Optimism, Conflicts, and Trade-offs

Data Mining - CdL CLAMSES

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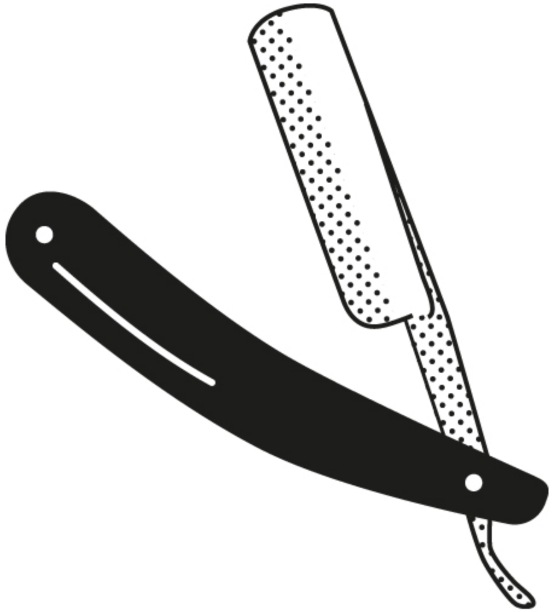


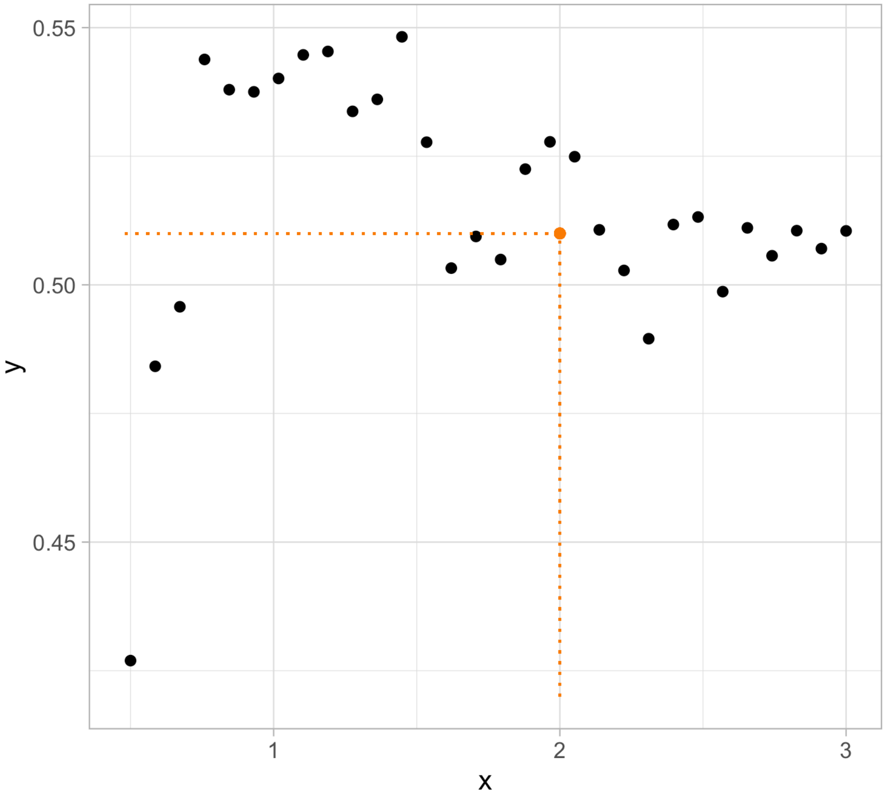
"Pluralitas non est ponenda sine necessitate."

William of Ockham

- This unit will cover the following **topics**:
  - Bias-variance trade-off
  - Cross-validation
  - Information criteria
  - Optimism
- You may have seen these notions before...
- ...but it is worth discussing the **details** of these ideas once again.
- They are indeed the **foundations** of **statistical learning**.

Yesterday's and tomorrow's data

Yesterday's data



- Let us presume that **yesterday** we observed $n = 30$ pairs of data (x_i, y_i).
- Data were generated according to

$$Y_i = f(x_i) + \epsilon_i, \quad i = 1, \dots, n,$$

  with each y_i being the realization of Y_i.
- The $\epsilon_1, \dots, \epsilon_n$ are iid "**error**" terms, such that $\mathbb{E}(\epsilon_i) = 0$ and $\text{var}(\epsilon_i) = \sigma^2 = 10^{-4}$.
- Here $f(x)$ is a regression function (**signal**) that we leave unspecified.
- **Tomorrow** we will get a new x. We wish to **predict** Y using $\mathbb{E}(Y) = f(x)$.

Polynomial regression

- The function $f(x)$ is unknown, therefore, it should be estimated.
- A simple approach is using the tools of Unit A, such as **polynomial regression**:

$$f(x; \beta) = \beta_1 + \beta_2 x + \beta_3 x^2 + \cdots + \beta_p x^{p-1},$$

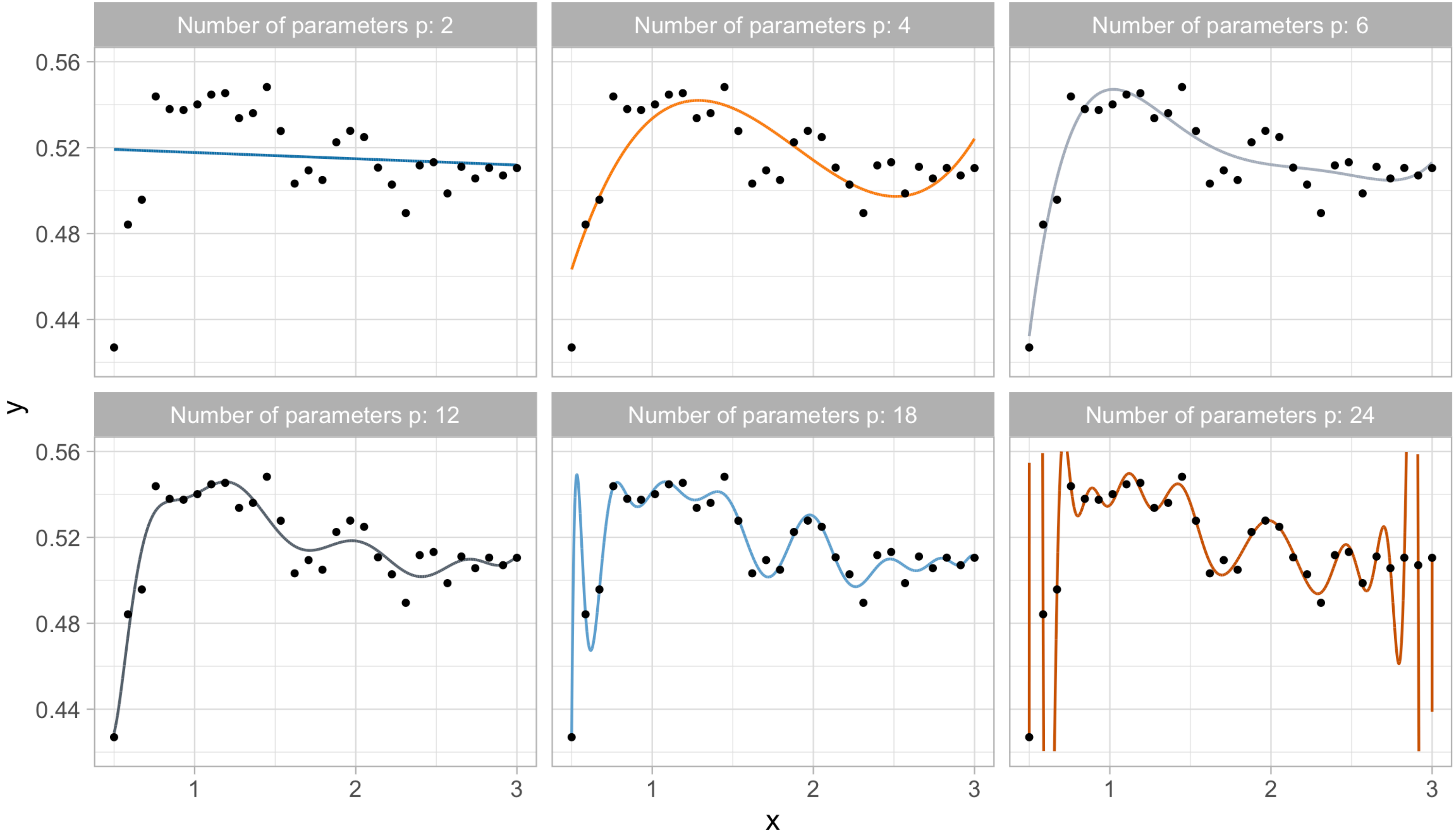
namely $f(x)$ is **approximated** with a polynomial of degree $p - 1$ (i.e., Taylor expansions).

