boldsymbol{\beta}\|^2 + \frac{1}{n} \|H_\alpha \mathbf{e}\|^2 + \frac{2}{n} \mathbf{e}^\top M_\alpha \mathbf{X} \boldsymbol{\beta} \quad (6)$$

From here, we emphasize four intermediate steps:

- i. Using Markov's inequality, for $\varepsilon > 0$,

$$\begin{aligned} \mathbb{P} \left\{ \|H_\alpha \mathbf{e}\|^2 \geq n\varepsilon \right\} &\leq \frac{\sigma^2 p_n(\alpha)}{n\varepsilon} \rightarrow 0 \\ \implies \frac{1}{n} \|H_\alpha \mathbf{e}\|^2 &= o_{\mathbb{P}}(1). \end{aligned}$$

- ii. Since M_α is a projection matrix, $\|M_\alpha \mathbf{X} \boldsymbol{\beta}\|^2 \leq \|\mathbf{X} \boldsymbol{\beta}\|^2 = O_{\mathbb{P}}(n)$, so that

$$\mathbb{E} \left[\left(\mathbf{e}^\top M_\alpha \mathbf{X} \boldsymbol{\beta} \right)^2 \mid \mathbf{X} \right] = \frac{4}{n^2} \sigma^2 \|M_\alpha \mathbf{X} \boldsymbol{\beta}\|^2 = o_{\mathbb{P}}(1).$$

Combining the latter with $\mathbb{E} [\mathbf{e}^\top M_\alpha \mathbf{X} \boldsymbol{\beta} \mid \mathbf{X}] = 0$, we obtain that

$$\frac{2}{n} \mathbf{e}^\top M_\alpha \mathbf{X} \boldsymbol{\beta} = o_{\mathbb{P}}(1).$$

- iii. Combining i. and ii. with (6) yields

$$\xi_{\alpha,n} = \frac{1}{n} \|\mathbf{e}\|^2 + \frac{1}{n} \|M_\alpha \mathbf{X} \boldsymbol{\beta}\|^2 + o_{\mathbb{P}}(1).$$

Furthermore, since $\|\mathbf{e}\|^2 = O_{\mathbb{P}}(n)$, we have that $\xi_{\alpha,n} = O_{\mathbb{P}}(1)$.

- iv. Finally, since $0 < h_{ii,\alpha} < 1$, $2h_{ii,\alpha} + O_{\mathbb{P}}(h_{ii,\alpha}^2) \leq O_{\mathbb{P}}(\max_i h_{ii,\alpha})$. Thus,

$$\zeta_{\alpha,n} \leq O_{\mathbb{P}} \left(\max_i h_{ii,\alpha} \right) \left(\frac{1}{n} \sum_{i=1}^n \left(y_i - \mathbf{x}_{i\alpha}^\top \hat{\boldsymbol{\beta}}_\alpha \right)^2 \right) = O_{\mathbb{P}} \left(\max_i h_{ii,\alpha} \right) \xi_{\alpha,n}.$$

From assumption **H3**, $\zeta_{\alpha,n} = o_{\mathbb{P}}(1) \xi_{\alpha,n} = o_{\mathbb{P}}(1)$.

It follows that

$$\hat{R}_n^{(1)}(\alpha) = \frac{1}{n}\|e\|^2 + \frac{1}{n}\|M_\alpha \mathbf{X}\boldsymbol{\beta}\|^2 + o_{\mathbb{P}}(1) \stackrel{(\text{LLN})}{=} \sigma^2 + \frac{1}{n}\|M_\alpha \mathbf{X}\boldsymbol{\beta}\|^2 + o_{\mathbb{P}}(1).$$

Noting that $R_n(\alpha) = \frac{1}{n}\|M_\alpha \mathbf{X}\boldsymbol{\beta}\|^2 + o_{\mathbb{P}}(1)$ yields the first case in (3).

