

Cross Validation, Monte Carlo Cross Validation, and Accumulated Prediction Errors: Asymptotic Properties

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Cross Validation (CV)

- Consider

$$y_i = \mathbf{x}'_i \boldsymbol{\beta} + e_i = \sum_{j=1}^p x_{ij} \beta_j + e_i,$$

where $\boldsymbol{\beta}' = (\beta_1, \dots, \beta_p)$ and e_i are i.i.d. r.v.s with $E(e_i) = 0$ and $E(e_i^2) = \sigma^2 > 0$.

- Suppose $\beta_i = 0$ for some $i \in \mathbb{P} = \{1, \dots, p\}$.
- We are interested in choosing the smallest true model

$$y_i = \mathbf{x}'_{i,\alpha^*} \boldsymbol{\beta}_{\alpha^*} + e_i,$$

where $\alpha^* = \{i : \beta_i \neq 0\}$, $\boldsymbol{\beta}'_{\alpha^*} = (\beta_i, i \in \alpha^*)$ and $\mathbf{x}'_{i,\alpha^*} = (x_{ij}, j \in \alpha^*)$, among the candidate models

$$E(\mathbf{y}) \in C(\mathbf{X}_\alpha),$$

where $\mathbf{y}' = (y_1, \dots, y_n)$, $\mathbf{X}'_\alpha = (\mathbf{x}_{i,\alpha}, \dots, \mathbf{x}_{n,\alpha})$ with $\mathbf{x}'_{i,\alpha} = (x_{ij}, j \in \alpha)$, and $\alpha \in 2^{\mathbb{P}}$.

Delete- n_v -out CV ($CV(n_v)$)

- Let (y_i, \mathbf{x}_i) , $i = 1, \dots, n$, be observations.
- $CV(n_v)$ splits the data into two parts:

$$\{(y_i, \mathbf{x}_i), i \in s\} \quad \text{and} \quad \{(y_i, \mathbf{x}_i), i \in s^c\},$$

where s and s^c are subsets of $\mathbb{N} = \{1, \dots, n\}$ with $s \cap s^c = \emptyset$ and $s \cup s^c = \mathbb{N}$.

- The first part is referred to as the validation (testing) sample, whereas the second part is referred to as the training sample.
- Denote $\sharp(s)$ and $\sharp(s^c)$ by n_v and n_c , respectively, noting that $n_v + n_c = n$.
- The CV evaluates the performance of α using

$$\begin{aligned} \hat{\Gamma}_{\alpha, n}(n_v) &= \frac{1}{n_v \binom{n}{n_v}} \sum_{\text{All } (s, s^c) \text{ combinations}} \sum_{i \in s} (y_i - \mathbf{x}'_{i, \alpha} \hat{\beta}_{\alpha, s^c})^2 \\ &= \frac{1}{n_v \binom{n}{n_v}} \sum_{\text{All } (s, s^c) \text{ combinations}} \|\mathbf{y}_s - \hat{\mathbf{y}}_{\alpha, s^c}\|^2, \quad (\hat{\mathbf{y}}_{\alpha, s^c} = \mathbf{X}_{\alpha, s} \hat{\beta}_{\alpha, s^c}) \end{aligned}$$

where $\mathbf{y}'_A = (y_i, i \in A)$, $A \subseteq \mathbb{N}$ and $\hat{\beta}_{\alpha, s^c} = (\mathbf{X}'_{\alpha, s^c} \mathbf{X}_{\alpha, s^c})^{-1} \mathbf{X}'_{\alpha, s^c} \mathbf{y}_{s^c}$ with $\mathbf{X}'_{\alpha, A} = (\mathbf{x}_{i, \alpha}, i \in A)$.

Some statistical properties of CV

Define $P_\alpha = X_\alpha(X'_\alpha X_\alpha)^{-1}X'_\alpha$ and $Q_{\alpha,A} = X_{\alpha,A}(X'_\alpha X_\alpha)^{-1}X'_{\alpha,A}$.

Fact 1

$$n_v^{-1} \|y_s - \hat{y}_{\alpha,sc}\|^2 = n_v^{-1} \|(I_{n_v} - Q_{\alpha,s})^{-1}(y_s - X_{\alpha,s}\hat{\beta}_\alpha)\|^2,$$

where I_{n_v} denotes the n_v -dimensional identity matrix and

$$\hat{\beta}_\alpha = (X'_\alpha X_\alpha)^{-1}X'_\alpha y,$$

which is the least squares estimate of β_α based on the "full" data.

Proof

Since

$$(X'_{\alpha,s^c} X_{\alpha,s^c})^{-1} = (X'_{\alpha} X_{\alpha} - X'_{\alpha,s} X_{\alpha,s})^{-1},$$

by making use of

$$(A - B'B)^{-1} = A^{-1} + A^{-1}B'(I - BA^{-1}B')^{-1}BA^{-1}, \quad (1)$$

(I : identity matrix of suitable dimension)

we obtain

$$\begin{aligned} \hat{y}_{\alpha,s^c} &= X_{\alpha,s} \hat{\beta}_{\alpha,s^c} \\ &= X_{\alpha,s} \hat{\beta}_{\alpha} + Q_{\alpha,s} (I - Q_{\alpha,s})^{-1} X_{\alpha,s} \hat{\beta}_{\alpha} - Q_{\alpha,s} y_s - Q_{\alpha,s} (I - Q_{\alpha,s})^{-1} Q_{\alpha,s} y_s, \end{aligned}$$

and hence

$$y_s - X_{\alpha,s} \hat{\beta}_{\alpha,s^c} = (I - Q_{\alpha,s})^{-1} (y_s - X_{\alpha,s} \hat{\beta}_{\alpha}).$$

This completes the proof.

Remark

By Fact 1, we have

$$\hat{\Gamma}_{\alpha,n}(1) = n^{-1} \sum_{i=1}^n \{(1 - w_{i\alpha})^{-1} (y_i - x'_{i,\alpha} \hat{\beta}_{\alpha})\}^2, \rightarrow \text{Delete-1-out CV (conventional CV)}$$

where $w_{i\alpha} = (P_{\alpha})_{ii}$, the i th diagonal element of P_{α} .

