Cross-Validation and Dimension Reduction Methods

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Statistical Analysis and Document Mining

Complementary Course, Master of Applied Mathematics in Grenoble

Outline

1. Previous Episode: Cross-Validation in linear regression
   - Training error versus test error
   - Test error in linear regression
   - The general model selection paradigm
   - K-Fold cross-validation
2. Cross-Validation: Right and Wrong Way
   - Test error in binary (supervised) classification
   - Cross-Validation for classification problems
   - Cross-Validation: right and wrong
   - Cross-Validation in multistep modeling procedure
3. Cross-Validation for Principal Components Regression
   - Linear model selection and regularization
   - Dimension reduction methods
   - An application to the credit data
   - An application to the prostate cancer

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In the next slide we will discuss this in more detail?

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Test error in linear regression

- We are given a **training dataset** $\mathcal{D} \equiv \{(\mathbf{x}_n, y_n)\}_{n \in [N]}$, $[N] \equiv 1, \ldots, N$, i.i.d. sampled from **the true (but unknown) joint PDF** of $(\mathbf{X}, Y)$.

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$$Y = \beta_0 + \sum_{p=1}^{P} \beta_p X_p + \epsilon \equiv r(\mathbf{X}) + \epsilon, \quad \boldsymbol{\beta} \equiv (\beta_0, \beta_1, \ldots, \beta_P).$$

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$$y_n \approx \widehat{r}_{\mathcal{D}}(\mathbf{x}_n), \text{ or equivalent, } \mathcal{L}(\widehat{r}_{\mathcal{D}}, \mathcal{D}) \equiv \frac{1}{N} \sum_{n=1}^{N} (y_n - \widehat{r}_{\mathcal{D}}(\mathbf{x}_n))^2 \approx 0. \quad (1)$$

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- **Test (generalization) error:** for any **new sample** $(\mathbf{x}^*, y^*)$, how can we guarantee

$$y^* \approx \widehat{r}_{\mathcal{D}}(\mathbf{x}^*), \text{ or equivalent, } \mathcal{L}(\widehat{r}_{\mathcal{D}}) \equiv \mathbb{E}_{\mathbf{X},Y}\left[(Y - \widehat{r}_{\mathcal{D}}(\mathbf{X}))^2\right] \approx 0? \quad (2)$$

Recall from CM3, in general, it holds that $\mathcal{L}(\widehat{r}_{\mathcal{D}}, \mathcal{D}) \leq \mathcal{L}(\widehat{r}_{\mathcal{D}})$. (3)

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  3. Non-asymptotic approach: **slope heuristic**[7] [8], which is particularly useful for high-dimensional small data sets, *e.g.*, $N \ll P$.

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- Estimates can be used to select best model, and to give an idea of the test error of the final chosen model.