- This model is linear in the parameters: ordinary least squares can be applied.
- How do we choose the **degree of the polynomial** $p - 1$?
- Without clear guidance, in principle, any value of $p \in \{1, \dots, n\}$ could be appropriate.
- Let us compare the **mean squared error** (MSE) on yesterday's data (**training**)

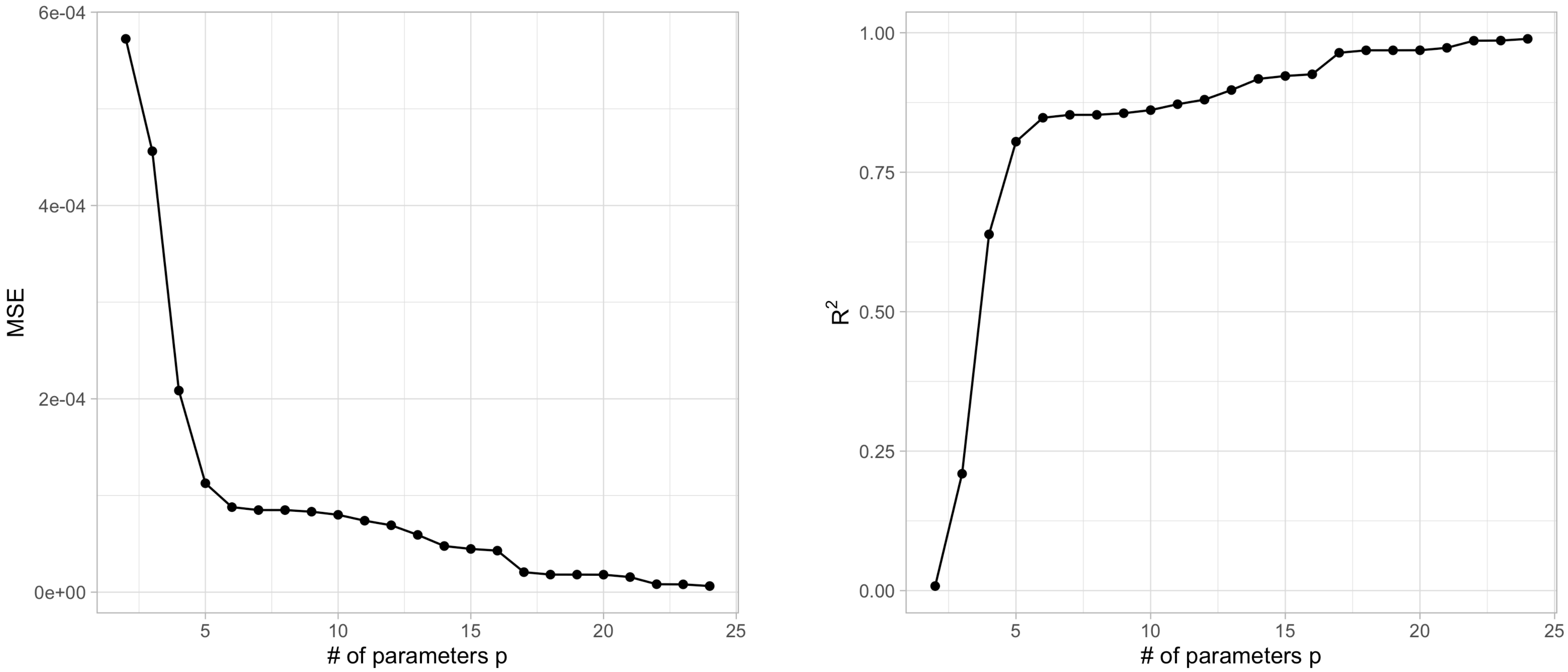
$$\text{MSE}_\text{train} = \frac{1}{n}\sum_{i=1}^{n}\{y_i - f(x_i; \hat{\beta})\}^2,$$

or alternatively R^2_train, for different values of p...