If $\alpha \in \mathcal{T}$, it is easy to see from (5) that $\xi_{\alpha,n} = 1/n\|M_\alpha e\|^2$, Furthermore,

$$\zeta_{\alpha,n} = \frac{2}{n}\sigma^2 p(\alpha) + o_{\mathbb{P}}(1), \quad (?)$$

proving the second case. □

Proposition 2.6 (Shao, 1993 [4]). *Suppose that \mathcal{T} is non-empty and let $\hat{\alpha}^{(1)}$ be the model minimizing $\hat{R}_n^{(1)}(\alpha)$.*

1. Under H1, H2, and H3,

$$\lim_{n \rightarrow \infty} \mathbb{P}\{\hat{\alpha}^{(1)} \in \mathcal{T}^c\} = 0.$$

2. For $\alpha \in \mathcal{T}$ with $\alpha \neq \alpha^*$,

$$\mathbb{P}\left\{\hat{R}_n^{(1)}(\alpha) \leq \hat{R}_n^{(1)}(\alpha^*)\right\} = \mathbb{P}\left\{2(p(\alpha) - p(\alpha^*))\sigma^2 < \mathbf{e}^\top (H_\alpha - H_{\alpha^*})\mathbf{e}\right\} + o_{\mathbb{P}}(1).$$

In particular, if $\mathbf{e} \sim \mathcal{N}(0_n, \sigma^2 I_n)$,

$$\mathbb{P}\left\{\hat{R}_n^{(1)}(\alpha) \leq \hat{R}_n^{(1)}(\alpha^*)\right\} = \mathbb{P}\{2k < \chi^2(k)\} + o_{\mathbb{P}}(1) > 0$$

for $k = p(\alpha) - p(\alpha^*)$.

3. If $p(\alpha^*) < p$,

$$\lim_{n \rightarrow \infty} \mathbb{P}\{\hat{\alpha}^{(1)} = \alpha^*\} \neq 1.$$

Proof.

1. Let $\bar{\alpha} \in \mathcal{T}$ and $\tilde{\alpha} \in \mathcal{T}^c$. By, Lemma 2.5, we have that

$$\begin{aligned} \mathbb{P}\left\{\hat{R}_n^{(1)}(\tilde{\alpha}) \leq \hat{R}_n^{(1)}(\bar{\alpha})\right\} &= \mathbb{P}\left\{\frac{1}{n}\sigma^2 p(\tilde{\alpha}) + \frac{1}{n}\|M_{\tilde{\alpha}} \mathbf{X}\boldsymbol{\beta}\|^2 + \sigma^2 + o_{\mathbb{P}}(1)\right. \\ &\quad \left.\leq \frac{1}{n}\|M_{\bar{\alpha}} \mathbf{e}\|^2 + \frac{1}{n}\sigma^2 p(\bar{\alpha}) + o_{\mathbb{P}}(n^{-1})\right\} \\ &= \mathbb{P}\left\{\frac{1}{n}\sigma^2 (p(\tilde{\alpha}) - p(\bar{\alpha})) + \sigma^2 + \frac{1}{n}\|M_{\tilde{\alpha}} \mathbf{X}\boldsymbol{\beta}\|^2 - \frac{1}{n}\|M_{\bar{\alpha}} \mathbf{e}\|^2 \leq o_{\mathbb{P}}(1)\right\} \end{aligned}$$

From **H1**, the latter probability goes to zero as $n \rightarrow \infty$. Therefore, $\mathbb{1}_{[\hat{R}_n^{(1)}(\tilde{\alpha}) \leq \hat{R}_n^{(1)}(\bar{\alpha})]} = o_{\mathbb{P}}(1)$.