Theorem 1

Assume

$$\frac{\mathbf{X}'\mathbf{X}}{n} \xrightarrow{n \rightarrow \infty} \mathbf{R}, \text{ a positive definite matrix,} \quad (2)$$

where $\mathbf{X}' = (\mathbf{x}_1, \dots, \mathbf{x}_n)$, and

$$\max_{1 \leq i \leq n} w_{i\alpha} \xrightarrow{n \rightarrow \infty} 0 \text{ for any } \alpha \in 2^{\mathbb{P}}. \quad (3)$$

Then

(1)

$$\hat{\Gamma}_{\alpha,n}(1) = \sigma^2 + \frac{1}{n} \boldsymbol{\beta}' \mathbf{X}' (\mathbf{I} - \mathbf{P}_{\alpha}) \mathbf{X} \boldsymbol{\beta} + o_p(1),$$

(\mathbf{I} : n -dimensional identity matrix)

if α is an incorrect model (namely $\alpha^* - \alpha \neq \emptyset$),

(2)

$$\hat{\Gamma}_{\alpha,n}(1) = n^{-1} \mathbf{e}' \mathbf{e} + \frac{2d_{\alpha}\sigma^2}{n} - \frac{1}{n} \mathbf{e}' \mathbf{P}_{\alpha} \mathbf{e} + o_p(n^{-1}),$$

if α is a correct model ($\alpha^* - \alpha = \emptyset$), where $d_{\alpha} = \sharp(\alpha)$ and $\mathbf{e}' = (e_1, \dots, e_n)$.

Proof

- Since

$$(1 - w_{i\alpha})^2 = 1 + 2w_{i\alpha} + O(w_{i\alpha}^2),$$

where $O(\cdot)$ denotes a bound uniform over $1 \leq i \leq n$, it holds that

$$\hat{\Gamma}_{\alpha,n}(1) = \frac{1}{n} \sum_{i=1}^n \gamma_{i\alpha}^2 + \frac{1}{n} \sum_{i=1}^n (2w_{i\alpha} + O(w_{i\alpha}^2)) \gamma_{i,\alpha}^2 \equiv (\text{I}) + (\text{II}),$$

where $\gamma_{i,\alpha} = y_i - \mathbf{x}'_{i,\alpha} \hat{\beta}_\alpha$.

- If α is incorrect, then

$$\begin{aligned} (\text{I}) &= n^{-1} \mathbf{y}' (\mathbf{I} - \mathbf{P}_\alpha) \mathbf{y} \\ &= n^{-1} (\mathbf{e}' + \beta' \mathbf{X}') (\mathbf{I} - \mathbf{P}_\alpha) (\mathbf{X} \beta + \mathbf{e}) \\ &= n^{-1} \mathbf{e}' (\mathbf{I} - \mathbf{P}_\alpha) \mathbf{e} + 2n^{-1} \mathbf{e}' (\mathbf{I} - \mathbf{P}_\alpha) \mathbf{X} \beta + n^{-1} \beta' \mathbf{X}' (\mathbf{I} - \mathbf{P}_\alpha) \mathbf{X} \beta \\ &\stackrel{\text{why?}}{=} \sigma^2 + n^{-1} \beta' \mathbf{X}' (\mathbf{I} - \mathbf{P}_\alpha) \mathbf{X} \beta + o_p(1), \end{aligned}$$

and $(\text{II}) = o_p(1)$. Then (1) follows.

If α is correct, then

$$(I) = n^{-1} \mathbf{e}'(\mathbf{I} - \mathbf{P}_\alpha) \mathbf{e},$$

and

$$\begin{aligned}
 (II) &= n^{-1} \sum_{i=1}^n (2w_{i\alpha} + O(w_{i\alpha}^2))(e_i - \mathbf{x}'_{i,\alpha}(\hat{\beta}_\alpha - \beta_\alpha))^2 \\
 &\stackrel{\text{why?}}{=} \frac{2}{n} \sum_{i=1}^n w_{i\alpha} e_i^2 + o_p(n^{-1}) \\
 &= \frac{2}{n} \sum_{i=1}^n w_{i\alpha} \sigma^2 + \frac{2}{n} \sum_{i=1}^n w_{i\alpha} (e_i^2 - \sigma^2) + o_p(n^{-1}) \\
 &\stackrel{\text{why?}}{=} \frac{2d_\alpha \sigma^2}{n} + o_p(1).
 \end{aligned}$$

This completes the proof.

Corollary 1

Let

$$\hat{\alpha} = \operatorname{argmin}_{\alpha \in 2^{\mathbb{P}}} \hat{\Gamma}_{\alpha,n}(1).$$

Then $\lim_{n \rightarrow \infty} P(\alpha^* - \hat{\alpha} = \emptyset) = 1$, but $\lim_{n \rightarrow \infty} P(\hat{\alpha} = \alpha^*)$ is in general less than 1.

Notation

- $b = \binom{n}{n_v}$
- $\mathcal{B}_{n_v} = \{s : s \subseteq \mathbb{N} \text{ and } \#(s) = n_v\}$
- $P_{\alpha,s} = \mathbf{X}_{\alpha,s}(\mathbf{X}'_{\alpha,s}\mathbf{X}_{\alpha,s})^{-1}\mathbf{X}'_{\alpha,s}$
- $\hat{R}_{\alpha,s} = \frac{1}{n_v} \sum_{t \in s} \mathbf{x}_{t,\alpha} \mathbf{x}'_{t,\alpha}$
- $\hat{R}_{\alpha,s^c} = \frac{1}{n_c} \sum_{t \in s^c} \mathbf{x}_{t,\alpha} \mathbf{x}'_{t,\alpha}$
- $\gamma_{\alpha,s} = \mathbf{y}_s - \mathbf{X}_{\alpha,s}\hat{\beta}_{\alpha}$