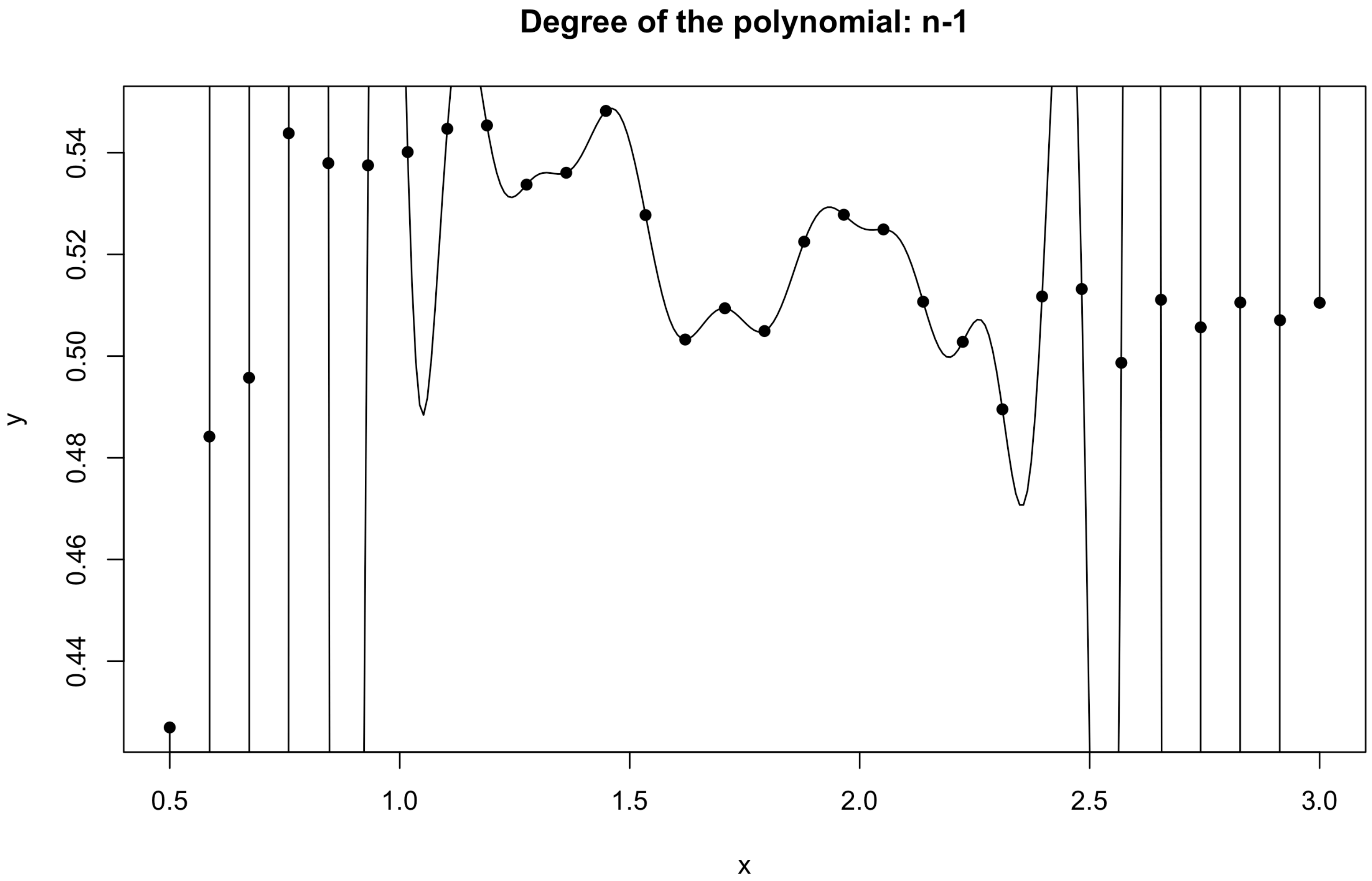
Yesterday's data, polynomial regression



Yesterday’s data, goodness of fit



Yesterday's data, polynomial interpolation ($p = n$)



Yesterday's data, tomorrow's prediction

- The **MSE** decreases as the number of parameter increases; similarly, the R^2 increases as a function of p. It can be **proved** that this **always happens** using ordinary least squares.
- One might be tempted to let p as large as possible to make the model more flexible...
- Taking this reasoning to the extreme would lead to the choice $p = n$, so that

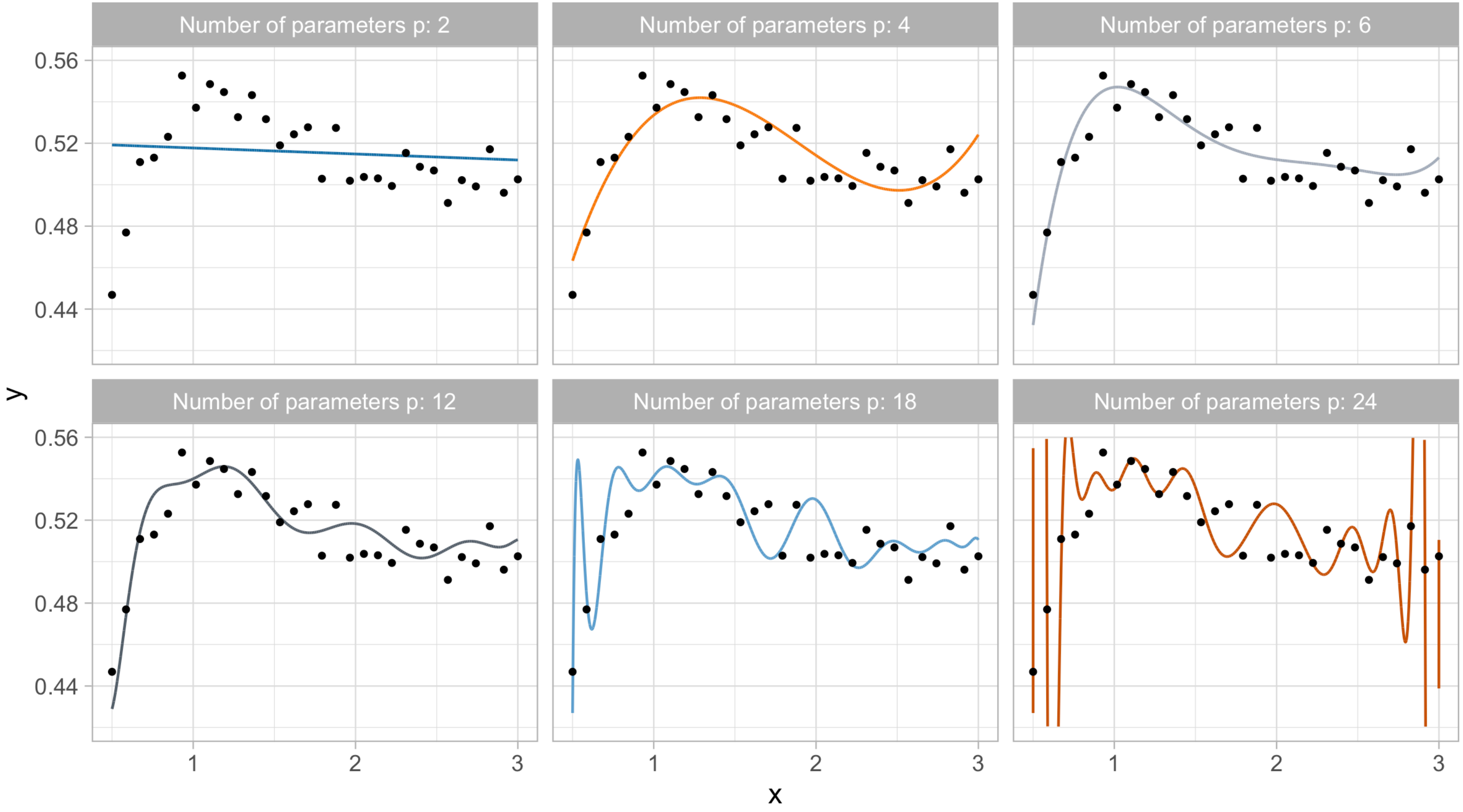
  $$\text{MSE}_\text{train} = 0, \qquad R^2_\text{train} = 1,$$

  i.e., a perfect fit. This procedure is called **interpolation**.
- However, we are **not** interested in predicting **yesterday** data. Our goal is to predict **tomorrow**'s data, i.e. a **new set** of $n = 30$ points:

