Model Assessment and Selection

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Statistical Analysis and Document Mining

Complementary Course, Master of Applied Mathematics in Grenoble

Outline

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☛ Recall that conditional on $X_{[P]} \equiv (X_1, ..., X_P)$, Y belongs to a certain family of distributions: Gaussian or normal distribution for linear regression, Bernoulli distribution for logistic regression and Poisson distribution for Poisson regression.

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Each approach models the mean of Y as a function of the predictors.

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HOW. $\eta(\mu) = \mu$, $\eta(\mu) = \log(\mu/(1-\mu))$, $\eta(\mu) = \log(\mu)$.

Test error in multinomial logistic regression

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

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- Multinomial logistic regression (LR) takes the form $p_K(\mathbf{X}) = 1 - \sum_{k=1}^{K-1} p_k(\mathbf{X})$, and models the probability that Y belongs to a particular category instead of the value of Y as follows:

$$\log\left(\frac{p_k(\mathbf{X})}{p_K(\mathbf{X})}\right) = \beta_{k0} + \sum_{p=1}^{P} \beta_{kp} x_p.$$

- **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 $\forall n \in [N]$,

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

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

$$y^* \approx \widehat{r}_{\mathcal{D}}(\mathbf{x}^*), \text{ or equivalent, } \mathcal{L}(\widehat{r}_{\mathcal{D}}) \equiv \mathbb{E}_{\mathbf{X},Y}\left[\mathbb{1}\left(Y \neq \widehat{r}_{\mathcal{D}}(\mathbf{X})\right)\right] \approx 0? \quad (2)$$

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   - Choosing the optimal model in subset selection
   - Estimating test error: two approaches
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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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Recall from CM3, in general, it holds that $\mathcal{L}(\widehat{r}_{\mathcal{D}}, \mathcal{D}) \leq \mathcal{L}(\widehat{r}_{\mathcal{D}})$. (5)

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- We wish to choose **a model with low test error, not a model with low training error.** Recall that training error is usually a poor estimate of test error.

Therefore, RSS **and** R^2 **are not suitable for selecting the best model among a collection of models with different numbers of predictors.**

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2. We can directly estimate the test error, using either a validation set approach or a cross-validation approach, as discussed in previous lectures (CM3 and CC4).

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  2. **Non-asymptotic approach: slope heuristic**[4] [5] particularly useful for high-dimensional small data sets, *e.g.,* $N \ll P$.
  3. **Cross-validation procedures:**[6] [7] [8] K-Fold, leave-one-out in CC4.

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2. The next few slides display C_p, AIC, BIC and Adjusted R^2, CV, ridge and Lasso for the best model of each size produced by best subset selection on the Credit data set.

Some details: C_p and AIC

1. Mallow's C_p: estimate of test MSE (unbiased one when and why?) and choosing the model with the lowest C_p value:

$$\mathrm{C_p} = \frac{1}{N}\left[\mathrm{RSS}(p) + 2p\widehat{\sigma}^2\right] \text{ or equivalent?} \frac{\mathrm{RSS}}{\widehat{\sigma}^2} + 2p - N. \tag{6}$$

Here p is the total number of parameters used (*e.g.*, number of predictors) $\widehat{\sigma}^2$ is an estimate of the variance of the error ϵ. Typically $\widehat{\sigma}^2$ is estimated using the full model containing all predictors.

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In the case of the linear model with Gaussian errors, MLE and least squares are the same thing, and $\mathrm{C_p}$ and AIC are equivalent (Prove this?).

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- Since $logN > 2$ for any $N > 7$, the BIC statistic generally places a heavier penalty on models with many variables, and hence results in the selection of smaller models than $\mathrm{C_p}$. To be verified in Figure 1 soon!

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- Unlike the R^2 statistic, the adjusted R^2 statistic pays a price for the inclusion of unnecessary variables in the model. To be verified in Figure 1 soon!

Outline

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What is the rationale for this? If a set of models appear to be more or less equally good, then we might as well choose the simplest model-that is, the model with the smallest number of predictors.

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

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

Previous episode: CV 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 $\widehat{r}^{(-k)}(\mathbf{x}, \mathbf{m})$, 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.
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   $K = ?$ Setting $K = N$ yields N-fold or leave-one out cross-validation (LOOCV, **high variance**). A common better choice $K = 5$ or 10.