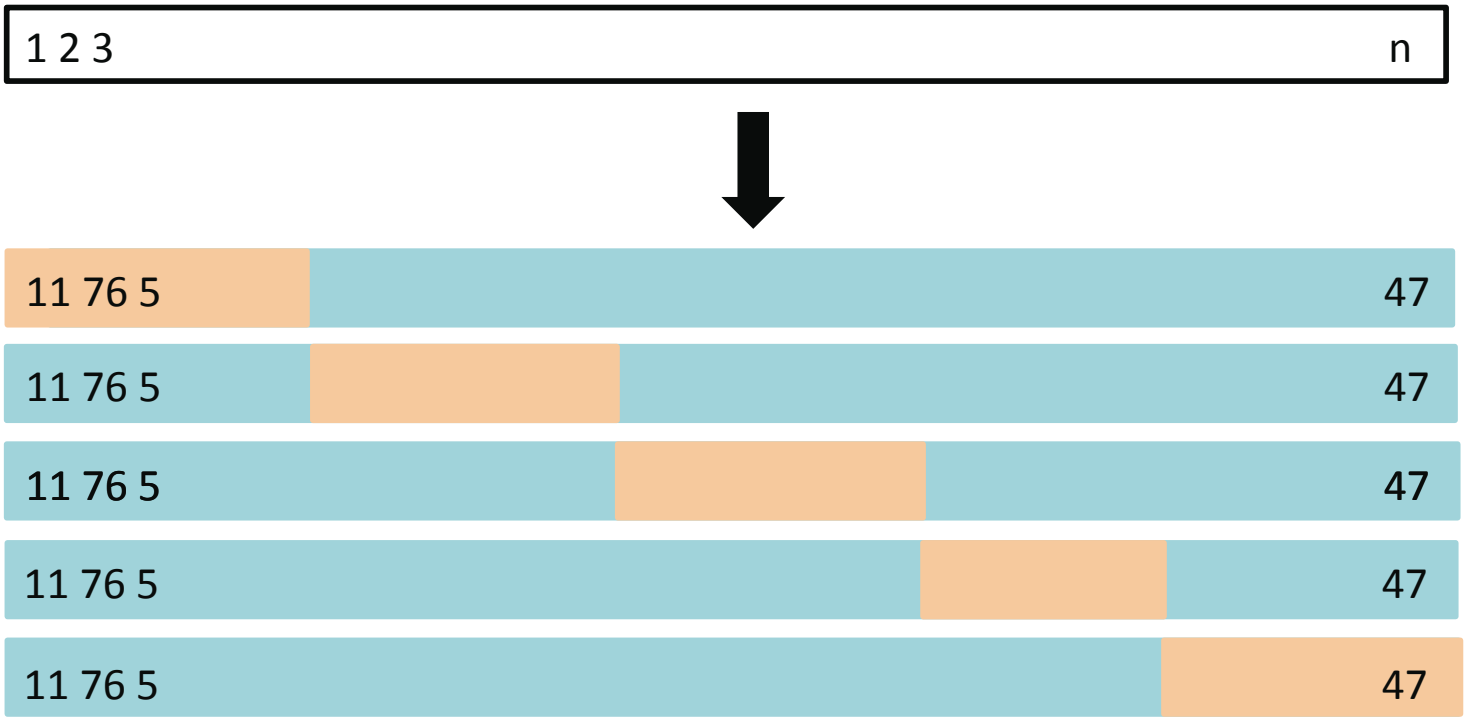

Figure 1: A schematic display of 5-fold CV. A set of N observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting estimates [James et al., 2021, Figure 5.5].

K-Fold cross-validation for linear regression in detail

1. Split the training dataset randomly into K folds so that we have $\mathcal{D}_1 \cup \cdots \cup \mathcal{D}_K = \mathcal{D}$, where $\mathcal{D}_k$ denotes the indices of the observations in part k. There are N_k observations in part k: if N is a multiple of K, then $N_k = N/K$.

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- The problem is that the predictors have an unfair advantage, as they were chosen in step (1) on the basis of all of the samples. Leaving samples out after the variables have been selected does not correctly mimic the application of the classifier to a completely independent test set, since these predictors "have already seen" the left out samples.

This error made in many high profile genomics papers [Hastie et al., 2009, Section 7.10.2].

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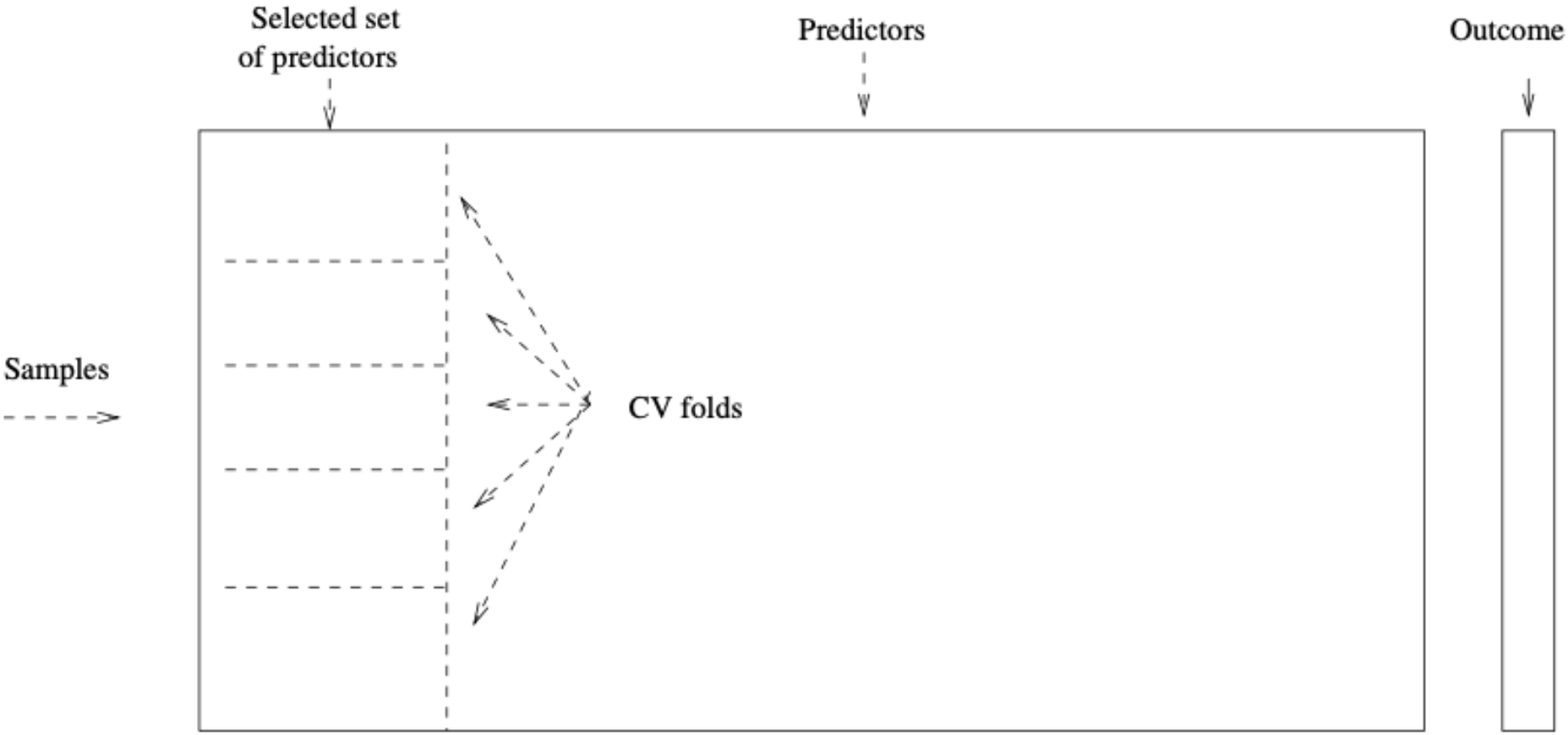