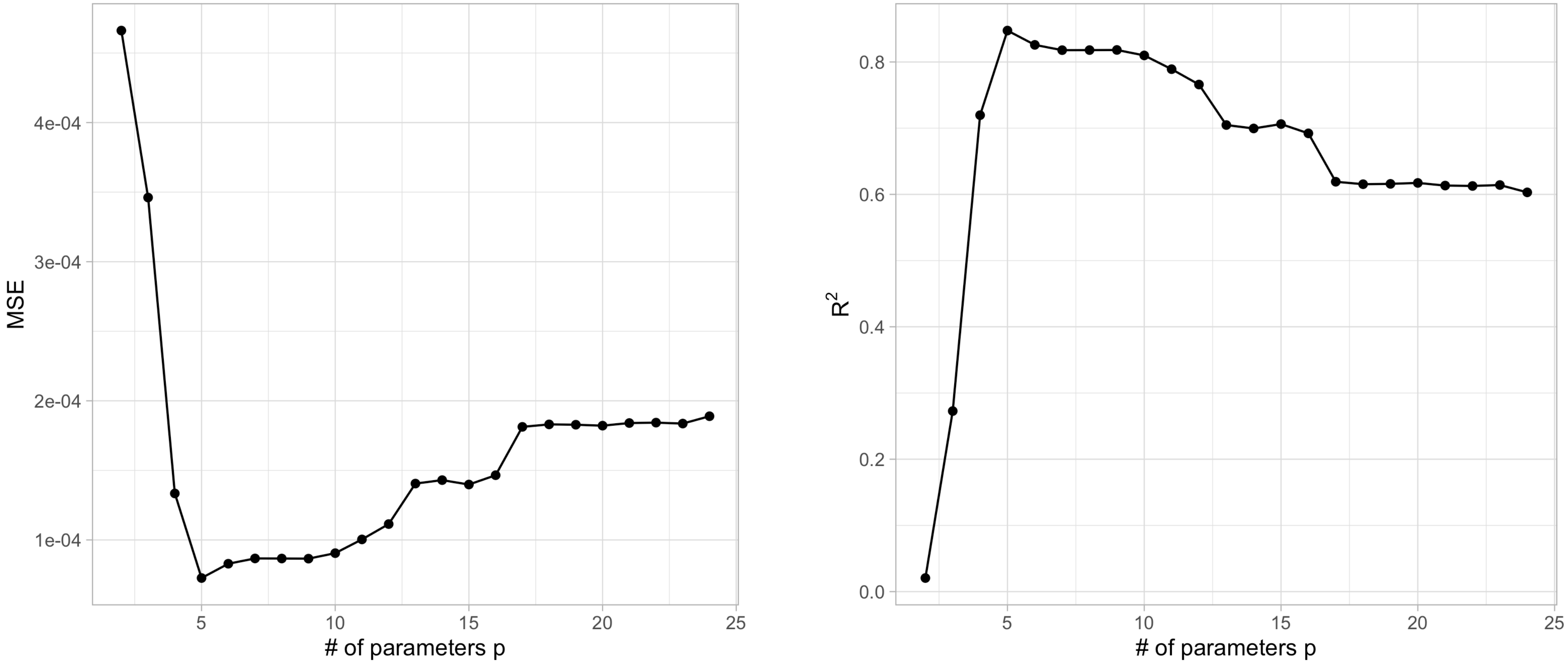
  $$(x_1, \tilde{y}_1), \dots, (x_n, \tilde{y}_n),$$

  using $\hat{y}_i = f(x_i; \hat{\beta})$, where $\hat{\beta}$ is obtained using yesterday's data.
- **Remark**. Tomorrow's r.v. $\tilde{Y}_1, \dots, \tilde{Y}_n$ follow the same scheme as yesterday's data.

Tomorrow’s data, polynomial regression



Tomorrow’s data, goodness of fit



Comments and remarks

- The mean squared error on tomorrow's data (**test**) is defined as

$$\mathrm{MSE}_{\text{test}} = \frac{1}{n}\sum_{i=1}^{n}\{\tilde{y}_i - f(x_i;\hat{\beta})\}^2,$$

  and similarly the R^2_{test}. We would like the $\mathrm{MSE}_{\text{test}}$ to be **as small as possible**.

- For **small values** of p, an increase in the degree of the polynomial **improves the fit**. In other words, at the beginning, both the $\mathrm{MSE}_{\text{train}}$ and the $\mathrm{MSE}_{\text{test}}$ decrease.
- For **larger values** of p, the improvement gradually ceases, and the polynomial follows **random fluctuations** in yesterday's data, which are **not observed** in the **new sample**.
- An over-adaptation to yesterday's data is called **overfitting**, which occurs when the training $\mathrm{MSE}_{\text{train}}$ is low but the test $\mathrm{MSE}_{\text{test}}$ is high.
- Yesterday's dataset is available from the textbook (A&S) website:
  - Dataset http://azzalini.stat.unipd.it/Book-DM/yesterday.dat
  - True $f(\boldsymbol{x})$ http://azzalini.stat.unipd.it/Book-DM/f_true.R

☠️ - Orthogonal polynomials

- When performing polynomial regression, the poly command computes an **orthogonal basis** of the original covariates $(1, x, x^2, \dots, x^{p-1})$ through the QR decomposition:

```
fit <- lm(y.yesterday ~ poly(x, degree = 3, raw = FALSE), data = dataset)
X <- model.matrix(fit)
colnames(X) = c("Intercept","x1","x2","x3")
round(t(X) %*% X, 8)
```

```
          Intercept x1 x2 x3
Intercept        30  0  0  0
x1                0  1  0  0
x2                0  0  1  0
x3                0  0  0  1
```

- Polynomial regression becomes numerically unstable when $p \geq 13$ (`raw = TRUE`, original polynomials) and $p \geq 25$ (`raw = FALSE`, orthogonal polynomials).

☠️ - Lagrange interpolating polynomials

- If the previous code does not work for $p \geq 25$, how was the plot of this slide computed?
- It turns out that for $p = n$ there exists an alternative way of finding the ordinary least square solution, based on Lagrange interpolating polynomials, namely:

$$\hat{f}(x) = \sum_{i=1}^{n} \ell_i(x) y_i, \qquad \ell_i(x) = \prod_{k \neq i} \frac{x - x_k}{x_i - x_k}.$$

- Interpolating polynomials are clearly **unsuitable** for regression purposes, but may have interesting applications in other contexts.

Errors, trade-offs, and optimism

Summary and notation (fixed-X)

- In the previous example, we consider two sets of **random variables**:
  - The **training set** (yesterday) $Y_1, \dots, Y_n$, whose realization is $y_1, \dots, y_n$.
  - The **test set** (tomorrow) $\tilde{Y}_1, \dots, \tilde{Y}_n$, whose realization is $\tilde{y}_1, \dots, \tilde{y}_n$.
- The **covariates** $\boldsymbol{x}_i = (x_{i1}, \dots, x_{ip})^T$ in this scenario are **deterministic**. This is the so-called **fixed-X** design, which is a common assumption in regression models.
- We also assume that the random variables Y_i and $\tilde{Y}_i$ are **independent**.
- In **regression** problems we customarily assume that

$$Y_i = f(\boldsymbol{x}_i) + \epsilon_i, \qquad \tilde{Y}_i = f(\boldsymbol{x}_i) + \tilde{\epsilon}_i, \quad i = 1, \dots, n,$$

  where ϵ_i and $\tilde{\epsilon}_i$ are iid "**error**" terms, with $\mathbb{E}(\epsilon_i) = 0$ and $\text{var}(\epsilon_i) = \sigma^2$.
- In **classification** problems the relationship between $\boldsymbol{x}_i$ and the **Bernoulli** r.v. $Y_i \in \{0, 1\}$ is

$$\mathbb{P}(Y_i = 1) = p(\boldsymbol{x}_i) = g\{f(\boldsymbol{x}_i)\}, \qquad i = 1, \dots, n,$$

  where $g(x) : \mathbb{R} \to (0, 1)$ is monotone transformation, such as the inverse logit.