We now observe that

$$\mathbb{P}\{\hat{\alpha}^{(1)} \in \mathcal{T}^c\} = \mathbb{E}\left[\mathbb{1}_{[\hat{\alpha}^{(1)} \in \mathcal{T}^c]}\right] = \mathbb{E}\left[\sum_{\tilde{\alpha} \in \mathcal{T}^c} \prod_{\alpha \in \mathcal{A}} \mathbb{1}_{[\hat{R}_n^{(1)}(\tilde{\alpha}) \leq \hat{R}_n^{(1)}(\alpha)]}\right] \rightarrow 0.$$

2. The first part follows from Lemma 2.1 by algebraic manipulation. The second part follows by noting that, if $\mathbf{e} \sim \mathcal{N}(0_n, \sigma^2 I_n)$, then

$$\frac{\mathbf{e}^\top}{\sigma} (H_\alpha - H_{\alpha^*}) \frac{\mathbf{e}}{\sigma} \sim \chi^2(\text{tr}(H_\alpha - H_{\alpha^*})).$$

3. It is easy to see that $p(\alpha^*) = p$ if and only if $\mathcal{T} = \{\alpha^*\}$. Thus, if $p(\alpha^*) < p$, there exists $\alpha \in \mathcal{T}^c$ with $\alpha \neq \alpha^*$. The result then follows by part 2 above. \square

Corollary 2.7. *Leave-one-out cross-validation is not consistent for selection. In particular, it overfits with non-vanishing probability.*

2.3 A General Perspective: Shao, 1997

[Brief intro to section]

For this section, we allow the number of candidates in \mathcal{A}_n , as well as the candidates $\alpha \in \mathcal{A}_n$ themselves, to vary with n (though we assume that both remain finite). To illustrate why this might be useful, we consider two examples from [3]:

If we wish to approximate a univariate regression function $x \mapsto f(x)$ by a polynomial of degree at most $p_n < n$, we may consider the models indexed by $\mathcal{A}_n := \{\alpha_d : d \in [p_n]\}$, with $\alpha_d = \{1, \dots, d\}$ and $f_{\alpha_d}(x) = \beta_0 + \beta_1 x + \dots + \beta_d x^d$. Clearly, the number of candidate models increases as more observations become available.

The *Generalized Information Criterion* (GIC), defined below, is a generalization of multiple empirical criteria for model selection. Various cross-validation methods can be seen as special cases of the GIC.

Definition 2.4. *We define the GIC loss estimator to be*

$$\hat{R}_{n,\lambda_n}(\alpha) := \frac{\|\mathbf{y} - \hat{m}(\mathbf{X})\|^2}{n} + \frac{1}{n} \lambda_n \hat{\sigma}_n^2 p_n(\alpha) \quad \text{for } \alpha \in \mathcal{A}_n,$$

where $\hat{\sigma}_n^2$ is an estimator of σ^2 and λ_n is a sequence of positive real numbers satisfying $\lambda_n \geq 2$ and $\lambda_n/n \rightarrow 0$.

2.3.1 The case of $\lambda_n \equiv 2$

Proposition 2.8 (Shao, 1997 [3]). *Suppose that $\lambda_n = 2$ for all $n \geq 1$ and that $\hat{\sigma}_n^2$ is a consistent estimator of σ^2 . Then,*

$$\hat{R}_{n,2}(\alpha) = \begin{cases} \frac{1}{n} \|\mathbf{e}\|^2 + \frac{2}{n} \hat{\sigma}_n^2 p_n(\alpha) - \frac{1}{n} \|H_\alpha \mathbf{e}\|^2 & \text{if } \alpha \in \mathcal{T}_n \\ \frac{1}{n} \|\mathbf{e}\|^2 + L_n(\alpha) + o_{\mathbb{P}}(L_n(\alpha)) & \text{if } \alpha \in \mathcal{T}_n^c \end{cases}$$

Theorem 2.9 (Shao, 1997 [3]). *Suppose that $H4$ holds and that $\hat{\sigma}_n^2$ is consistent for σ^2 .*

1. *If $|\mathcal{T}_n| \leq 1$ for all but finitely many n , then $\hat{\alpha}_n^2$ asymptotically loss efficient.*

2. Suppose that $|\mathcal{T}_n| > 1$ for all but finitely many n . If there exists a positive integer m such that $\mathbb{E} [y_1 - \mathbf{x}_1^\top \boldsymbol{\beta}]^{4m} < \infty$ and

$$\sum_{\alpha \in \mathcal{T}_n} \frac{1}{(p_n(\alpha))^m} \rightarrow 0 \quad \text{or} \quad \sum_{\substack{\alpha \in \mathcal{T}_n, \\ \alpha \neq \alpha^*}} \frac{1}{(p_n(\alpha) - p_n(\alpha^*))^m}, \quad (7)$$

then $\hat{\alpha}_n^2$ is asymptotically loss efficient.