Figure 2: Cross-validation: the wrong path diagram [James et al., 2021, Figure 7.5].

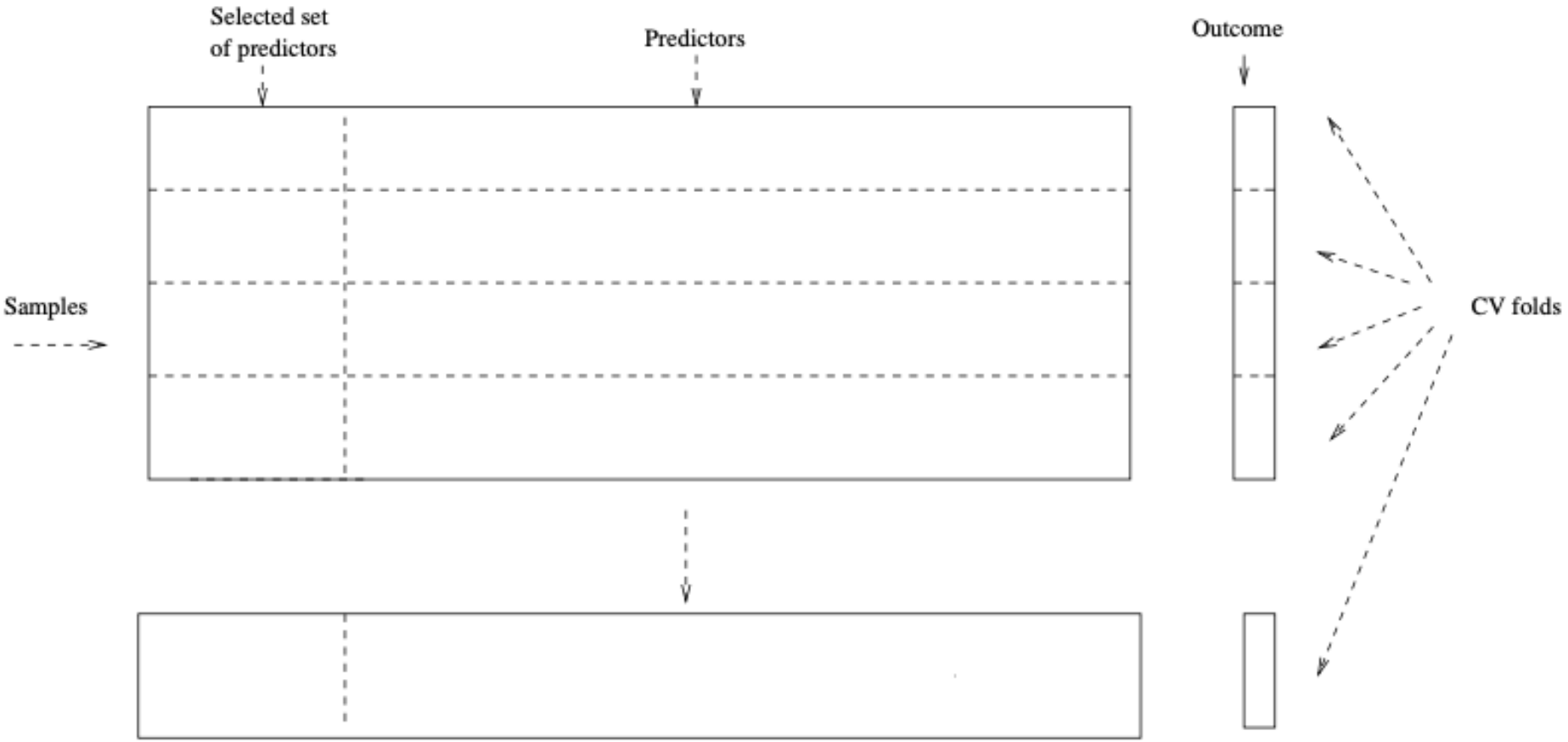

Figure 3: Cross-validation: the true path diagram [James et al., 2021, Figure 7.5].