The in-sample prediction error

- The **training data** is used to estimate a function of the covariates $\hat{f}(\boldsymbol{x}_i)$. We hope our predictions work well on the **test set**.
- A measure of quality for the predictions is the **in-sample prediction error**:

$$\text{ErrF} = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\mathscr{L}\{\tilde{Y}_i; \hat{f}(\boldsymbol{x}_i)\}\right],$$

  where $\mathscr{L}\{\tilde{Y}_i; \hat{f}(\boldsymbol{x}_i)\}$ is a **loss function**. The "**F**" is a reminder of the **f**ixed-X design.
- The expectation is taken with respect to training random variable $Y_1, \dots, Y_n$, implicitly appearing in $\hat{f}(\boldsymbol{x})$, and the new data points $\tilde{Y}_1, \dots, \tilde{Y}_n$.
- The in-sample prediction error is measuring the **average** "discrepancy" between the **new data points** and the corresponding predictions based on the training.

Loss functions

- Examples of loss functions for **regression problems** $Y \in \mathbb{R}$ are:
  - The **quadratic loss** $\mathscr{L}\{\tilde{Y}_i; \hat{f}(\boldsymbol{x}_i)\} = \{\tilde{Y}_i - \hat{f}(\boldsymbol{x}_i)\}^2$, leading to the MSE.
  - The **absolute loss** $\mathscr{L}\{\tilde{Y}_i; \hat{f}(\boldsymbol{x}_i)\} = |\tilde{Y}_i - \hat{f}(\boldsymbol{x}_i)|$, leading to the MAE.
- Examples of loss functions for **binary classification problems** $Y \in \{0, 1\}$ are:
  - The **misclassification loss**, which is defined as

    $$\mathscr{L}\{\tilde{Y}_i; \hat{f}(\boldsymbol{x}_i)\} = \mathbb{I}(\tilde{Y}_i \neq \hat{y}_i).$$

    The predictions are obtained by dichotomizing the probabilities $\hat{y}_i = \mathbb{I}(\hat{p}(\boldsymbol{x}_i) > 1/2)$.
  - The **deviance** or **cross-entropy** loss functions are defined as

    $$\mathscr{L}\{\tilde{Y}_i; \hat{f}(\boldsymbol{x}_i)\} = -2\left[\mathbb{I}(Y_i = 1)\log \hat{p}(\boldsymbol{x}_i) + \mathbb{I}(Y_i = 0)\log\{1 - \hat{p}(\boldsymbol{x}_i)\}\right].$$

Regression under quadratic loss I

Error decomposition (reducible and irreducible)

In a regression problem, under a quadratic loss, **each element** of the **in-sample prediction error** admits the following decomposition

$$\begin{aligned}\mathbb{E}\left[\{\tilde{Y}_i - \hat{f}(\boldsymbol{x}_i)\}^2\right] &= \mathbb{E}\left[\{f(\boldsymbol{x}_i) + \tilde{\epsilon}_i - \hat{f}(\boldsymbol{x}_i)\}^2\right] \\ &= \mathbb{E}\left[\{f(\boldsymbol{x}_i) - \hat{f}(\boldsymbol{x}_i)\}^2\right] + \mathbb{E}(\tilde{\epsilon}_i^2) + 2\,\mathbb{E}\left[\tilde{\epsilon}_i\,\{f(\boldsymbol{x}_i) - \hat{f}(\boldsymbol{x}_i)\}\right] \\ &= \underbrace{\mathbb{E}\left[\{\hat{f}(\boldsymbol{x}_i) - f(\boldsymbol{x}_i)\}^2\right]}_{\text{reducible}} + \underbrace{\sigma^2}_{\text{irreducible}},\end{aligned}$$

recalling that $\mathbb{E}(\tilde{\epsilon}_i^2) = \text{var}(\tilde{\epsilon}_i) = \sigma^2$ and for any $i = 1, \dots, n$.

Regression under quadratic loss II

- We would like to make the **mean squared error** as **small** as possible, e.g., by choosing an "optimal" degree of the polynomial $p - 1$ that minimizes it.
- Let us recall the previous decomposition

$$\mathbb{E}\left[\{\tilde{Y}_i - \hat{f}(\boldsymbol{x}_i)\}^2\right] = \underbrace{\mathbb{E}\left[\{\hat{f}(\boldsymbol{x}_i) - f(\boldsymbol{x}_i)\}^2\right]}_{\text{reducible}} + \underbrace{\sigma^2}_{\text{irreducible}}, \qquad i = 1\dots,n.$$

- The **best case scenario** is when the estimated function coincides with the mean of $\tilde{Y}_i$, i.e.

$$\hat{f}(\boldsymbol{x}_i) = f(\boldsymbol{x}_i) = \mathbb{E}(\tilde{Y}_i),$$

  but even in this (overly optimistic) situation, we would still commit mistakes, due to the presence of $\tilde{\epsilon}_i$ (unless $\sigma^2 = 0$). Hence, the variance σ^2 is called the **irreducible error**.
- Since we do not know $f(\boldsymbol{x}_i)$, we seek for an estimate $\hat{f}(\boldsymbol{x}_i) \approx f(\boldsymbol{x}_i)$, in the attempt of minimizing the **reducible error**.

Classification under misclassification loss

- In **classification problems**, under a **misclassification loss**, the in-sample prediction error is

$$\text{ErrF} = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\mathscr{L}\{\tilde{Y}_i; \hat{f}(\boldsymbol{x}_i)\}\right] = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\{\mathbb{I}(\tilde{Y}_i \neq \hat{y}_i)\} = \frac{1}{n}\sum_{i=1}^{n}\mathbb{P}(\tilde{Y}_i \neq \hat{y}_i).$$

- The above error is **minimized** whenever $\hat{y}_i$ corresponds to **Bayes classifier**

$$\hat{y}_{i,\text{bayes}} = \arg\max_{y \in \{0,1\}} \mathbb{P}(\tilde{Y}_i = y) = \mathbb{I}(p(\boldsymbol{x}_i) > 0.5),$$

  which depends on the unknown probabilities $p(\boldsymbol{x}_i)$.

- We call the **Bayes rate** the optimal in-sample prediction error:

$$\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\mathscr{L}\{\tilde{Y}_i; p(\boldsymbol{x}_i)\}\right] = \frac{1}{n}\sum_{i=1}^{n}\min\{p(\boldsymbol{x}_i), 1 - p(\boldsymbol{x}_i)\}.$$

- The **Bayes rate** is the error rate we would get if we knew the true $p(\boldsymbol{x})$ and can be regarded as the **irreducible error** for classification problems.