3. Suppose that $|\mathcal{T}_n| > 1$ for all but finitely many n . Suppose, furthermore, that for some constant $c > 2$,

$$\liminf_{n \rightarrow \infty} \inf_{Q_n \in \mathcal{Q}_{n,q}} \mathbb{P} \{ \|Q_n \mathbf{e}\|^2 > c\sigma^2 q \} > 0, \quad (8)$$

where $\mathcal{Q}_{n,q}$ is the set of all projection matrices of rank q . Then, if $|\mathcal{T}_n|$ is bounded or \mathcal{A}_n is embedded, the condition that

$$p_n(\alpha^*) \rightarrow \infty \quad \text{or} \quad \min_{\substack{\alpha \in \mathcal{T}_n, \\ \alpha \neq \alpha^*}} (p_n(\alpha) - p_n(\alpha^*)) \rightarrow \infty \quad (9)$$

is necessary and sufficient for the asymptotic loss efficiency of $\hat{\alpha}_n^2$.

Proof. The proof for 1. is given in the last paragraph of page 226. I don't understand it. \square

Note that condition (8) is satisfied if $\mathbf{e} \sim \mathcal{N}(0_n, \sigma^2 I_n)$. Condition (9) is satisfied if \mathcal{A}_n does not contain two correct models with fixed dimension for all but finitely many n .

Corollary 2.10 (Shao, 1997). *If \mathcal{T}_n contains exactly one model with fixed dimension for all but finitely many n , then $\hat{\alpha}_n^2$ is consistent.*

Proof. This follows immediately from Theorem 2.9 and Proposition 2.8. \square

2.3.2 The case of $\lambda_n \rightarrow \infty$

The proofs are missing here.

We now consider the case of the GIC $\hat{R}_{n,n}(\lambda_n)$ with $\lambda \rightarrow \infty$ as $n \rightarrow \infty$. Unlike in the previous case, the following results do not require that $\hat{\sigma}_n^2$ be consistent for σ^2 .

Proposition 2.11 (Shao, 1997 [3]). *Suppose that $\lambda_n = 2$ for all $n \geq 1$ and that $\hat{\sigma}_n^2$ is a consistent estimator of σ^2 . Then,*

$$\hat{R}_{n,2}(\alpha) = \begin{cases} \frac{1}{n} \|\mathbf{e}\|^2 + \frac{2}{n} \hat{\sigma}_n^2 p_n(\alpha) - \frac{1}{n} \|H_\alpha \mathbf{e}\|^2 & \text{if } \alpha \in \mathcal{T}_n \\ \frac{1}{n} \|\mathbf{e}\|^2 + L_n(\alpha) + \frac{1}{n} p_n(\lambda_n \hat{\sigma}_n^2 - 2\sigma^2) + o_{\mathbb{P}}(L_n(\alpha)) & \text{if } \alpha \in \mathcal{T}_n^c \end{cases}$$

Theorem 2.12 (Shao, 1997 [3]). *Suppose that **H4** holds and that*

$$\limsup_{n \rightarrow \infty} \sum_{\alpha \in \mathcal{T}_n} \frac{1}{p_n(\alpha)^m} \quad (10)$$

for some m with $\mathbb{E}[e_i^{4m}] < \infty$.

1. If **H1**, $\lambda_n \rightarrow \infty$, and $\lambda_n p_n/n \rightarrow 0$ are satisfied, then $\hat{R}_{n,n}(\lambda_n)$ is asymptotically loss efficient.
2. If there exists $\alpha_0 \in \mathcal{T}_n$ with $p_n(\alpha_0)$ constant for all but finitely many n , $\lambda_n \rightarrow \infty$, and $\lambda_n/n \rightarrow 0$, then $\hat{R}_{n,n}(\lambda_n)$ is consistent.