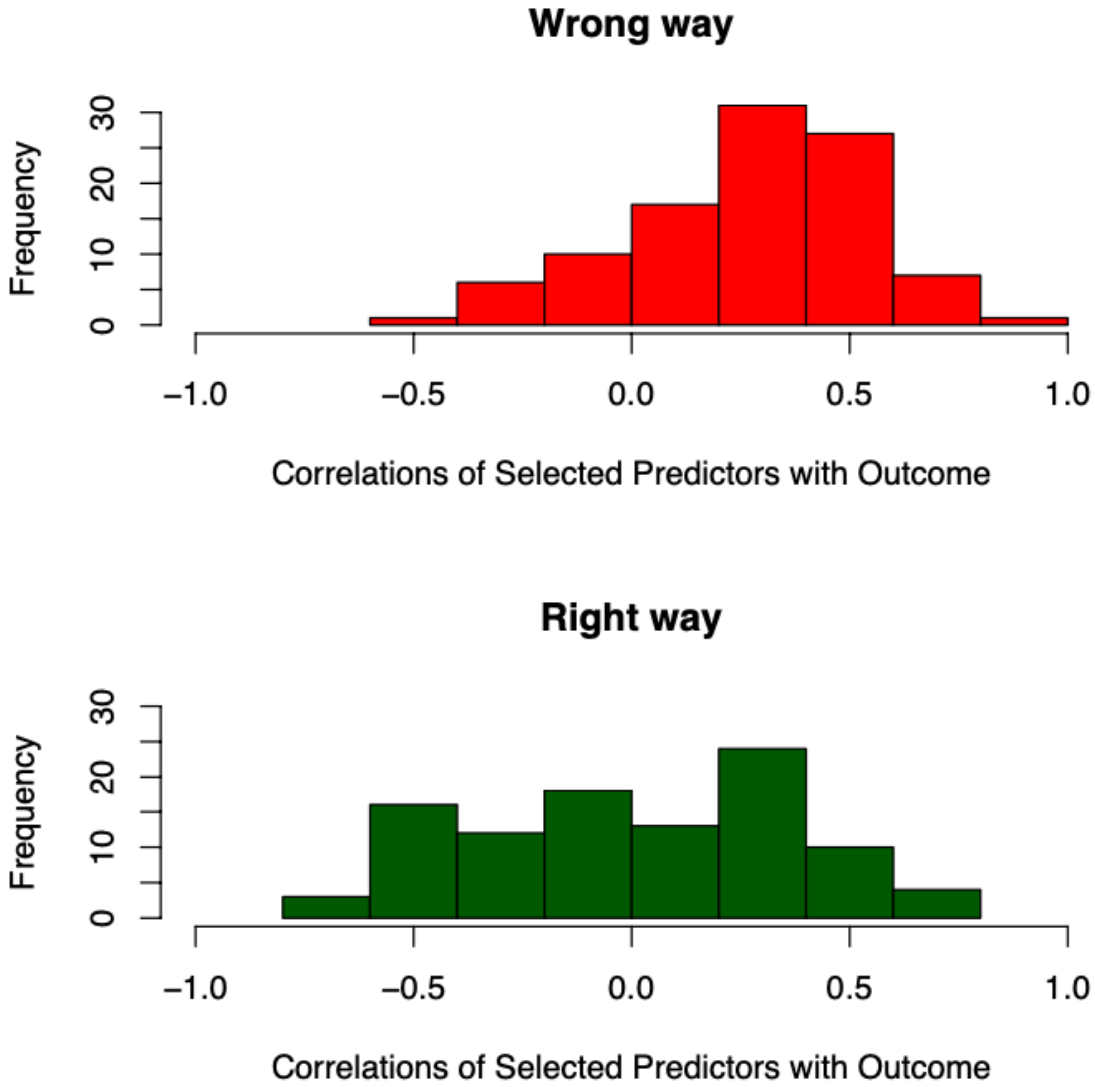

Figure 4: Cross-validation the wrong and right way: histograms shows the correlation of class labels, in 10 randomly chosen samples, with the 100 predictors chosen using the incorrect (upper red) and correct (lower **green**) versions of cross-validation [Hastie et al., 2009, Figure 7.5].

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Cross-Validation in multistep modeling procedure

- In multistep modeling procedure, cross-validation must be applied to the entire sequence of modeling steps.
- Samples must be "left out" before any selection or filtering steps are applied.
- Exceptional case: **Initial unsupervised screening steps can be done before samples are left out**.
  For example, we could select the 1000 predictors with highest variance across all 50 samples (using PCA & PCR as in CM4), before starting cross-validation.

