#### Cross-Validation and Dimension Reduction Methods

#### TrungTin Nguyen

STATIFY team, Inria centre at the University Grenoble Alpes, France











#### **Statistical Analysis and Document Mining**

Complementary Course, Master of Applied Mathematics in Grenoble

- 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

- 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
- 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

## Previous episode: Training error versus test error

- The training error can be easily calculated by applying the statistical learning method to the observations used in its training.
- In contrast, the test error is the average error that results from using a statistical learning method to predict the response on a new observation, one that was not used in training the method.
- ★ The training error rate often is quite different from the test error rate, and in particular the former can dramatically underestimate the latter.
- **?** Not clear enough for you?
- In the next slide we will discuss this in more detail?

- 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
- 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

## Test error in linear regression

- We are given a training dataset  $\mathcal{D} \equiv \{(\mathbf{x}_n, y_n)\}_{n \in [N]}, [N] \equiv 1, \dots, N$ , i.i.d. sampled from the true (but unknown) joint PDF of  $(\mathbf{X}, Y)$ .
- ightharpoonup Given any error term  $\epsilon$ , multiple linear regression function takes the form

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

**Training error:** using ordinary least squares (OLS), we obtain coefficient estimates  $\widehat{\beta}$  and  $\widehat{r}_{\mathcal{D}}(\mathbf{x}_n) \equiv \widehat{\beta}_0 + \sum_{p=1}^P \widehat{\beta}_p \mathbf{x}_{np}$  such that  $\forall n \in [N]$ ,

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

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

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

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

- 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
- 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

# Previous episode: the general model selection paradigm

- Model selection problem: let  $(S_m)_{m \in \mathcal{M}}$  be a family of models. For every  $m \in \mathcal{M}$ , let  $\widehat{s}_m(\mathcal{D}_N)$  be a minimum contrast estimator, e.g., least-squares contrast in LS, over  $S_m$ .  $\textcircled{\bullet}$ Our goal is to choose the best data-driven model  $\widehat{m} \equiv \widehat{m}(\mathcal{D}_N) \in \mathcal{M}$  from data.
- Some model selection criteria:
  - **1** Asymptotic approach: Mallows's  $C_p^1$ , Akaike information criterion<sup>2</sup> (AIC), Bayesian information criterion<sup>3</sup> (BIC): no finite sample guarantees.
  - Cross-validation procedures: 4 5 6 K-Fold, leave-one-out.
    - Non-asymptotic approach: **slope heuristic**<sup>7 8</sup>, which is particularly useful for high-dimensional small data sets, e.g.,  $N \ll P$ .

 $<sup>^{1}</sup>$ Mallows, C. L. (1973). "Some Comments on  $C_{P}$ ". Technometrics.

<sup>&</sup>lt;sup>2</sup>Akaike, H. (1974). "A new look at the statistical model identification". IEEE Transactions on Automatic Control.

<sup>&</sup>lt;sup>3</sup>Schwarz, G. (1978). "Estimating the dimension of a model". The Annals of Statistics.

<sup>&</sup>lt;sup>4</sup>Stone, M. (1974). "Cross-validatory choice and assessment of statistical predictions". JRSSSB.

<sup>&</sup>lt;sup>5</sup>Geisser, S. (1975). "The predictive sample reuse method with applications". J. Amer. Statist. Assoc.

<sup>&</sup>lt;sup>6</sup> Arlot, S., & Celisse, A. (2010). "A survey of cross-validation procedures for model selection". Statist. Surv.

<sup>&</sup>lt;sup>7</sup>Birgé, L. and Massart, P. (2007). "Minimal penalties for Gaussian model selection". Probability Theory and Related Fields.

<sup>&</sup>lt;sup>8</sup> Nguyen, T., Nguyen, H. D., Chamroukhi, F., & Forbes, F. (2022). "A non-asymptotic approach for model selection via penalization in high-dimensional mixture of experts models". Electronic Journal of Statistics.