Remark: Condition (10) is satisfied whenever $|\mathcal{T}_n|$ is bounded or \mathcal{A}_n is embedded. It implies that

$$\max_{\alpha \in \mathcal{T}_n} \frac{\|H_\alpha \mathbf{e}\|^2}{\lambda_n \hat{\sigma}_n^2 p_n(\alpha)} \xrightarrow{\mathbb{P}} 0.$$

2.3.3 Cross-validation

Theorem 2.13 (Shao, 1997 [3]). 1. If **H3** holds, then Theorem 2.9 applies for the leave-one-out estimator.

2. Suppose that **H1**, **H4**, and (10) hold. If the splits are “balanced”, and d is chosen so that $d/n \rightarrow 1$ and $p_n/(n-d) \rightarrow 0$, then the delete- d cross-validation estimator is asymptotically loss efficient

MISSING: Discussion.

3 CV for Nonparametric Model Selection

3.1 Comparison of Distinct Procedures: Yang, 2007

Here we consider two regression procedures, denoted δ_1 and δ_2 , that yield estimators $\hat{f}_{n,1}$ and $\hat{f}_{n,2}$ of the regression function satisfying

$$y_i = f(\mathbf{x}_i) + \epsilon_i \quad i \in [n], \tag{11}$$

for \mathbf{x}_i iid, $\mathbb{E}[\epsilon_i | \mathbf{X}] \stackrel{\text{a.s.}}{=} 0$ and $\mathbb{E}[\epsilon_i^2 | \mathbf{X}] \stackrel{\text{a.s.}}{<} \infty$.

Definition 3.1. We say δ_1 is asymptotically better than δ_2 under the loss function L if, for $0 < \varepsilon < 1$, there exists $c_\varepsilon > 0$ such that

$$\mathbb{P} \left\{ L_n(\hat{f}_{n,2}) \geq (1 + c_\varepsilon) L_n(\hat{f}_{n,1}) \right\} \geq 1 - \varepsilon.$$

Given that δ_1 is asymptotically better than δ_2 , we say that a selection procedure is consistent if it selects δ_1 with probability tending to 1 as $n \rightarrow \infty$.

3.1.1 Single-split cross-validation (the Hold-out)

For this section, we assume that the first n_1 elements in \mathcal{D}_n are used as a training/estimation sample and the remaining n_2 elements make up the validation sample. We write p_n and q_n for the rates of convergence of the estimators $\hat{f}_{n,1}$ and $\hat{f}_{n,2}$, respectively. That is,

$$O_{\mathbb{P}}(p_n) = \|f - \hat{f}_{n,1}\|_2 \quad \text{and} \quad O_{\mathbb{P}}(q_n) = \|f - \hat{f}_{n,2}\|_2.$$

The hold-out cross-validation method consists in selecting the estimator that minimizes the hold-out loss

$$L_{\text{ho}}(\hat{f}_{n,j}) = \sum_{i=n_1+1}^n \left(y_i - \hat{f}_{n,j}(\mathbf{x}_i) \right)^2 \quad \text{for } j = 1, 2.$$

The propositions in this section rely on the following conditions:

- **A3.1:** $\mathbb{E}[\epsilon_i^2 \mid \mathbf{x}_i]$ is bounded a.s. for $i \in [n]$.
- **A3.2:** There exists A_n such that $\|f - \hat{f}_{n,j}\|_\infty = O_{\mathbb{P}}(A_n)$ for $j = 1, 2$.
- **A3.3:** One procedure is asymptotically better than the other.
- **A3.4:** There exists M_n such that $\|f - \hat{f}_{n,j}\|_4 / \|f - \hat{f}_{n,j}\|_4 = o_{\mathbb{P}}(M_n)$ for $j = 1, 2$.

Theorem 3.1 (Yang, 2007 [6]). *Suppose that **A3.1–A3.4** hold. Suppose, furthermore, that*

1. $n_1 \rightarrow \infty$
2. $n_2 \rightarrow \infty$
3. $n_2 M_n^{-4} \rightarrow \infty$
4. $\sqrt{n_2} \max(p_{n_1}, q_{n_1})$

Then, the hold-out CV procedure is consistent.