Bias-variance trade-off

- In many textbooks, including A&S, the starting point of the analysis is the **reducible error**, because it is the only one we can control and has a transparent interpretation.
- The reducible error measures the **discrepancy** between the unknown function $f(\boldsymbol{x})$ and its estimate $\hat{f}(\boldsymbol{x})$ and therefore it is a **natural measure** of the goodness of fit.
- What follows holds both for **regression** and **classification** problems.

Bias-variance decomposition

For any covariate value $\boldsymbol{x}$, it holds the following bias-variance decomposition:

$$\mathbb{E}\left[\{\hat{f}(\boldsymbol{x}) - f(\boldsymbol{x})\}^2\right] = \underbrace{\mathbb{E}\left[\hat{f}(\boldsymbol{x}) - f(\boldsymbol{x})\right]^2}_{\text{Bias}^2} + \underbrace{\text{var}\{\hat{f}(\boldsymbol{x})\}}_{\text{variance}}.$$

Example: bias-variance in linear regression models

- In **regression problems** the **in-sample prediction error** under **squared loss** is

$$\text{ErrF} = \sigma^2 + \frac{1}{n}\sum_{i=1}^n \mathbb{E}\left[\hat{f}(\boldsymbol{x}_i) - f(\boldsymbol{x}_i)\right]^2 + \frac{1}{n}\sum_{i=1}^n \text{var}\{\hat{f}(\boldsymbol{x}_i)\}.$$

- In **ordinary least squares** the above quantity can be computed in closed form, since each element of the **bias** term equals

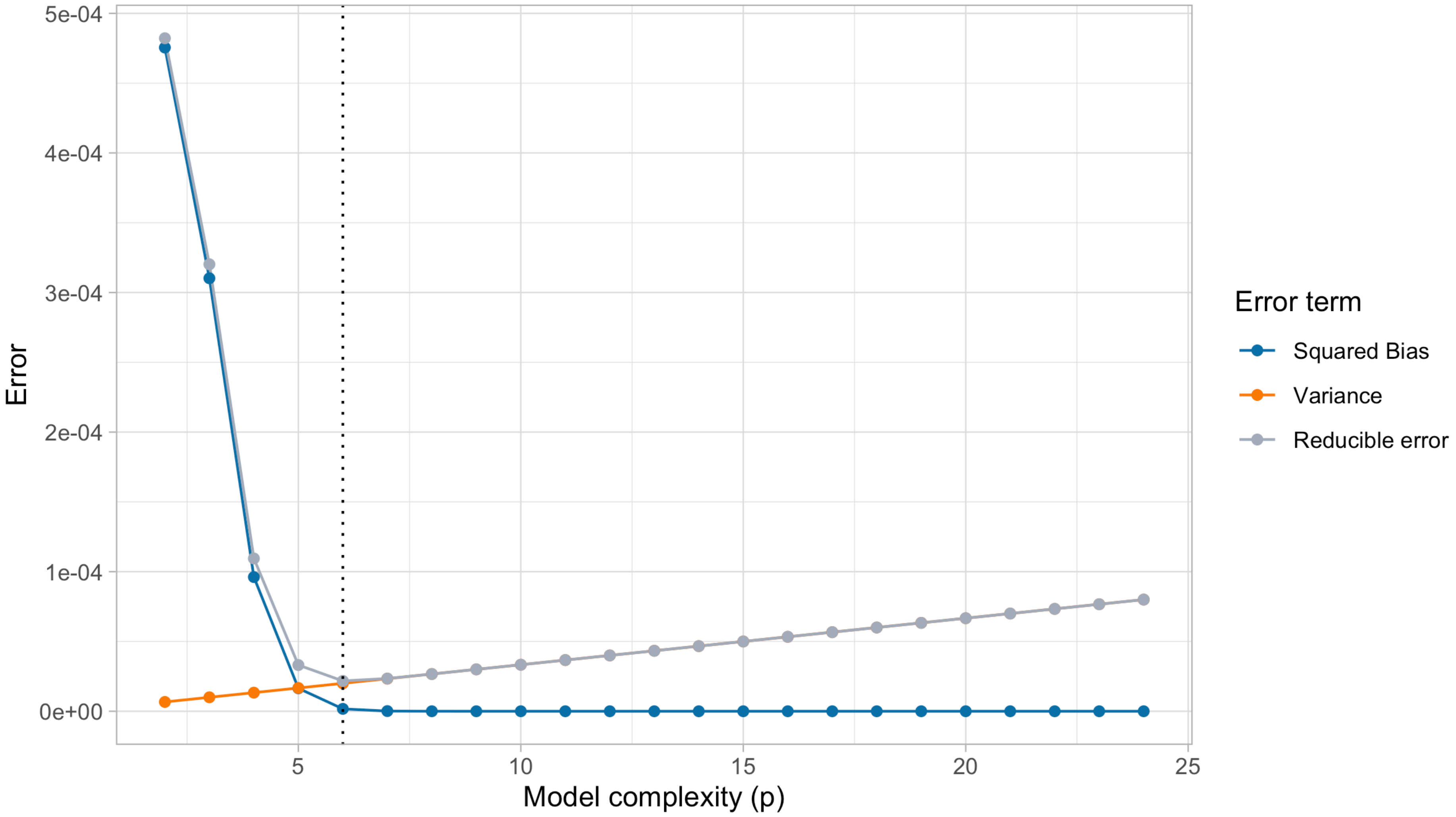
$$\mathbb{E}\left[f(\boldsymbol{x}_i;\hat{\beta}) - f(\boldsymbol{x}_i)\right] = \boldsymbol{x}_i^T(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{f} - f(\boldsymbol{x}_i).$$

  where $\boldsymbol{f} = (f(\boldsymbol{x}_1),\dots,f(\boldsymbol{x}_n))^T$. Note that **if** $f(\boldsymbol{x}) = \boldsymbol{x}^T\beta$, then the bias is zero.

- Moreover, in **ordinary least squares** the **variance** term equals

$$\frac{1}{n}\sum_{i=1}^n \text{var}\{f(\boldsymbol{x}_i;\hat{\beta})\} = \frac{\sigma^2}{n}\sum_{i=1}^n \boldsymbol{x}_i^T(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{x}_i = \frac{\sigma^2}{n}\text{tr}(\boldsymbol{H}) = \sigma^2\frac{p}{n}.$$

If we knew $f(x)$...


5e-04
4e-04
3e-04
2e-04
1e-04
0e+00
Error
5
10
15
20
25
Model complexity (p)
Error term
Squared Bias
Variance
Reducible error

Bias-variance trade-off

- When p grows, the mean squared error first decreases and then it increases. In the example, the **theoretical optimum** is $p = 6$ (5th degree polynomial).
- The **bias** measures the ability of $\hat{f}(\boldsymbol{x})$ to reconstruct the true $f(\boldsymbol{x})$. The bias is due to **lack of knowledge** of the data-generating mechanism. It equals zero when $\mathbb{E}\{\hat{f}(\boldsymbol{x})\} = f(\boldsymbol{x})$.
- The **bias** term can be reduced by increasing the flexibility of the model (e.g., by considering a high value for p).
- The **variance** measures the variability of the estimator $\hat{f}(\boldsymbol{x})$ and its tendency to follow random fluctuations of the data.
- The **variance** increases with the model complexity.
- It is not possible to minimize both the bias and the variance, there is a **trade-off**.
- We say that an estimator is **overfitting** the data if an increase in variance comes without important gains in terms of bias.