❓ **BUT WHY**:

[9] Ambroise, C. and McLachlan, G. (2002). "Selection bias in gene extraction on the basis of microarray gene-expression data", Proceedings of the National Academy of Sciences.

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  For example, we could select the 1000 predictors with highest variance across all 50 samples (using PCA & PCR as in CM4), before starting cross-validation.
- **BUT WHY**: Since this filtering does not involve the class labels, it does not give the predictors an unfair advantage. See Ambroise and McLachlan (2002)[9] for a detailed discussion of this issue.

[9] Ambroise, C. and McLachlan, G. (2002). "Selection bias in gene extraction on the basis of microarray gene-expression data", Proceedings of the National Academy of Sciences.

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Previous episode: methods for linear model selection and regularization

Subset Selection: by best subset or stepwise selection of $\mathcal{P} \equiv$ all possible subset models of P predictors, $\text{card}(\mathcal{P}) = 2^P$.

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1. **Dimension Reduction:** project the P predictors into a lower dimensional subspace, *e.g.*, principal components regression, partial least squares. (In CM4, we learned how to do this).

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Previous episode: methods for linear model selection and regularization

3. **Shrinkage Methods:**
   - **Fit a model involving all P predictors**, using a technique that **constrains** or **regularizes** the coefficient estimates, or equivalently, that the **estimated coefficients are shrunken towards zero**.

[11] Hoerl, A. E., & Kennard, R. W. (1970). "Ridge Regression: Biased Estimation for Nonorthogonal Problems", Technometrics.

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   Not immediately obvious why such a constraint should improve the fit.

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The two best-known techniques: ridge regression[11] and Lasso [12] [13].

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- We now explore a class of approaches that transform the predictors and then fit a least squares model using the transformed variables. We will refer to these techniques as dimension reduction methods.

Dimension reduction methods: details

- Let $Z_1, \ldots, Z_Q$ represent $Q < P$ linear combinations of our original predictors. That is, for each $q \in [Q]$, it holds that

$$Z_q = \sum_{p=1}^{P} W_{qp} X_p, \text{ for some matrices } \mathbf{W} \equiv (W_{qp})_{q \in [Q], p \in [P]}. \tag{6}$$

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- Via using OLS, we can then fit the following linear regression model

$$y_n = \gamma_0 + \sum_{q=1}^{Q} \gamma_q z_{nq} + \epsilon_n, n \in [N], \quad \boldsymbol{\gamma} = (\gamma_0, \gamma_1, \ldots, \gamma_Q)$$

$$= \gamma_0 + \sum_{q=1}^{Q} \gamma_q \sum_{p=1}^{P} W_{qp} X_p + \epsilon_n = \gamma_0 + \sum_{p=1}^{P} \underbrace{\sum_{q=1}^{Q} \gamma_q W_{qp}}_{\beta_p} X_p + \epsilon_n. \tag{7}$$

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If $\mathbf{W}$ are chosen wisely, *e.g.*, using PCA from CM4 to have Principal Components Regression, then such dimension reduction approaches can often outperform OLS regression!

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An application to the credit data

- **Description:** the response is balance (average credit card debt for 400 individuals) and there are 6 quantitative predictors: income (in thousands of dollars), limit (credit limit), rating (credit rating), cards (number of credit cards), age, education (years of education), and 4 qualitative variables: own (house ownership), student (student status), married (Yes or No), and region (East, West or South). [James et al., 2021, Section 3.3].

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- **Goal:** develop an accurate model that can be used to **predict balance** on the basis of 10 predictors $\leftarrow$ Using glmnet package in $\boldsymbol{R}$.

```
> head(Credit)                                                          Y
  Income Limit Rating Cards Age Education Own Student Married Region Balance
1 14.891  3606    283     2  34        11  No      No     Yes  South     333
2 106.025 6645    483     3  82        15 Yes     Yes     Yes   West     903
3 104.593 7075    514     4  71        11  No      No      No   West     580
4 148.924 9504    681     3  36        11 Yes     No      No   West     964
5 55.882  4897    357     2  68        16  No      No     Yes  South     331
6 80.180  8047    569     4  77        10  No      No      No  South    1151
```