- 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
- 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
- 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

#### K-Fold cross-validation

- **► Widely used approach** for estimating test error  $\mathcal{L}(\hat{r}_{\mathcal{D}})$ .
  - **1** Idea is to randomly divide the data  $\mathcal{D}$  into K parts.
  - ② We leave out part k, fit the model to the other K-1 parts (combined).
  - We obtain predictions for the left-out kth part.
  - **1** This is done in turn for each part  $k \in [K]$  and then the results are combined.
- Estimates can be used to select best model, and to give an idea of the test error of the final chosen model.

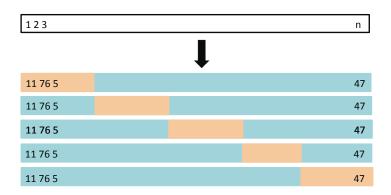


Figure 1: A schematic display of 5-fold CV. A set of *N* observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting estimates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

## K-Fold cross-validation for linear regression in detail

- 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  $N_k = N/K$ .
- ② For each  $k \in [K]$ , fit a model  $\hat{r}^{(-k)}(\mathbf{x}, \mathbf{m})$ , indexed by a tuning parameter (or a model)  $\mathbf{m} \in \mathcal{M}$ , on all samples from the training set except those in the kth fold.
- **3** Estimating test error  $\mathcal{L}(\hat{r}_{\mathcal{D}})$  via averaging the final resulting MSE estimates

$$\mathcal{L}(\widehat{r}_{\mathcal{D}}) \approx \underbrace{\frac{1}{K} \sum_{k=1}^{K}}_{\text{average over } K \text{ folds}} \underbrace{\left[ \frac{1}{N_k} \sum_{n \in \mathcal{D}_k} \left( y_n - \widehat{r}^{(-k)}(\mathbf{x}_n) \right)^2 \right]}_{\text{Estimate test error for each fold}} \equiv \mathsf{CV}(\widehat{r}, K, \mathbf{m}).$$

● Best data-driven model:  $\widehat{\mathbf{m}} \equiv \operatorname{argmin}_{\mathbf{m} \in \mathcal{M}} \operatorname{CV}(\widehat{r}, K, \mathbf{m})$ . K = ? Setting K = N yields N-fold or leave-one out cross-validation (LOOCV, **high variance**). A common better choice K = 5 or 10.

- 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
- 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
- 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

- 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
- 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

## Test error in binary classification: more details in CM5

- We are given a training dataset  $\mathcal{D} \equiv \{(\mathbf{x}_n, y_n)\}_{n \in [N]}, \ y_{[N]} \in [2] \equiv \mathcal{C},$  i.i.d. sampled from the true (but unknown) joint PDF of  $(\mathbf{X}, Y)$ .
- ? How to model relationship between  $p_c(\mathbf{X}) = \mathbb{P}(Y = c | \mathbf{X}), c \in \mathcal{C}$ , and  $\mathbf{X}$ ?
- ... The multiple logistic regression (MLR) takes the form  $p_2(\mathbf{X}) = 1 p_1(\mathbf{X})$ , where

$$\log\left(\frac{p_{1}(\mathbf{X})}{1-p_{1}(\mathbf{X})}\right) = \beta_{0} + \sum_{p=1}^{P} \beta_{p} X_{p}, \text{ or } p_{1}(\mathbf{X}) = \frac{\exp(\beta_{0} + \sum_{p=1}^{P} \beta_{p} X_{p})}{1 + \exp(\beta_{0} + \sum_{p=1}^{P} \beta_{p} X_{p})}.$$

**Training error:** using non-linear LS or maximum likelihood estimation (MLE), we obtain  $\widehat{\beta}$  and  $\widehat{r}_{\mathcal{D}}(\mathbf{x}_n) = \operatorname{argmax}_{c \in \mathcal{C}} p_c(\mathbf{x}_n)$  such that  $\forall n \in [N]$ ,

$$y_n \approx \hat{r}_{\mathcal{D}}(\mathbf{x}_n)$$
, or equivalent,  $\mathcal{L}(\hat{r}_{\mathcal{D}}, \mathcal{D}) \equiv \frac{1}{N} \sum_{n=1}^{N} \mathbb{1} \left[ y_n \neq \hat{r}_{\mathcal{D}}(\mathbf{x}_n) \right] \approx 0.$  (4)

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

$$y^* pprox \widehat{r}_{\mathcal{D}}(\mathbf{x}^*)$$
, or equivalent,  $\mathcal{L}(\widehat{r}_{\mathcal{D}}) \equiv \mathbb{E}_{\mathbf{X},Y} \left[\mathbb{1}\left(Y 
eq \widehat{r}_{\mathcal{D}}(\mathbf{X})\right)\right] pprox 0$ ?