Then, Fact 1 yields

$$\hat{\Gamma}_{\alpha,n}(n_v) = \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} (I_{n_v} - Q_{\alpha,s})^{-1} (I_{n_v} - Q_{\alpha,s})^{-1} \gamma_{\alpha,s} = \text{(I)} + \text{(II)} + \cdots + \text{(VI)}, \quad (4)$$

where

$$\begin{aligned} \text{(I)} &= \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} \gamma_{\alpha,s}, & \text{(II)} &= \frac{n_v^2}{n_c^2} \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} P_{\alpha,s} \gamma_{\alpha,s}, \\ \text{(III)} &= \frac{1}{n_c^2} \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} X_{\alpha,s} (\hat{R}_{\alpha,s^c}^{-1} - \hat{R}_{\alpha,s}^{-1}) X'_{\alpha,s} X_{\alpha,s} (\hat{R}_{\alpha,s^c}^{-1} - \hat{R}_{\alpha,s}^{-1}) X'_{\alpha,s} \gamma_{\alpha,s}, \\ \text{(IV)} &= 2 \frac{n_v}{n_c} \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} P_{\alpha,s} \gamma_{\alpha,s}, \\ \text{(V)} &= \frac{2}{n_c} \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} X_{\alpha,s} (\hat{R}_{\alpha,s^c}^{-1} - \hat{R}_{\alpha,s}^{-1}) X'_{\alpha,s} \gamma_{\alpha,s}, \\ \text{(VI)} &= \frac{2n_v}{n_c^2} \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} P_{\alpha,s} X_{\alpha,s} (\hat{R}_{\alpha,s^c}^{-1} - \hat{R}_{\alpha,s}^{-1}) X'_{\alpha,s} \gamma_{\alpha,s}. \quad (P_{\alpha,s} X_{\alpha,s} = X_{\alpha,s}) \end{aligned}$$

Hint

Using (1), one gets

$$(I_{n_v} - Q_{\alpha,s})^{-1} = I_{n_v} + \frac{n_v}{n_c} P_{\alpha,s} + \frac{1}{n_c} X_{\alpha,s} (\hat{R}_{\alpha,s^c}^{-1} - \hat{R}_{\alpha,s}^{-1}) X'_{\alpha,s}.$$

Theorem 2

Assume the same assumptions as in Theorem 1. Assume also that

$$\lim_{n \rightarrow \infty} \max_{s \in \mathcal{B}_{n_v}} \|\hat{\mathbf{R}}_s - \hat{\mathbf{R}}_{s^c}\| = 0, \quad (5)$$

where $\hat{\mathbf{R}}_A = \frac{1}{\#(A)} \sum_{t \in A} \mathbf{x}_t \mathbf{x}_t'$ with $A \subseteq \mathbb{N}$. Suppose

$$\frac{n_v}{n} \rightarrow 1 \quad \text{and} \quad n_c = n - n_v \rightarrow \infty. \quad (6)$$

Then

(i) For $\alpha^* - \alpha \neq \emptyset$,

$$\hat{\Gamma}_{\alpha, n}(n_v) = n^{-1} \mathbf{e}' \mathbf{e} + n^{-1} \boldsymbol{\beta}' \mathbf{X}' (\mathbf{I} - \mathbf{P}_\alpha) \mathbf{X} \boldsymbol{\beta} + o_p(1) + R_n, \quad (7)$$

where R_n is a non-negative random variable.

(ii) For $\alpha^* - \alpha = \emptyset$,

$$\hat{\Gamma}_{\alpha, n}(n_v) = n^{-1} \mathbf{e}' \mathbf{e} + \frac{d_\alpha \sigma^2}{n_c} + o_p(n_c^{-1}). \quad (8)$$

(iii) $\lim_{n \rightarrow \infty} P(\hat{\alpha}_{n_v} = \alpha^*) = 1$, where $\hat{\alpha}_{n_v} = \operatorname{argmin}_{\alpha \in 2^{\mathbb{P}}} \hat{\Gamma}_{\alpha, n}(n_v)$.

Proof

- We begin by considering the case of $\alpha^* - \alpha = \emptyset$.
- We will first show that

$$\hat{\Gamma}_{\alpha,n}(n_v) = (\text{I}) + (\text{II})(1 + o(1)), \quad (9)$$

via proving

$$|(K)| = (\text{II})o(1), \quad (10)$$

where $K = \text{III}, \text{IV}, \text{V}, \text{and VI}$.

To show (10) holds with $K = \text{VI}$, note that

$$(\text{VI}) \leq 2\{(A) + (B)\}, \quad (11)$$

where

$$\begin{aligned} (A) &= \frac{n_v}{n_c^2} \frac{1}{n_v b} \left| \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} \mathbf{X}_{\alpha,s} (\hat{\mathbf{R}}_{\alpha,s^c}^{-1} - \hat{\mathbf{R}}_{\alpha,s}^{-1}) (\hat{\mathbf{R}}_{\alpha,s} - \hat{\mathbf{R}}_{\alpha,s^c}) \hat{\mathbf{R}}_{\alpha,s}^{-1} \mathbf{X}'_{\alpha,s} \gamma_{\alpha,s} \right|, \\ (B) &= \frac{n_v}{n_c^2} \frac{1}{n_v b} \left| \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} \mathbf{X}_{\alpha,s} \hat{\mathbf{R}}_{\alpha,s}^{-1} (\hat{\mathbf{R}}_{\alpha,s} - \hat{\mathbf{R}}_{\alpha,s^c}) \hat{\mathbf{R}}_{\alpha,s}^{-1} \mathbf{X}'_{\alpha,s} \gamma_{\alpha,s} \right|. \end{aligned}$$