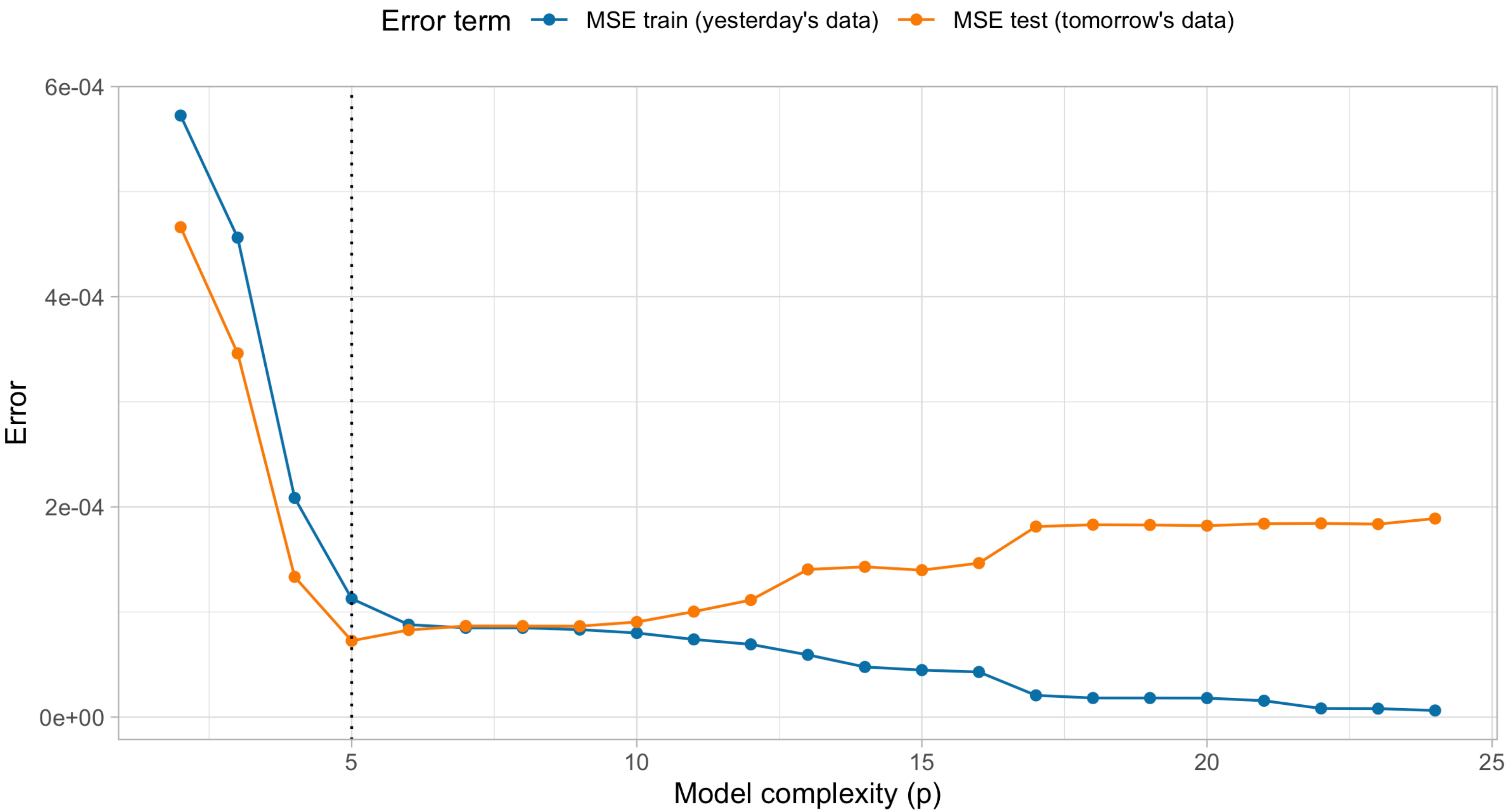
But since we do not know $f(x)$...

- We just concluded that we must expect a trade-off between error and variance components. In practice, however, we cannot do this because, of course, $f(x)$ is **unknown**.
- A simple solution consists indeed in **splitting** the observations in two parts: a **training set** $(y_1, \dots, y_n)$ and a **test set** $(\tilde{y}_1, \dots, \tilde{y}_n)$, having the same covariates $x_1, \dots, x_n$.
- We fit the model $\hat{f}$ using n observations of the training and we use it to predict the n observations on the test set.
- This leads to an **unbiased estimate** of the **in-sample prediction error**, i.e.:

$$\widehat{\mathrm{ErrF}} = \frac{1}{n}\sum_{i=1}^{n} \mathscr{L}\{\tilde{y}_i; \hat{f}(\boldsymbol{x}_i)\}.$$

- This is precisely what we already did with yesterday's and tomorrow's data!

MSE on training and test set (recap)



Optimism I

- Let us investigate this discrepancy between training and test more in-depth.
- In **regression problems**, under a **squared loss function**, the **in-sample prediction error** is

$$\text{ErrF} = \mathbb{E}(\text{MSE}_{\text{test}}) = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\left[\{\tilde{Y}_i - \hat{f}(\boldsymbol{x}_i)\}^2\right]$$

- Similarly, the **in-sample training error** can be defined as follows

$$\mathbb{E}(\text{MSE}_{\text{train}}) = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\left[\{Y_i - \hat{f}(\boldsymbol{x}_i)\}^2\right].$$

- We already know that $\mathbb{E}(\text{MSE}_{\text{train}})$ provides a very optimistic assessment of the model performance. For example when $p = n$ then $\mathbb{E}(\text{MSE}_{\text{train}}) = 0$.
- We call **optimism** the difference between these two quantities:

$$\text{Opt} = \mathbb{E}(\text{MSE}_{\text{test}}) - \mathbb{E}(\text{MSE}_{\text{train}}).$$

Optimism II

- It can be proved (see Exercises) that the **optimism** has a very simple form:

$$\mathrm{Opt} = \frac{2}{n}\sum_{i=1}^{n}\mathrm{cov}(Y_i, \hat{f}(\boldsymbol{x}_i))$$

- If **ordinary least squares** are employed, then the predictions are $\boldsymbol{H}\boldsymbol{Y}$, therefore