A very detailed proof of this result is provided in Yang [6], so it will be skipped here.

3.1.2 Voting cross-validation with multiple splits

The (theoretical) majority-vote cross-validation method proceeds as follows: for each permutation $i \mapsto \pi(i)$ of the data, we compute the estimators $\hat{f}_{n_1,1}$ and $\hat{f}_{n_1,2}$ using the first n_1 data points $(y_{\pi(1)}, \mathbf{x}_{\pi(1)}), \dots, (y_{\pi(n_1)}, \mathbf{x}_{\pi(n_1)})$ as the training sample and the remaining $n_2 = n - n_1$ elements as the validation sample. We then find the estimator that minimizes the hold-out loss

$$L_\pi(\hat{f}_{n_1,j}) = \sum_{i=n_1+1}^n \left(y_{\pi(i)} - \hat{f}_{n_1,j}(\mathbf{x}_{\pi(i)}) \right)^2 \quad \text{for } j = 1, 2.$$

The chosen estimator is the one favored by the majority of the permutations. More formally, we define

$$\tau_\pi = \mathbb{1}_{[L_\pi(\hat{f}_{n_1,1}) \leq L_\pi(\hat{f}_{n_1,2})]}$$

We then define our selection criterion as follows:

$$\hat{f}_n = \begin{cases} \hat{f}_{n,1} & \text{if } \sum_{\pi \in \Pi} \tau_\pi \geq n!/2, \\ \hat{f}_{n,2} & \text{otherwise,} \end{cases}$$

where Π denotes the set of all permutations of $[n]$.

Theorem 3.2 (Yang, 2007 [6]). *Under the conditions of Theorem 4.1 and the condition that the data is iid, the majority-vote cross-validation method is consistent.*

Proof. Suppose that δ_1 is asymptotically better than δ_2 . For $\pi \in \Pi$, we have that

$$\mathbb{P} \left\{ L_\pi \left(\hat{f}_{n1,1} \right) \leq L_\pi \left(\hat{f}_{n1,2} \right) \right\} = \mathbb{E} [\tau_\pi] \stackrel{(*)}{=} \mathbb{E} \left[\frac{1}{n!} \sum_{\pi \in \Pi} \tau_\pi \right].$$

The equality at $(*)$ follows from the fact that the data are iid, hence exchangeable, and thus the τ_π are identically distributed. By Theorem 3.1, the right-hand side converges to 1 as $n \rightarrow \infty$. Since the average $1/n! \sum_{\pi} \tau_\pi$ is almost surely at most 1, it follows that $1/n! \sum_{\pi} \tau_\pi \rightarrow 1$ in probability, and the majority-vote cross-validation method is consistent. \square

The proof of Theorem 3.2 does not require using the entire set Π of permutations for the majority vote. In fact, Theorem 3.1 establishes that even a single data split suffices for consistency, provided the splitting conditions are met. Moreover, Yang [6] presents a counterexample demonstrating that these conditions are not merely sufficient but necessary, hence showing that the number of splits does not affect consistency. In other words, multiple splits in cross-validation cannot rescue an inconsistent single-split procedure. A natural question, then, is: if multiple splits do not improve consistency, what is their benefit? This will be explored in a simulation later on.

4 Aggregation

4.1 Bunea et al., 2007

As before, we consider independent pairs in $\mathcal{D}_n := \{(y_i, \mathbf{x}_i) : i \in [n]\}$ satisfying (11). Suppose that we have M candidate estimators of the regression function, denoted $\hat{f}_{n,1}, \hat{f}_{n,2}, \dots, \hat{f}_{n,M}$. Instead of selecting a single estimator, we combine them into an *aggregate* \tilde{f}_λ given by

$$\tilde{f}_\lambda = \sum_{j=1}^M \hat{\lambda}_j \hat{f}_{n,j},$$

with $\hat{\lambda} := (\hat{\lambda}_1, \dots, \hat{\lambda}_M) \in \Lambda \subset \mathbb{R}^M$ chosen to satisfy

$$\hat{\lambda} = \arg \min_{\lambda \in \Lambda} \left\{ \frac{1}{n} \|y - f_\lambda(\mathbf{x})\|^2 - \text{pen}(\lambda) \right\} \quad (12)$$

for some penalty $\text{pen}(\lambda)$ on the coefficients.