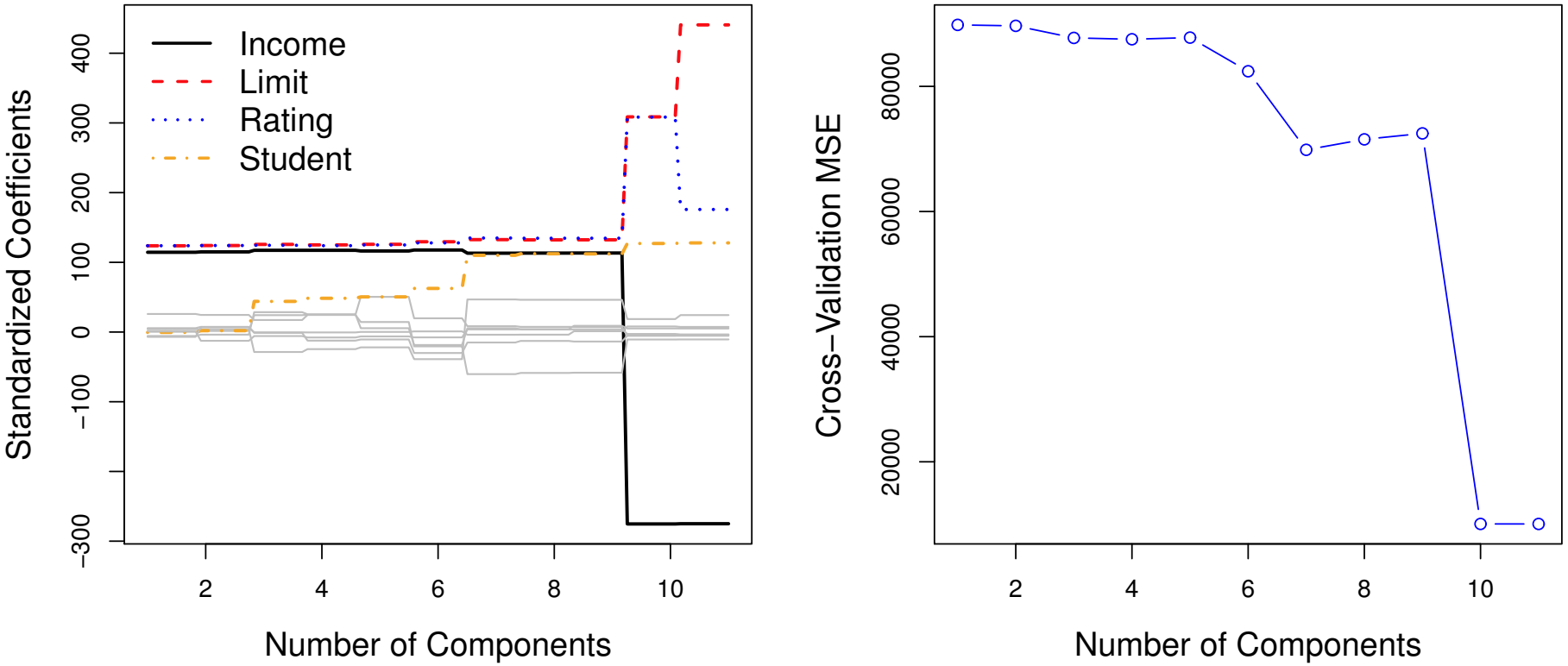

Figure 5: **Choosing the number of directions Q via cross-validation** on the Credit data. Left: PCR standardized coefficient estimates on the Credit data set for different values of Q. Right: The ten-fold cross-validation MSE obtained using PCR, as a function of Q [James et al., 2021, Figure 6.20].

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- **Description:** represent the correlation between the **level of prostate specific antigen** (PSA) and a number of **clinical measures**, in 97 men who were about to receive a radical prostatectomy[14].

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An application to the prostate cancer

- **Description:** represent the correlation between the **level of prostate specific antigen** (PSA) and a number of **clinical measures**, in 97 men who were about to receive a radical prostatectomy[14].
- **Goal:** predict the log of PSA (lpsa) from a number of measurements including log cancer volume (lcavol), log prostate weight (lweight), age, log of benign prostatic hyperplasia amount (lbph), seminal vesicle invasion (svi), log of capsular penetration (lcp), Gleason score (gleason), and percent of Gleason scores 4 or 5 (pgg45).

```
> head(df)
     lcavol  lweight age      lbph svi       lcp gleason pgg45       lpsa
1 -0.5798185 2.769459  50 -1.386294   0 -1.386294       6     0 -0.4307829
2 -0.9942523 3.319626  58 -1.386294   0 -1.386294       6     0 -0.1625189
3 -0.5108256 2.691243  74 -1.386294   0 -1.386294       7    20 -0.1625189
4 -1.2039728 3.282789  58 -1.386294   0 -1.386294       6     0 -0.1625189
5  0.7514161 3.432373  62 -1.386294   0 -1.386294       6     0  0.3715636
6 -1.0498221 3.228826  50 -1.386294   0 -1.386294       6     0  0.7654678
```

[14] Stamey et al. (1989). "Prostate specific antigen in the diagnosis and treatment of adenocarcinoma of the prostate II radical prostatectomy treated patients", Journal of Urology.