Outline

An empirical comparison on 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 ← 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
```

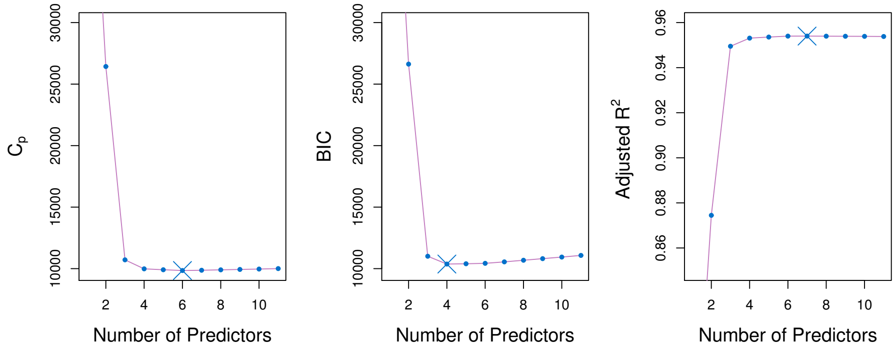

Figure 1: C_p (or AIC), BIC and Adjusted R^2 are shown for the best models of each size for the Credit data set [James et al., 2021, Figure 6.2]. Cp and BIC are estimates of test MSE.

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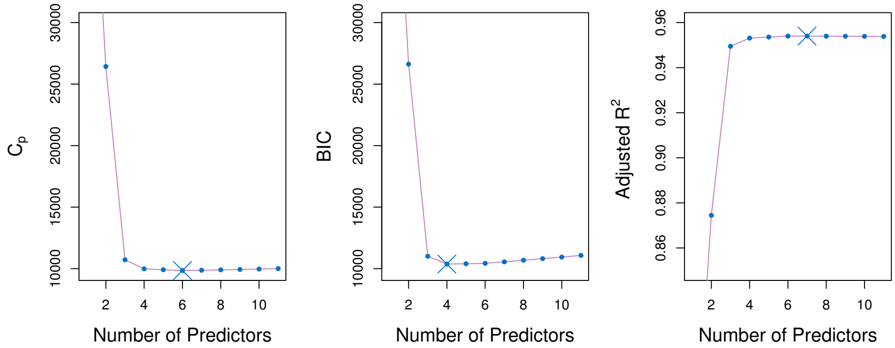

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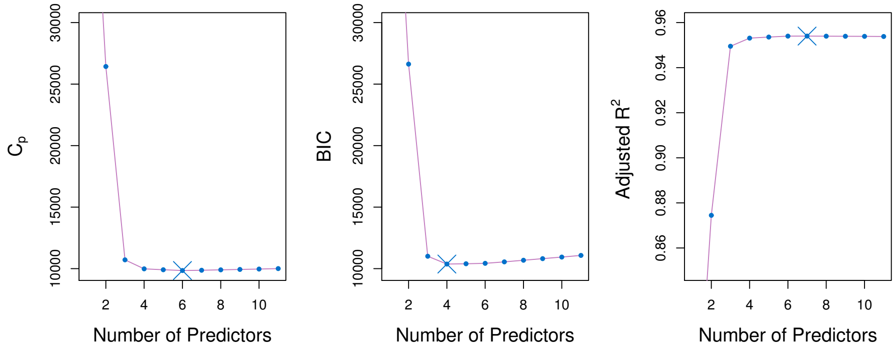

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The other two plots are rather flat after four variables are included.

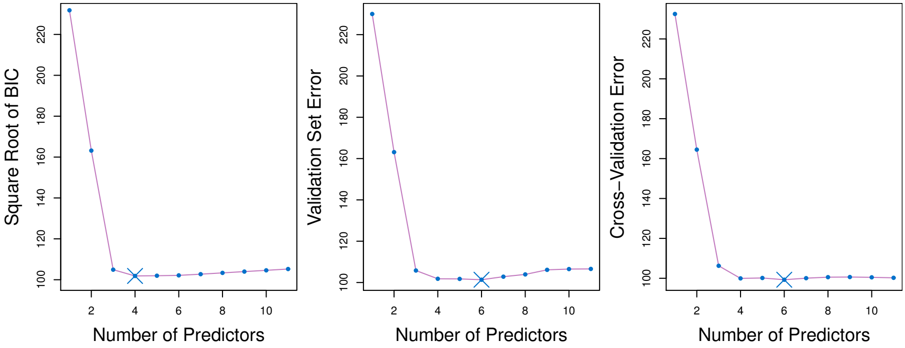

Figure 2: The overall best model, based on each of these quantities, is shown as a blue cross 'x'. [James et al., 2021, Figure 6.3].

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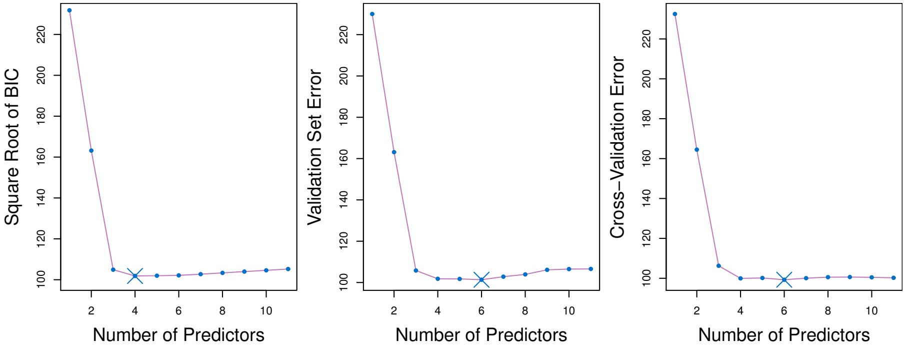

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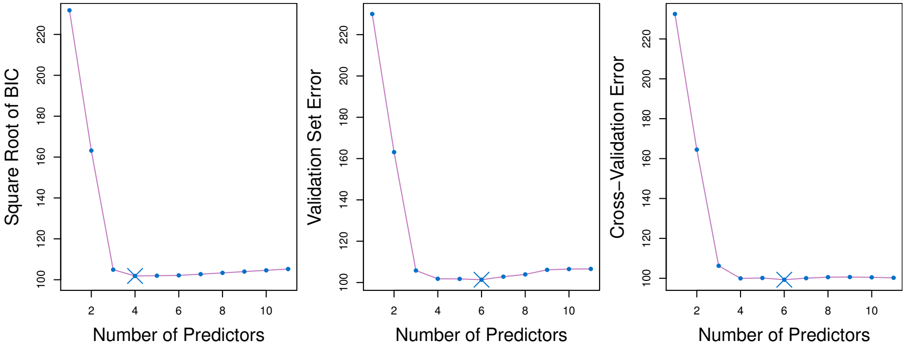
❓ Some comments. . . However, all three approaches suggest that the four-, five-, and six-variable models are roughly equivalent in terms of their test errors.



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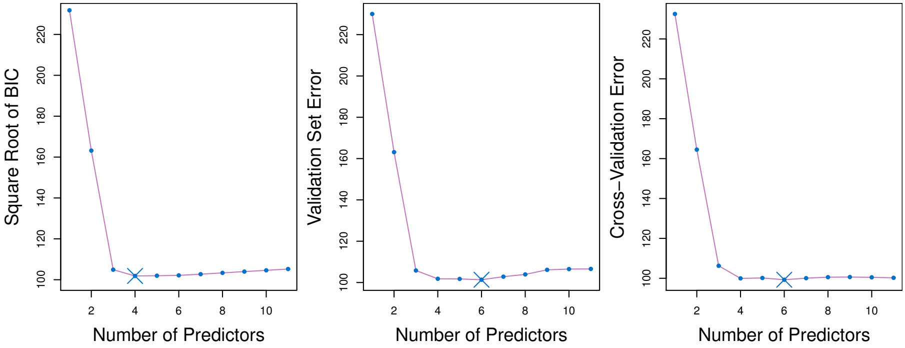