4.1.1 Four types of aggregation

There are four aggregation schemes considered in Bunea et al. [1], each of which is characterized by a different set Λ of admissible weights $\hat{\lambda}$:

- Model Selection Aggregation (MS): A single estimator is selected. That is,

$$\Lambda_{\text{MS}} = \{\lambda \in \mathbb{R}^M : \lambda = \mathbf{e}_j \text{ for some } j \in [M]\}.$$

- Linear Aggregation (L): $\tilde{f}_{\hat{\lambda}}$ is chosen among all linear combinations of the estimators. That is,

$$\Lambda_{\text{L}} = \mathbb{R}^M.$$

- Convex Aggregation (C): $\tilde{f}_{\hat{\lambda}}$ is chosen among all convex combinations of the estimators. That is,

$$\Lambda_{\text{C}} = \left\{ \lambda \in \mathbb{R}^M : \lambda \geq 0, \sum_{j=1}^M \lambda_j = 1 \right\}.$$

- Subset Selection (S): We select and aggregate at most D estimators from the pool, for a given $D \leq M$. That is,

$$\Lambda_{\text{S}} = \{\lambda \in \mathbb{R}^M : \lambda \text{ has at most } D \text{ non-zero entries}\}.$$

4.1.2 Evaluating the aggregate

In an ideal scenario, we would like to select weights λ^* satisfying

$$\lambda^* = \arg \min_{\lambda \in \Lambda} \mathbb{E} \left[d(f, \tilde{f}_{\lambda}) \right]$$

for some distance function d (e.g., the L_2 norm). However, since the true regression function f is unknown, this approach is clearly not feasible. Another way of constructing an estimator is to minimize its maximum risk on a class of functions Θ containing f . That is, we would like to find $\hat{\lambda}$ satisfying

$$\sup_{f \in \Theta} \mathbb{E} \|f - \tilde{f}_{\hat{\lambda}}\|_2^2 = \inf_{\lambda \in \Lambda} \sup_{f \in \Theta} \mathbb{E} \|f - \tilde{f}_{\lambda}\|_2^2.$$

This is known as *minimax* estimation. However, once again, there is no obvious way to compute the expectation $\mathbb{E} \|f - \tilde{f}_{\hat{\lambda}}\|_2^2$ for an arbitrary $f \in \Theta$.

For these reasons, we instead adopt the least-squares approach in (12). But how can we know if this approach is any good? We need a tool to evaluate the performance of our aggregate against *any* possible of regression function f . Oracles provide us with such a tool.

Definition 4.1 (adapted from Tsybakov, 2009 [5]). *Suppose that there exists $\lambda^* \in \Lambda$ such that*

$$\mathbb{E} \|f - \tilde{f}_{\lambda^*}\|_2^2 = \inf_{\lambda \in \Lambda} \mathbb{E} \|f - \tilde{f}_{\lambda}\|_2^2.$$

The function $f \mapsto \tilde{f}_{\lambda^}$ is called the oracle of aggregation under L_2 .*

We say that the aggregate $\tilde{f}_{\hat{\lambda}}$ mimics the oracle if

$$\mathbb{E} \|f - \tilde{f}_{\hat{\lambda}}\|_2 \leq \inf_{\lambda \in \Lambda} \mathbb{E} \|f - \tilde{f}_{\lambda}\|_2 + \Delta_{n,M}. \quad (13)$$

for the smallest possible $\Delta_{n,M} > 0$ independent of f .

In what follows, the goal is to find lower bounds on $\Delta_{n,M}$ for each of the aggregation schemes.