In addition,

$$(B) \stackrel{\text{why?}}{\leq} \frac{n_v^2}{n_c^2} \frac{1}{n_v b} \max_{s \in \mathcal{B}_{n_v}} \|\hat{\mathbf{R}}_{\alpha,s} - \hat{\mathbf{R}}_{\alpha,s^c}\| \max_{s \in \mathcal{B}_{n_v}} \|\hat{\mathbf{R}}_{\alpha,s}^{-1}\| \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} \mathbf{P}_{\alpha,s} \gamma_{\alpha,s}, \quad (12)$$

and

$$(A) \stackrel{\text{why?}}{\leq} \frac{n_v^2}{n_c^2} \frac{1}{n_v b} \max_{s \in \mathcal{B}_{n_v}} \|\hat{\mathbf{R}}_{\alpha,s} - \hat{\mathbf{R}}_{\alpha,s^c}\|^2 \max_{s \in \mathcal{B}_{n_v}} \|\hat{\mathbf{R}}_{\alpha,s}^{-1}\| \max_{s \in \mathcal{B}_{n_v}} \|\hat{\mathbf{R}}_{\alpha,s^c}^{-1}\| \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} \mathbf{P}_{\alpha,s} \gamma_{\alpha,s}. \quad (13)$$

- By (2), we have

$$\max_{s \in \mathcal{B}_{n_v}} \|\hat{\mathbf{R}}_{\alpha,s}^{-1}\| = O(1),$$

which, together with (5), and (11)–(13), yields

$$|(\text{VI})| = (\text{II})o(1). \quad (14)$$

- Similarly, it can be shown that

$$|(\text{V})| = (\text{II})o(1). \quad (15)$$

- Since $\frac{n_v}{n_c} \rightarrow \infty$, it is easy to see that

$$|(\text{IV})| = (\text{IV}) = (\text{II})o(1). \quad ((\text{IV}) \text{ is non-negative}) \quad (16)$$

Now, for (III), we have

$$\begin{aligned}
 |(III)| &\leq \frac{n_v}{n_c^2} \frac{1}{n_v b} \left| \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} \mathbf{X}_{\alpha,s} \hat{\mathbf{R}}_{\alpha,s^c}^{-1} (\hat{\mathbf{R}}_{\alpha,s} - \hat{\mathbf{R}}_{\alpha,s^c}) \hat{\mathbf{R}}_{\alpha,s^c}^{-1} (\hat{\mathbf{R}}_{\alpha,s} - \hat{\mathbf{R}}_{\alpha,s^c}) \hat{\mathbf{R}}_{\alpha,s}^{-1} \mathbf{X}'_{\alpha,s} \gamma_{\alpha,s} \right| \\
 &\leq \frac{n_v}{n_c^2} \frac{1}{n_v b} \left| \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} \mathbf{X}_{\alpha,s} \hat{\mathbf{R}}_{\alpha,s}^{-1} (\hat{\mathbf{R}}_{\alpha,s} - \hat{\mathbf{R}}_{\alpha,s^c}) \hat{\mathbf{R}}_{\alpha,s^c}^{-1} (\hat{\mathbf{R}}_{\alpha,s} - \hat{\mathbf{R}}_{\alpha,s^c}) \hat{\mathbf{R}}_{\alpha,s}^{-1} \mathbf{X}'_{\alpha,s} \gamma_{\alpha,s} \right| \\
 &\quad + \frac{n_v}{n_c^2} \frac{1}{n_v b} \left| \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} \mathbf{X}_{\alpha,s} \hat{\mathbf{R}}_{\alpha,s}^{-1} (\hat{\mathbf{R}}_{\alpha,s} - \hat{\mathbf{R}}_{\alpha,s^c}) \hat{\mathbf{R}}_{\alpha,s^c}^{-1} \right. \\
 &\quad \left. (\hat{\mathbf{R}}_{\alpha,s} - \hat{\mathbf{R}}_{\alpha,s^c}) \hat{\mathbf{R}}_{\alpha,s^c}^{-1} (\hat{\mathbf{R}}_{\alpha,s} - \hat{\mathbf{R}}_{\alpha,s^c}) \hat{\mathbf{R}}_{\alpha,s}^{-1} \mathbf{X}'_{\alpha,s} \gamma_{\alpha,s} \right|.
 \end{aligned}$$

This and an argument similar to that used to prove (14) give

$$|(III)| = (II)o(1). \quad (17)$$

Hence, (10) follows from (14)–(17). Now, by an argument similar to that use to prove (14) again, we have

$$(II) = \frac{n_v^2}{n_c^2} \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} \mathbf{Q}_{\alpha,s} \gamma_{\alpha,s} + (II)o(1). \quad (18)$$

Moreover,

$$\begin{aligned}
 & \frac{n_v^2}{n_c^2} \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha, s} \mathbf{Q}_{\alpha, s} \gamma_{\alpha, s} \\
 &= \frac{n_v^2}{n_c^2} \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \sum_{(i, j) \in s \times s} P_{\alpha, ij} \gamma_{i, \alpha} \gamma_{j, \alpha} \quad ([P_{\alpha, ij}]_{i, j \in s} = \mathbf{P}_{\alpha}) \\
 &= \frac{n_v^2}{n_c^2} \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \sum_{i \in s} P_{\alpha, ii} \gamma_{i, \alpha}^2 + \frac{n_v^2}{n_c^2} \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \sum_{(i, j) \in s \times s, i \neq j} P_{\alpha, ij} \gamma_{i, \alpha} \gamma_{j, \alpha} \quad (P_{\alpha, ii} = w_{i\alpha}) \\
 &\stackrel{\text{why?}}{=} \frac{n_v^2}{n_c^2} \frac{1}{n} \sum_{i=1}^n w_{i\alpha} \gamma_{i, \alpha}^2 - \frac{n_v^2}{n_c^2} \frac{n_v - 1}{n - 1} \frac{1}{n} \sum_{i=1}^n w_{i\alpha} \gamma_{i, \alpha}^2 \\
 &= \frac{n_v^2}{n_c^2} \frac{1}{n} \frac{n_c}{n - 1} \sum_{i=1}^n w_{i\alpha} \sigma^2 + O\left(\frac{1}{n_c} \sum_{i=1}^n w_{i\alpha} (\gamma_{i, \alpha}^2 - \sigma^2)\right) \\
 &\stackrel{\text{why?}}{=} \frac{d_{\alpha} \sigma^2}{n_c} + o_p(n_c^{-1}). \tag{19}
 \end{aligned}$$