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Applying the one-standard-error rule to the validation set or cross-validation approach? leads to selection of the three-variable model.

In the left-hand panel, each curve corresponds to the ridge regression coefficient estimate for one of the ten variables, plotted as a function of λ.

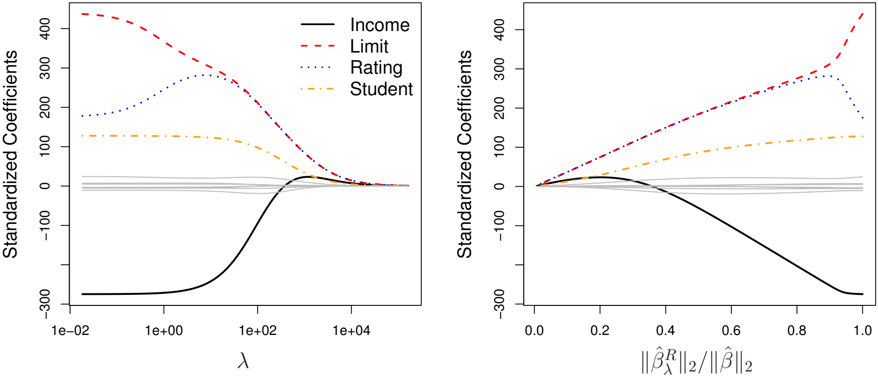

Figure 3: The standardized ridge regression coefficients are displayed for the Credit data set, as a function of λ and $\|\widehat{\beta}_\lambda^{\text{ridge}}\|_2/\|\widehat{\beta}^{\text{ls}}\|_2$ [James et al., 2021, Figure 6.4].

In the right-hand panel, a small value of the x-axis indicates that the ridge regression coefficient estimates have been shrunken very close to zero.

In the left-hand panel, each curve corresponds to the Lasso regression coefficient estimate for one of the ten variables, plotted as a function of λ.

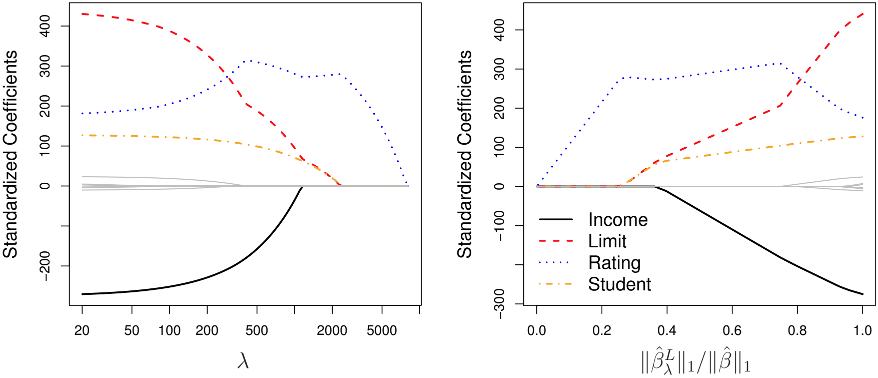

Figure 4: The standardized Lasso coefficients are displayed for the Credit data set, as a function of λ and $\|\widehat{\beta}^{\text{lasso}}_\lambda\|_1/\|\widehat{\beta}^{\text{ls}}\|_1$ [James et al., 2021, Figure 6.6].

In the right-hand panel, a small value of the x-axis indicates that the Lasso regression coefficient estimates have been shrunken to zero.

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   - Generalized linear models
   - Test error in multiple linear regression
   - Choosing the optimal model in subset selection