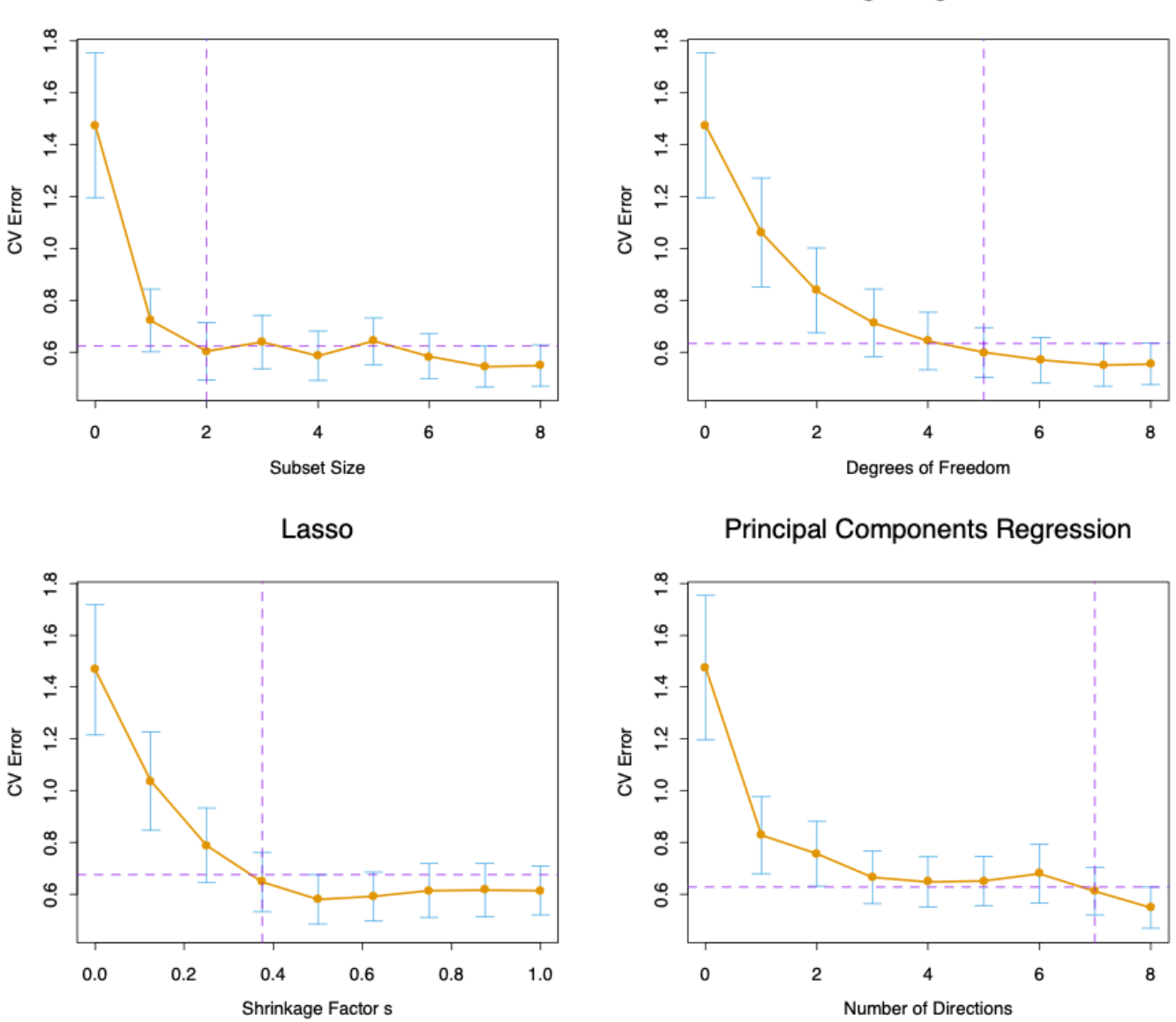


Figure 6: **Estimated prediction error curves and their standard errors for the various selection and shrinkage methods** on the Prostate Cancer data. The estimates of prediction error and their standard errors were obtained by 10-folds cross-validation. [Hastie et al., 2009, Figure 3.7].