- By (18) and (19), we have

$$(II) = \frac{d_{\alpha}\sigma^2}{n_c} + o_p(n_c^{-1}). \quad (20)$$

- Moreover,

$$(I) = \frac{1}{n} \mathbf{y}'(\mathbf{I} - \mathbf{P}_{\alpha})\mathbf{y} = \frac{1}{n} \mathbf{e}'(\mathbf{I} - \mathbf{P}_{\alpha})\mathbf{e} = n^{-1} \mathbf{e}'\mathbf{e} + O_p(n^{-1}). \quad (21)$$

- In view of (20), (21) and (9), the desired conclusion (8) follows.

- To show (7), note that (4) implies (why?)

$$\hat{\Gamma}_{\alpha,n}(n_v) \geq \frac{1}{n_v b} \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha,s} \gamma_{\alpha,s} = \frac{1}{n} \mathbf{y}'(\mathbf{I} - \mathbf{P}_{\alpha})\mathbf{y}. \quad (22)$$

- Since $\alpha^* - \alpha \neq \emptyset$,

$$\begin{aligned} \frac{1}{n} \mathbf{y}'(\mathbf{I} - \mathbf{P}_{\alpha})\mathbf{y} &= n^{-1} \mathbf{e}'\mathbf{e} + n^{-1} \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P}_{\alpha})\mathbf{X}\boldsymbol{\beta} + 2n^{-1} \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P}_{\alpha})\mathbf{e} \\ &= n^{-1} \mathbf{e}'\mathbf{e} + n^{-1} \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P}_{\alpha})\mathbf{X}\boldsymbol{\beta} + o_p(1), \end{aligned} \quad (23)$$

and hence (7) is ensured by (22) and (23).

- Finally, (iii) is an immediate consequence of (i) and (ii).

Monte Carlo Cross Validation (MCCV)

- Let $s_i \stackrel{\text{i.i.d.}}{\sim} U(\mathcal{B}_{n_v})$, where \mathcal{B}_{n_v} is defined in the note for CV.
- Define MCCV as follows:

$$\hat{\Gamma}_{\alpha,n}^{\text{MCCV}} = \frac{1}{n_v b} \sum_{i=1}^b \|\mathbf{y}_{s_i} - \hat{\mathbf{y}}_{\alpha, s_i^c}\|^2,$$

where b is the number of Monte Carlo simulations used to calculate CV.

Theorem 3

Assume the same assumptions as in Theorem 1. Suppose

$$\max_{1 \leq j \leq b} \left\| \frac{1}{n_v} \sum_{i \in s_j} \mathbf{x}_i \mathbf{x}_i' - \frac{1}{n_c} \sum_{i \notin s_j} \mathbf{x}_i \mathbf{x}_i' \right\| = o_p(1), \quad (24)$$

and

$$Ee_1^4 < \infty, \quad \frac{n^2}{bn_c^2} \rightarrow 0, \quad \frac{n_v}{n} \rightarrow 1, \quad \text{and} \quad n_c \rightarrow \infty. \quad (25)$$

Then,

(i) for $\alpha^* - \alpha \neq \emptyset$,

$$\hat{\Gamma}_{\alpha, n}^{\text{MCCV}} = \frac{1}{n_v b} \sum_{i=1}^b \mathbf{e}_{s_i}' \mathbf{e}_{s_i} + \frac{1}{n} \boldsymbol{\beta}' \mathbf{X}' (\mathbf{I} - \mathbf{P}_\alpha) \mathbf{X} \boldsymbol{\beta} + o_p(1) + R_n,$$

where $\mathbf{e}_{s_i}' = (e_j, j \in s_i)$ and R_n is some positive r.v.,

(ii) for $\alpha^* - \alpha = \emptyset$,

$$\hat{\Gamma}_{\alpha, n}^{\text{MCCV}} = \frac{1}{n_v b} \sum_{i=1}^b \mathbf{e}_{s_i}' \mathbf{e}_{s_i} + n_c^{-1} d_\alpha \sigma^2 + o_p(n_c^{-1}),$$

(iii) $\lim_{n \rightarrow \infty} P(\hat{\alpha}_{\text{MCCV}} = \alpha^*) = 1$, where $\hat{\alpha}_{\text{MCCV}} = \operatorname{argmin}_{\alpha \in 2^{\mathcal{P}}} \hat{\Gamma}_{\alpha, n}^{\text{MCCV}}$.

Proof

By an argument similar to that used to prove (9) and (18) in the note for CV, one has for $\alpha^* - \alpha = \emptyset$,

$$\hat{\Gamma}_{\alpha,n}^{\text{MCCV}} = \frac{1}{n_v b} \sum_{i=1}^b \gamma'_{\alpha,s_i} \gamma_{\alpha,s_i} + \frac{n_v^2}{n_c^2} \frac{1}{n_v b} \sum_{i=1}^b \gamma'_{\alpha,s_i} P_{\alpha,s_i} \gamma_{\alpha,s_i} (1 + o_p(1)), \quad (26)$$

and

$$\frac{n_v^2}{n_c^2} \frac{1}{n_v b} \sum_{i=1}^b \gamma'_{\alpha,s_i} P_{\alpha,s_i} \gamma_{\alpha,s_i} (1 + o_p(1)) = \frac{n_v^2}{n_c^2} \frac{1}{n_v b} \sum_{i=1}^b \gamma'_{\alpha,s_i} Q_{\alpha,s_i} \gamma_{\alpha,s_i}. \quad (27)$$