   - Estimating test error: two approaches
2. Generalized Linear Model Selection and Regularization
   - General model selection paradigm
   - Asymptotic approach: C_p, AIC, BIC and Adjusted R^2
   - Validation and cross-validation
   - An empirical comparison on Credit data
   - Non-asymptotic approach: slope heuristic ...
3. High-Dimensional Setting
   - Previous episode: multiple impact of high-dimensionality on statistics
4. Perspectives

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Multiple impact of high-dimensionality on statistics

1. High-dimensional spaces are vast and data points are isolated in their immensity (CC5).
2. The accumulation of small fluctuations in many different directions can produce a large global fluctuation.
3. An event that is an accumulation of rare events may not be rare.
4. Numerical computations and optimizations in high-dimensional spaces can be overly intensive.

For more details, see [Giraud, 2021, Chapter 1].

Outline

Perspectives

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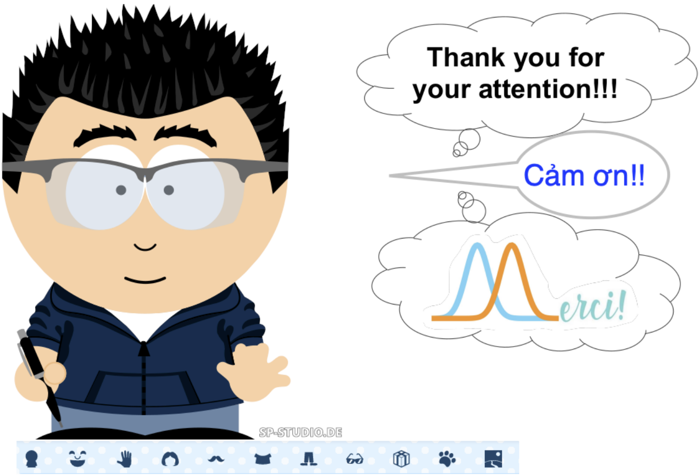
4. $\boxed{\text{Week 11 (25/04/2023):}}$ **Last CC with questions**.

“Essentially, all models are wrong, but some are useful”.[9]



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

[9] 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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