8/26

TrungTin Nguyen CV and Dimension Reduction Methods February 28, 2023

- 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
- 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
- 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

## Cross-Validation for classification problems

- 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  $N_k = N/K$ .
- ② For each  $k \in [K]$ , fit a model  $\hat{r}^{(-k)}(\mathbf{x}, \mathbf{m})$ , indexed by a tuning parameter (or a model)  $\mathbf{m} \in \mathcal{M}$ , on all samples from the training set except those in the kth fold.
- **3** Estimating test error  $\mathcal{L}(\hat{r}_{\mathcal{D}})$  via averaging the final resulting MSE estimates

$$\mathcal{L}(\widehat{r}_{\mathcal{D}}) \approx \underbrace{\frac{1}{K} \sum_{k=1}^{K}}_{\text{average over } K \text{ folds}} \underbrace{\left[ \frac{1}{N_k} \sum_{n \in \mathcal{D}_k} \mathbb{1}\left(y_n \neq \widehat{r}^{(-k)}(\mathbf{x}_n)\right)\right]}_{\text{Estimate test error for each fold}} \equiv \text{CV}(\widehat{r}, K, \mathbf{m}).$$

● Best data-driven model:  $\widehat{\mathbf{m}} \equiv \operatorname{argmin}_{\mathbf{m} \in \mathcal{M}} \operatorname{CV}(\widehat{r}, K, \mathbf{m})$ . K = ? Setting K = N yields N-fold or leave-one out cross-validation (LOOCV, **high variance**). A common better choice K = 5 or 10.

# Cross-Validation: right and wrong

Consider a simple classifier applied to some two-class data with a large number of 5000 predictors and a small number of 50 samples. This may arise in genetics (TP2-TP3) or proteomic applications, for example.

How do we estimate the test set performance of this classifier?

The **right way** to do cross-validation:

- Screen the predictors: find a subset of "good" predictors that show fairly strong (univariate) correlation with the class labels.
- Using just this subset of predictors, build a multivariate classifier, e.g., MLR.
- Use cross-validation to estimate the unknown tuning parameters m and to estimate the prediction error, e.g.,  $CV(\hat{r}, K, \hat{\mathbf{m}})$ , of the final model.

Wait! Is this a correct application of cross-validation? Can we apply cross-validation in step 2, forgetting about step 1? 🛖 NO!

- 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
- 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
- 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

# Cross-Validation: right and wrong

#### The wrong way to do cross-validation:

- Screen the predictors: find a subset of "good" predictors that show fairly strong (univariate) correlation with the class labels.
- ② Using just this subset of predictors, build a multivariate classifier.
- Use cross-validation to estimate the unknown tuning parameters m and to estimate the prediction error of the final model.

#### **8** BUT why:

- We can simulate realistic data with the class labels independent of the outcome, so that true test error =50%, but the CV error estimate that ignores Step 1 is almost zero! What has happened?
- 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].

## The **right way** to do cross-validation

- Divide the samples into K cross-validation folds (groups) at random.
- 2 For each fold k = 1, ..., K:
  - Screen the predictors: find a subset of "good" predictors that show fairly strong (univariate) correlation with the class labels, using all of the samples except those in fold k.
  - Using just this subset of predictors, build a multivariate classifier, using all of the samples except those in fold k.
  - lacktriangle Use the classifier to predict the class labels for the samples in fold k.
- The error estimates from step 2(c) are then accumulated over all K folds, to produce the cross-validation estimate of prediction error CV(r̂, K, m) for each model m ∈ M.
- **3** Best data-driven model:  $\widehat{\mathbf{m}} \equiv \operatorname{argmin}_{\mathbf{m} \in \mathcal{M}} \operatorname{CV}(\widehat{r}, K, \mathbf{m})$  leads to the prediction error, e.g.,  $\operatorname{CV}(\widehat{r}, K, \widehat{\mathbf{m}})$ , of the final model.