In addition, by (19) in the note for CV,

$$\begin{aligned}
 & E \left[\frac{n_v^2}{n_c^2} \frac{1}{n_v b} \sum_{i=1}^b \gamma'_{\alpha, s_i} \mathbf{Q}_{\alpha, s_i} \gamma_{\alpha, s_i} \middle| (y_1, \mathbf{x}_1), \dots, (y_n, \mathbf{x}_n) \right] \\
 &= \frac{n_v^2}{n_c^2} \frac{1}{n_v} E[\gamma'_{\alpha, s_1} \mathbf{Q}_{\alpha, s_1} \gamma_{\alpha, s_1} | (y_1, \mathbf{x}_1), \dots, (y_n, \mathbf{x}_n)] \\
 &\stackrel{\text{why?}}{=} \frac{n_v^2}{n_c^2} \frac{1}{n_v} \frac{1}{\binom{n}{n_v}} \sum_{s \in \mathcal{B}_{n_v}} \gamma'_{\alpha, s} \mathbf{Q}_{\alpha, s} \gamma_{\alpha, s} \\
 &= \frac{d_{\alpha} \sigma^2}{n_c} + o_p(n_c^{-1}),
 \end{aligned}$$

implying

$$E[n_c V_n | \mathcal{F}_n] \xrightarrow{pr.} d_{\alpha} \sigma^2, \quad (28)$$

where

$$V_n = \frac{n_v^2}{n_c^2} \frac{1}{n_v b} \sum_{i=1}^b \gamma'_{\alpha, s_i} \mathbf{Q}_{\alpha, s_i} \gamma_{\alpha, s_i}$$

and \mathcal{F}_n is the σ -field generated by $(y_1, \mathbf{x}_1), \dots, (y_n, \mathbf{x}_n)$.

- We also have

$$\begin{aligned}
 \text{Var}(n_c V_n | \mathcal{F}_n) &= \frac{n_v^2}{n_c^2} \frac{1}{b^2} \sum_{i=1}^b \text{Var}(\gamma'_{\alpha, s_i} \mathbf{Q}_{\alpha, s_i} \gamma_{\alpha, s_i} | \mathcal{F}_n) \\
 &\leq \frac{n_v^2}{n_c^2} \frac{1}{b} E((\gamma'_{\alpha, s_1} \mathbf{Q}_{\alpha, s_1} \gamma_{\alpha, s_1})^2 | \mathcal{F}_n) \\
 &= \frac{n_v^2}{n_c^2} \frac{1}{b} \frac{1}{\binom{n}{n_v}} \sum_{s \in \mathcal{B}_{n_v}} (\gamma'_{\alpha, s} \mathbf{Q}_{\alpha, s} \gamma_{\alpha, s})^2.
 \end{aligned}$$

- Since $Ee_1^4 < \infty$, we have

$$E((\gamma'_{\alpha, s} \mathbf{Q}_{\alpha, s} \gamma_{\alpha, s})^2) \leq C < \infty \text{ for all } s \in \mathcal{B}_{n_v}, \quad (C : \text{some positive constant})$$

which, together with $\frac{n_v^2}{n_c^2} \frac{1}{b} \rightarrow 0$, yields

$$\text{Var}[n_c V_n | \mathcal{F}_n] \xrightarrow{pr.} 0. \quad (29)$$

- It is shown in the Appendix that

$$(28) + (29) \quad \text{implies} \quad n_c V_n \xrightarrow{pr.} d_\alpha \sigma^2. \quad (30)$$

- In view of (26), (27) and (30), (ii) is proved once

$$\frac{1}{n_v b} \sum_{i=1}^b \gamma'_{\alpha, s_i} \gamma_{\alpha, s_i} = \frac{1}{n_v b} \sum_{i=1}^b e'_{s_i} e_{s_i} + o_p(n_c^{-1}). \quad (31)$$

- To show (31), note first that

$$\gamma_{\alpha, s_i} = e_{s_i} - \mathbf{X}_{\alpha, s_i} (\hat{\beta}_\alpha - \beta_\alpha),$$

yielding

$$\begin{aligned} \frac{1}{n_v b} \sum_{i=1}^b \gamma'_{\alpha, s_i} \gamma_{\alpha, s_i} &= \frac{1}{n_v b} \sum_{i=1}^b e'_{s_i} e_{s_i} - \frac{2}{n_v b} \sum_{i=1}^b (\hat{\beta}_\alpha - \beta_\alpha)' \mathbf{X}'_{\alpha, s_i} e_{s_i} \\ &\quad + (\hat{\beta}_\alpha - \beta_\alpha)' \left(\frac{1}{n_v b} \sum_{i=1}^b \mathbf{X}'_{\alpha, s_i} \mathbf{X}_{\alpha, s_i} \right) (\hat{\beta}_\alpha - \beta_\alpha). \end{aligned} \quad (32)$$

Since

$$\begin{aligned}
 \left| \frac{1}{n_v b} \sum_{i=1}^b (\hat{\beta}_\alpha - \beta_\alpha)' \mathbf{X}'_{\alpha, s_i} \mathbf{e}_{s_i} \right| &\leq \|\hat{\beta}_\alpha - \beta_\alpha\| \left\| \frac{1}{n_v b} \sum_{i=1}^b \mathbf{X}'_{\alpha, s_i} \mathbf{e}_{s_i} \right\|, \\
 E \left(\left\| \frac{1}{n_v b} \sum_{i=1}^b \mathbf{X}'_{\alpha, s_i} \mathbf{e}_{s_i} \right\| \right) &\leq \frac{1}{n_v b} \sum_{i=1}^b E(\|\mathbf{X}'_{\alpha, s_i} \mathbf{e}_{s_i}\|) \\
 &= \frac{1}{n_v} E[E(\|\mathbf{X}'_{\alpha, s_1} \mathbf{e}_{s_1}\| | \mathcal{F}_n)] \\
 &= \frac{1}{n_v} E \left(\frac{1}{\binom{n}{n_v}} \sum_{s \in \mathcal{B}_{n_v}} \|\mathbf{X}'_{\alpha, s} \mathbf{e}_s\| \right) \\
 &\stackrel{\text{why?}}{=} O(n_v^{-\frac{1}{2}}),
 \end{aligned}$$

and

$$\|\hat{\beta}_\alpha - \beta_\alpha\| = O_p(n^{-\frac{1}{2}}),$$

one has

$$\frac{2}{n_v b} \sum_{i=1}^b (\hat{\beta}_\alpha - \beta_\alpha)' \mathbf{X}'_{\alpha, s_i} \mathbf{e}_{s_i} \stackrel{\text{why?}}{=} O_p(n^{-1}). \quad (33)$$