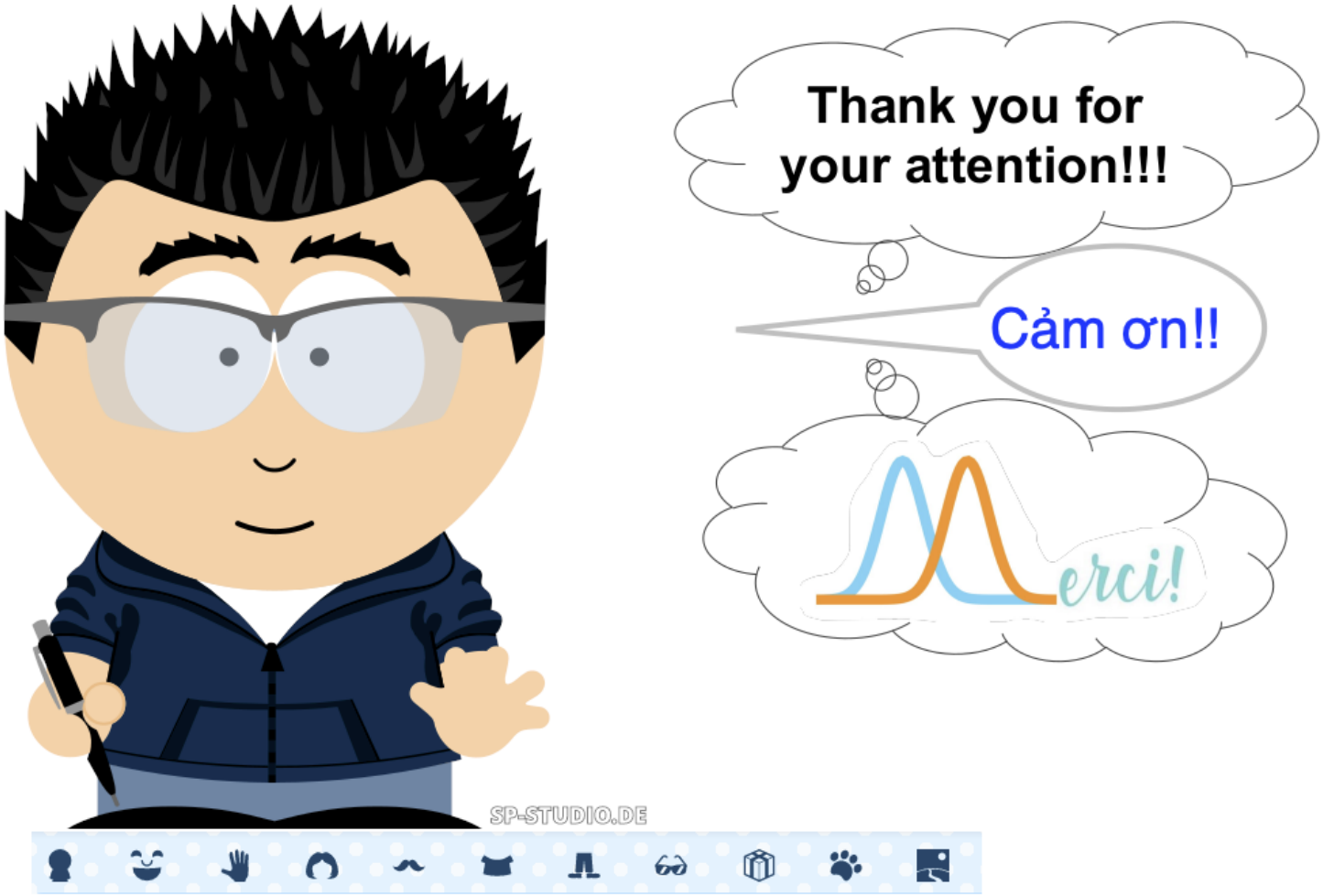
Term	LS	Best Subset	Ridge	Lasso	PCR	PLS
Intercept	2.465	2.477	2.452	2.468	2.497	2.452
lcavol	0.680	0.740	0.420	0.533	0.543	0.419
lweight	0.263	0.316	0.238	0.169	0.289	0.344
age	−0.141		−0.046		−0.152	−0.026
lbph	0.210		0.162	0.002	0.214	0.220
svi	0.305		0.227	0.094	0.315	0.243
lcp	−0.288		0.000		−0.051	0.079
gleason	−0.021		0.040		0.232	0.011
pgg45	0.267		0.133		−0.056	0.084
Test Error	0.521	0.492	0.492	0.479	0.449	0.528
Std Error	0.179	0.143	0.165	0.164	0.105	0.152

Figure 7: Estimated coefficients and test error results, for different subset and shrinkage methods applied to the prostate data. The blank entries correspond to variables omitted [Hastie et al., 2009, Table 3.3].

Each method has a **complexity parameter**, and this was chosen to minimize an estimate of prediction error based on **model selection criteria, *e.g.,*** 10-**folds cross-validation.**

Original data (97) = training set (67, cross-validation) + test set (30, juge performance of the selected model).

"Essentially, all models are wrong, but some are useful".[15]



⬆ This is my best data-driven model to approximate myself.

[15] Box, G. E.P. (1979). "Robustness in the strategy of scientific model building". In Robustness in Statistics (pp. 201-236). Academic Press.

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(Cited on pages 58, 59, 60, 61, 62, 71, 98, and 99.)

James, G., Witten, D., Hastie, T., & Tibshirani, R. (2021). *An Introduction to Statistical Learning: with Applications in R*, volume 2 of *Springer Texts in Statistics*. Springer.

(Cited on pages 27, 69, 70, 92, 93, and 94.)