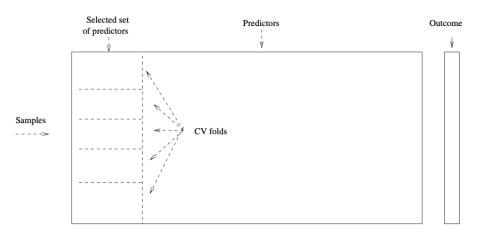


Figure 2: Cross-validation: the wrong path diagram [James et al., 2021, Figure 7.5].

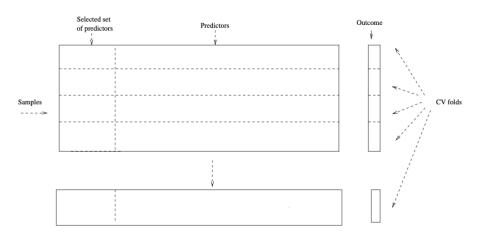
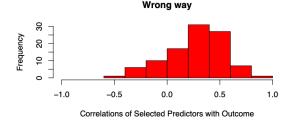


Figure 3: Cross-validation: the true path diagram [James et al., 2021, Figure 7.5].



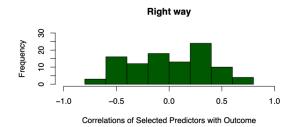


Figure 4: Cross-validation the wrong and right way: histograms shows the correlation of class labels, in 10 randomly chosen samples, with the 100 predictors chosen using the incorrect (upper red) and correct (lower green) versions of cross-validation [Hastie et al., 2009, Figure 7.5].

- 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
- 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
- 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

## 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.
- **3 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)<sup>9</sup> for a detailed discussion of this issue.

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.

- 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

- 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

# 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,  $card(\mathcal{P}) = 2^{P}$ .

- **•** Define a suitable collection of model  $\mathcal{M} = \{m : m \in \mathcal{P}\} \subset \mathcal{P}$  and fit models using LS, maximum likelihood estimation (MLE) or method of moments<sup>10</sup>.
- ② Identify the best model m∈ M via suitable model selection criteria. (Pedro talked about this in CM3).
- **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).

<sup>&</sup>lt;sup>10</sup> Pearson, K (1894). "Contributions to the mathematical theory of evolution". Philosophical Transactions of the Royal Society of London.

# Previous episode: methods for linear model selection and regularization

#### 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.
- Not immediately obvious why such a constraint should improve the fit.
- **This shrinkage (also known as regularization)** has the effect of reducing variance and can also perform variable selection.
- The two best-known techniques: ridge regression<sup>11</sup> and Lasso <sup>12</sup> <sup>13</sup>.

<sup>&</sup>lt;sup>11</sup>Hoerl, A. E., & Kennard, R. W. (1970). "Ridge Regression: Biased Estimation for Nonorthogonal Problems", Technometrics.

 $<sup>^{12}</sup>$ Tibshirani, R. (1996). "Regression Shrinkage and Selection via the lasso". JRSS. Series B.

 $<sup>^{13}</sup>$ Santosa, F., & Symes, W. W. (1986). "Linear inversion of band-limited reflection seismograms". SIAM journal on scientific and statistical computing.

- 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

#### Dimension reduction methods

- The methods that we have discussed so far in this chapter have involved fitting linear regression models, via least squares or a shrunken approach, using the **original predictors**,  $X_1, X_2, \ldots, X_P$ .
- 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

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

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

$$y_{n} = \gamma_{0} + \sum_{q=1}^{Q} \gamma_{q} z_{nq} + \epsilon_{n}, n \in [N], \quad \gamma = (\gamma_{0}, \gamma_{1}, \dots, \gamma_{Q})$$

$$= \gamma_{0} + \sum_{q=1}^{Q} \gamma_{q} \sum_{p=1}^{P} W_{qp} X_{p} + \epsilon_{n} = \gamma_{0} + \sum_{p=1}^{P} \sum_{\substack{q=1 \ \beta_{p}}}^{Q} \gamma_{q} W_{qp} X_{p} + \epsilon_{n}.$$

$$(7)$$

Note that in model (7), of as a special case of the original linear regression model via constraining the estimated  $\beta_p$  coefficients  $\stackrel{\bullet}{L}$  win in the bias-variance tradeoff! If 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!