- Similarly, it can be shown that

$$(\hat{\beta}_{\alpha} - \beta_{\alpha})' \left(\frac{1}{n_v b} \sum_{i=1}^b \mathbf{X}'_{\alpha, s_i} \mathbf{X}_{\alpha, s_i} \right) (\hat{\beta}_{\alpha} - \beta_{\alpha}) = O_p(n^{-1}). \quad (34)$$

- Combining (32)–(34), we obtain the desired conclusion (31). Thus, (ii) is proved.
- The proof of (i) is left as an exercise.
- Finally, we note that (iii) is an immediate consequence of (i) & (ii).

Appendix: the proof of (30)

To prove (30), we need the so-called conditional Chebyshev's inequality, which is stated as follows.

Conditional Chebyshev's inequality

Let X be a positive r.v., $\epsilon > 0$, and \mathcal{F} be a σ -field. Then

$$P(X > \epsilon | \mathcal{F}) \leq \frac{E(X | \mathcal{F})}{\epsilon} \quad \text{a.s. (almost surely)}. \quad (35)$$

Proof

Let $D \in \mathcal{F}$. Then, by the definition of conditional expectation,

$$\begin{aligned} \int_D P(X > \epsilon | \mathcal{F}) \, d\mathcal{P} &= \int_D E(I_{X>\epsilon} | \mathcal{F}) \, d\mathcal{P} = \int_D I_{X>\epsilon} \, d\mathcal{P} \leq \int_D \frac{X}{\epsilon} I_{X>\epsilon} \, d\mathcal{P} \\ &\leq \int_D \frac{X}{\epsilon} \, d\mathcal{P} \\ &= \int_D \frac{E(X | \mathcal{F})}{\epsilon} \, d\mathcal{P}. \end{aligned}$$

Hence (35) follows.

Now, (30) is ensured by the following fact.

Fact

Let $\{X_n\}$ and $\{\mathcal{F}_n\}$ be sequences of r.v.s and σ -field, respectively. If

$$\text{Var}(X_n|\mathcal{F}_n) \xrightarrow{pr.} 0, \quad (36)$$

and

$$E(X_n|\mathcal{F}_n) \xrightarrow{pr.} C \text{ (a constant)}, \quad (37)$$

then

$$X_n \xrightarrow{pr.} C. \quad (38)$$

Proof

By the conditional Chebyshev's inequality and (36), it holds that for any $\epsilon > 0$

$$P(|X_n - E(X_n|\mathcal{F}_n)| > \epsilon|\mathcal{F}_n) \leq \frac{\text{Var}(X_n|\mathcal{F}_n)}{\epsilon^2} \xrightarrow{pr.} 0,$$

which, together with the dominated convergence theorem, yields

$$X_n - E(X_n|\mathcal{F}_n) \xrightarrow{pr.} 0. \quad (\text{why?})$$

This and (37) give (38).

Accumulated Prediction Errors (APE)

Consider the following stochastic regression model

$$y_t = \sum_{i=1}^p \beta_i x_{ti} + \epsilon_t, \quad (39)$$

where $\epsilon_t \stackrel{\text{i.i.d.}}{\sim} (0, \sigma^2)$ and $\mathbf{x}_t = (x_{t1}, \dots, x_{tp})'$ is \mathcal{F}_{t-1} -measurable, meaning that \mathbf{x}_t can be completely decided by the information collected at time $t - 1$.

Example 1: Autoregressive (AR) models

$$y_t = a_1 y_{t-1} + \dots + a_p y_{t-p} + \epsilon_t,$$

where $A(z) = 1 - a_1 z - a_2 z^2 - \dots - a_p z^p \neq 0, \forall |z| \leq 1$.

Example 2: Autoregressive exogenous models

$$y_t = a_1 y_{t-1} + \dots + a_p y_{t-p} + \eta_1 Z_{t1} + \dots + \eta_q Z_{tq} + \epsilon_t,$$

where $A(z) \neq 0, \forall |z| \leq 1$, and $(\epsilon_t, Z_{t1}, \dots, Z_{tq})$ are i.i.d..

- Let α and α^* be defined as in the note for CV.
- We are interested in choosing α^* based on APE, which assigns α to a positive value:

$$\text{APE}_\alpha = \sum_{t=M+1}^n (y_t - \mathbf{x}'_{t,\alpha} \hat{\boldsymbol{\beta}}_{t-1,\alpha})^2,$$

where

$$\hat{\boldsymbol{\beta}}_{t,\alpha} = \left(\sum_{j=1}^t \mathbf{x}_{j,\alpha} \mathbf{x}'_{j,\alpha} \right)^{-1} \left(\sum_{j=1}^t \mathbf{x}_{j,\alpha} y_j \right)$$

and M is some integer to be specified later.

Theorem 4

Assume

$$\frac{1}{n} \sum_{t=1}^n \mathbf{x}_t \mathbf{x}_t' \xrightarrow{pr.} \mathbf{R} \text{ (p.d.)}, \quad E|\epsilon_1|^{q_1} < \infty \text{ for some large } q_1, \quad (40)$$

and

$$\max_{1 \leq t \leq n, 1 \leq i \leq p} E|x_{ti}|^{q_2} < \infty \text{ for some large } q_2, \quad E\|\sqrt{t}(\hat{\beta}_t - \beta)\|^{q_3} < \bar{k} < \infty, \quad (41)$$

for all $t \geq M$ and some large q_3 .