Definition 4.2 (Tsybakov, 2009 [5]). *For a class of functions Θ , a sequence $\{\psi_n\}_{n \geq 1}$ of positive numbers is called an optimal rate of convergence of estimators \hat{f} on Θ under L_2 if there exist constants $c, C > 0$ such that*

$$\limsup_{n \rightarrow \infty} \left(\psi_n^{-2} \inf_{\hat{f}} \sup_{f \in \Theta} \mathbb{E} \left[\|f - \hat{f}\|_2^2 \right] \right) \leq C \quad (14)$$

$$\text{and} \quad \liminf_{n \rightarrow \infty} \left(\psi_n^{-2} \inf_{\hat{f}} \sup_{f \in \Theta} \mathbb{E} \left[\|f - \hat{f}\|_2^2 \right] \right) \geq c \quad (15)$$

An estimator \hat{f}_n is said to be rate-optimal if

$$\sup_{f \in \Theta} \mathbb{E} \left[\|f - \hat{f}_n\|_2^2 \right] \leq C' \psi_n^2$$

for some $C' > 0$. It is called asymptotically efficient of Θ under L_2 if

$$\lim_{n \rightarrow \infty} \frac{\sup_{f \in \Theta} \mathbb{E} \|f - \hat{f}_n\|_2^2}{\inf_{\hat{f}} \sup_{f \in \Theta} \mathbb{E} \|f - \hat{f}\|_2^2} = 1.$$

We adapt Theorem 5.1 in [1] to consider exclusively the L_2 norm:

Theorem 4.1 (Bunea et al., 2007 [1]). *(Statement of lower bounds)*

$$\sup_{f_1, \dots, f_2 \in \mathcal{F}_0} \inf_{T_n} \sup_{f \in \mathcal{F}_0} \left\{ \mathbb{E} \|f - T_n\|_2^2 - \min_{\lambda \in \Lambda} \|f - \tilde{f}_\lambda\|_2^2 \right\} \geq c \psi_n$$

INCOMPLETE SECTION

4.1.3 A BIC-type penalty

Definition 4.3. Let $M(\lambda) := \|\lambda\|_0$ (i.e., the number of non-zero coefficients in λ). For $a > 0$, we define the Bunea-Tsybakov-Wegkamp *(I don't know what to call it)* penalty to be

$$\text{pen}_{\text{BIC}}(\lambda) := \frac{2\sigma^2}{n} M(\lambda) \left(1 + \frac{2+a}{1+a} \sqrt{2 \log \left(\frac{eM}{M(\lambda) \vee 1} \right)} + \frac{1+a}{a} \left[2 \log \left(\frac{eM}{M(\lambda) \vee 1} \right) \right] \right).$$

This penalty yields the BIC-type least-squares aggregate $\tilde{f}_{\hat{\lambda}_{\text{BIC}}} =: \tilde{f}_{\text{BIC}}$ with

$$\hat{\lambda}_{\text{BIC}} = \arg \min_{\lambda \in \mathbb{R}^M} \left\{ \frac{1}{n} \|\mathbf{y} - f_\lambda(\mathbf{x})\|^2 - \text{pen}_{\text{BIC}}(\lambda) \right\}$$

Theorem 4.2 (Bunea et al., 2007 [1]). Assume that the e_i are iid $\mathcal{N}(0, \sigma^2)$ and that the functions $f, \hat{f}_{n,1}, \dots, \hat{f}_{n,M}$ are uniformly bounded. Then, for all $a > 0$, $M \geq 2$, and $n \geq 1$,

$$\mathbb{E} \|\tilde{f}_{\text{BIC}} - f\|^2 \leq (1+a) \inf_{\lambda \in \mathbb{R}^M} \left\{ \|\tilde{f}_\lambda - f\|^2 + \frac{\sigma^2}{n} \left(5 + \frac{2+3a}{a} \left(2 \log \left(\frac{eM}{M(\lambda) \vee 1} \right) \right) \right) M(\lambda) \right\} + \frac{6\sigma^2(1+a)^2}{an(e-1)}$$

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