- 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

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

```
> head(Credit)
   Income Limit Rating Cards Age Education Own Student Married Region Balance
   14.891
           3606
                   283
                               34
                                         11
                                             No
                                                      Nο
                                                             Yes
                                                                  South
                                                                             333
2 106.025
          6645
                   483
                               82
                                         15 Yes
                                                     Yes
                                                             Yes
                                                                   West
                                                                             903
3 104.593 7075
                   514
                           4 71
                                         11 No.
                                                                             580
                                                      No
                                                              No
                                                                   West
4 148,924 9504
                   681
                               36
                                                                            964
                                         11 Yes
                                                      No
                                                              No
                                                                   West
   55.882
                                                             Yes
           4897
                   357
                               68
                                         16
                                             No
                                                      No
                                                                  South
                                                                             331
   80.180
           8047
                   569
                               77
                                         10
                                             No
                                                      Nο
                                                              No
                                                                  South
                                                                            1151
```

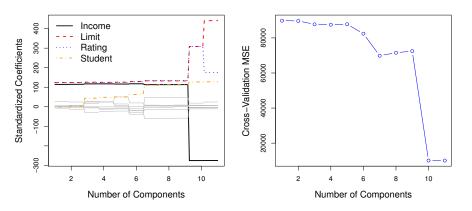


Figure 5: Choosing the number of directions Q via cross-validation on the Credit data. Left: PCR standardized coefficient estimates on the Credit data set for different values of Q. Right: The ten-fold cross-validation MSE obtained using PCR, as a function of Q [James et al., 2021, Figure 6.20].

- 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
- 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

## 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<sup>14</sup>.
- 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)

	nedu(ui)									
	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	

<sup>&</sup>lt;sup>14</sup>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.

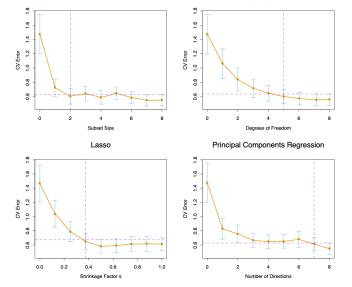


Figure 6: Estimated prediction error curves and their standard errors for the various selection and shrinkage methods on the Prostate Cancer data. The estimates of prediction error and their standard errors were obtained by 10-folds cross-validation. [Hastie et al., 2009, Figure 3.7].

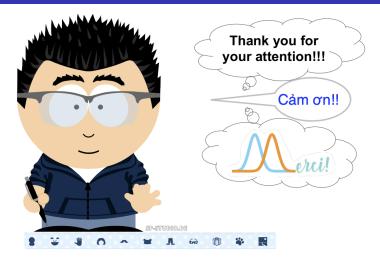
Term	LS	Best Subset	Ridge	Lasso	PCR	PLS
Intercept	2.465	2.477	2.452	2.468	2.497	2.452
lcavol	0.680	0.740	0.420	0.533	0.543	0.419
lweight	0.263	0.316	0.238	0.169	0.289	0.344
age	-0.141		-0.046		-0.152	-0.026
lbph	0.210		0.162	0.002	0.214	0.220
svi	0.305		0.227	0.094	0.315	0.243
lcp	-0.288		0.000		-0.051	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.

 $<sup>^{15}</sup>$ Box, G. E.P. (1979). "Robustness in the strategy of scientific model building". In Robustness in Statistics (pp. 201-236). Academic Press.

#### References



Hastie, T., Tibshirani, R., Friedman, J. H., & Friedman, J. H. (2009). *The elements of statistical learning: data mining, inference, and prediction*, volume 2 of *Springer Texts in Statistics*. Springer.

(Cited on pages 20, 24, 39, and 40.)



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 11, 22, 23, 35, and 36.)