(i) For $\alpha^* - \alpha = \emptyset$,

$$\text{APE}_\alpha = \sum_{t=M+1}^n \epsilon_t^2 + \sigma^2 d_\alpha \log n + o_p(\log n),$$

(ii) For $\alpha^* - \alpha \neq \emptyset$,

$$\text{APE}_\alpha \geq \sum_{t=M+1}^n \epsilon_t^2 + \Delta_n(\alpha) + O_p(1),$$

where $\frac{1}{n} \Delta_n(\alpha) \xrightarrow{pr.} \gamma > 0$.

(iii) $\lim_{n \rightarrow \infty} P(\hat{\alpha}_{\text{APE}} = \alpha^*) = 1$, where $\hat{\alpha}_{\text{APE}} = \operatorname{argmin}_{\alpha \in 2\mathbb{P}} \text{APE}_\alpha$.

Proof

- We first prove (i). Define

$$\mathbf{V}_{t,\alpha} = \left(\sum_{i=1}^t \mathbf{x}_{i,\alpha} \mathbf{x}_{i,\alpha}' \right)^{-1}, \quad Q_{t,\alpha} = \left(\sum_{j=1}^t \mathbf{x}_{j,\alpha} \epsilon_j \right)' \mathbf{V}_{t,\alpha} \left(\sum_{j=1}^t \mathbf{x}_{j,\alpha} \epsilon_j \right),$$

and $d_{t,\alpha} = \mathbf{x}_{t,\alpha}' \mathbf{V}_{t,\alpha} \mathbf{x}_{t,\alpha}$.

- By making use of

$$\mathbf{V}_{t,\alpha} = \mathbf{V}_{t-1,\alpha} - \frac{\mathbf{V}_{t-1,\alpha} \mathbf{x}_{t,\alpha} \mathbf{x}_{t,\alpha}' \mathbf{V}_{t-1,\alpha}}{1 + \mathbf{x}_{t,\alpha}' \mathbf{V}_{t-1,\alpha} \mathbf{x}_{t,\alpha}}$$

and

$$\frac{1}{1 + \mathbf{x}_{t,\alpha}' \mathbf{V}_{t-1,\alpha} \mathbf{x}_{t,\alpha}} = 1 - d_{t,\alpha},$$

one gets

$$\begin{aligned} & \sum_{t=M+1}^n \left(\mathbf{x}_{t,\alpha}' \mathbf{V}_{t-1,\alpha} \sum_{j=1}^{t-1} \mathbf{x}_{j,\alpha} \epsilon_j \right)^2 (1 - d_{t,\alpha}) + Q_{n,\alpha} - Q_{M,\alpha} \\ &= \sum_{t=M+1}^n d_{t,\alpha} \epsilon_t^2 + 2 \sum_{t=M+1}^n \mathbf{x}_{t,\alpha}' (\hat{\beta}_{t-1,\alpha} - \beta_\alpha) \epsilon_t (1 - d_{t,\alpha}). \end{aligned} \quad (42)$$

- Moreover, by (40) and (41), it can be shown that

$$\sum_{t=M+1}^n \left(\mathbf{x}'_{t,\alpha} \mathbf{V}_{t-1,\alpha} \sum_{j=1}^{t-1} \mathbf{x}_{j,\alpha} \epsilon_j \right)^2 d_{t,\alpha} = O_p(1), \quad (43)$$

$$Q_n = O_p(1), \quad Q_M = O_p(1), \quad (44)$$

$$\sum_{t=M+1}^n \mathbf{x}'_{t,\alpha} (\hat{\beta}_{t-1,\alpha} - \beta_\alpha) \epsilon_t (1 - d_{t,\alpha}) = o_p(\log n). \quad (45)$$

- Also, we have

$$\begin{aligned} \sum_{t=M+1}^n d_{t,\alpha} \epsilon_t^2 &= \sum_{t=M+1}^n d_{t,\alpha} \sigma^2 + \sum_{t=M+1}^n d_{t,\alpha} (\epsilon_t^2 - \sigma^2) \\ &= \sigma^2 d_\alpha \log n + o_p(\log n) + O_p(1). \end{aligned} \quad (46)$$

- Consequently, (i) follows from (42)–(46), and the fact that

$$\begin{aligned}
 \text{APE}_\alpha &= \sum_{t=M+1}^n (\epsilon_t - \mathbf{x}'_{t,\alpha}(\hat{\beta}_{t-1,\alpha} - \beta_\alpha))^2 \\
 &= \sum_{t=M+1}^n \epsilon_t^2 - 2 \sum_{t=M+1}^n (\hat{\beta}_{t-1,\alpha} - \beta_\alpha) \mathbf{x}_{t,\alpha} \epsilon_t + \sum_{t=M+1}^n [\mathbf{x}'_{t,\alpha}(\hat{\beta}_{t-1,\alpha} - \beta_\alpha)]^2 \\
 &= \sum_{t=M+1}^n \epsilon_t^2 + \sum_{t=M+1}^n [\mathbf{x}'_{t,\alpha}(\hat{\beta}_{t-1,\alpha} - \beta_\alpha)]^2 + o_p(\log n).
 \end{aligned}$$

- To show (ii), note that by Theorem 2.1 of Wei (1992), we have

$$\begin{aligned}
 \sum_{t=M+1}^n (y_t - \mathbf{x}'_{t,\alpha} \hat{\beta}_{t-1,\alpha})^2 &\geq \sum_{t=1}^n (y_t - \mathbf{x}'_{t,\alpha} \hat{\beta}_{n,\alpha})^2 - \sum_{t=1}^M (y_t - \mathbf{x}'_{t,\alpha} \hat{\beta}_{M,\alpha})^2 \\
 &= \mathbf{y}'(\mathbf{I} - \mathbf{P}_\alpha)\mathbf{y} + O_p(1),
 \end{aligned}$$

which implies (ii) (why?).

- Now, (iii) follows directly from (i) and (ii).

References

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