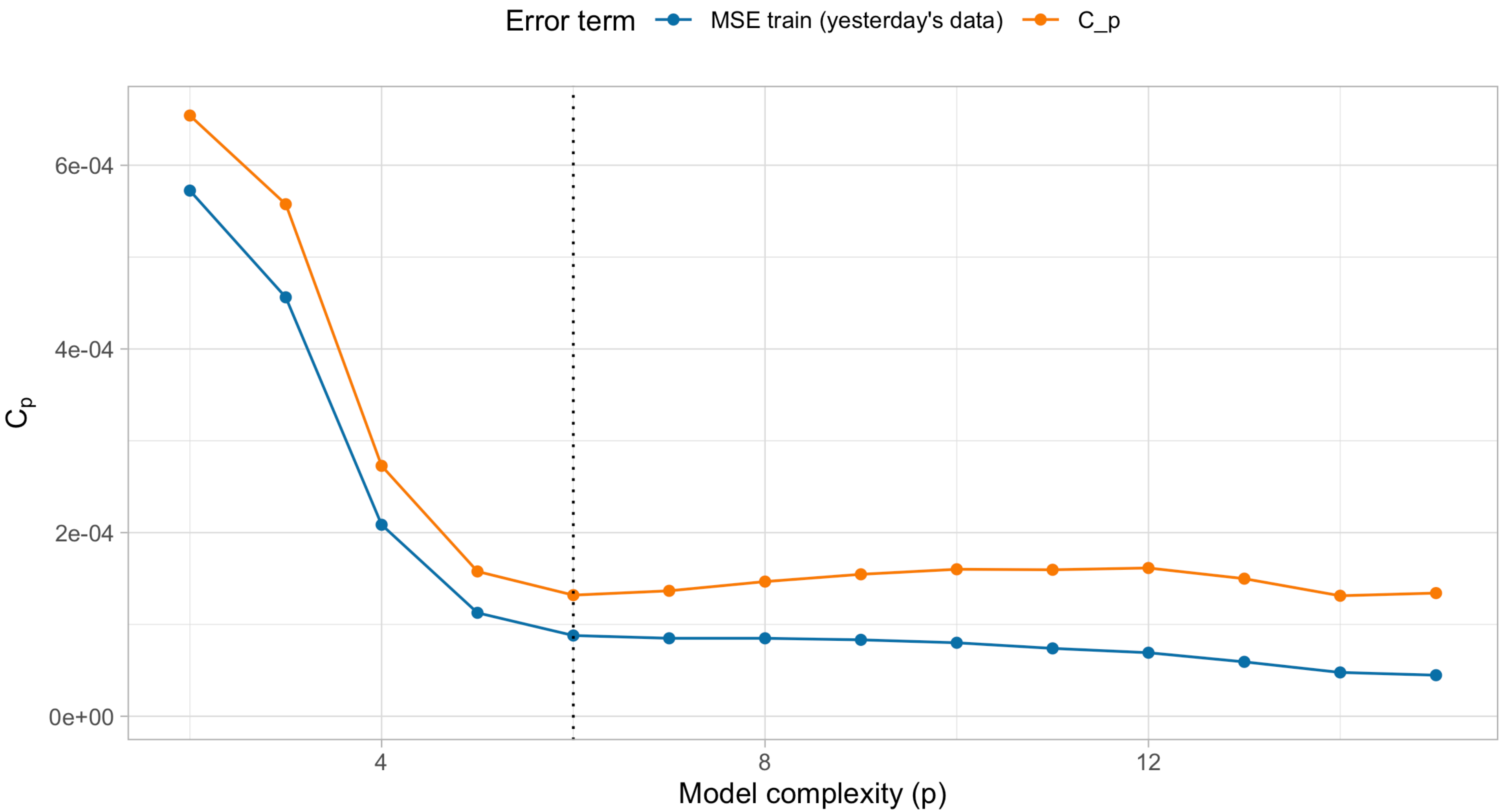
$$\mathrm{Opt}_{\mathrm{ols}} = \frac{2}{n}\mathrm{tr}\{\mathrm{cov}(\boldsymbol{Y}, \boldsymbol{H}\boldsymbol{Y})\} = \frac{2}{n}\mathrm{tr}\{\mathrm{cov}(\boldsymbol{Y}, \boldsymbol{Y})\boldsymbol{H}^T\} = \frac{2\sigma^2}{n}\mathrm{tr}(\boldsymbol{H}) = \frac{2\sigma^2 p}{n}.$$

- This leads to an estimate for the in-sample prediction error, known as C_p **of Mallows**:

$$\widehat{\mathrm{ErrF}} = \mathrm{MSE}_{\mathrm{train}} + \mathrm{Opt}_{\mathrm{ols}} = \frac{1}{n}\sum_{i=1}^{n}\{y_i - f(\boldsymbol{x}_i; \hat{\beta})\}^2 + \frac{2\sigma^2 p}{n}.$$

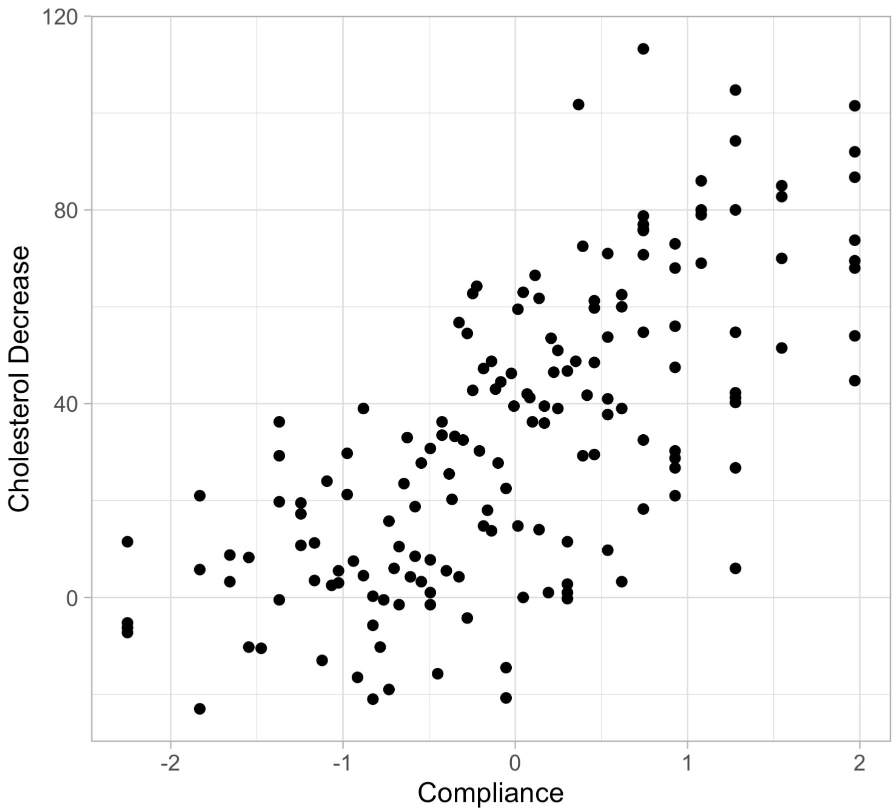
- If σ^2 is unknown, then it must be **estimated** using for instance s^2.

Optimism III



Cross-validation

Another example: cholesterol data



- A drug called "cholestyramine" is administered to $n = 164$ men.
- We observe the pair (x_i, y_i) for each man.
- The response y_i is the **decrease in cholesterol level** over the experiment.
- The covariate x_i is a measure of **compliance**.
- We assume, as before, that the data are generated according to

$$Y_i = f(x_i) + \epsilon_i, \quad i = 1, \ldots, n.$$

- The original data can be found here.

Summary and notation (random-X)

- A slight change to the previous setup is necessary. In fact, there are no reasons to believe that the **compliance** is a fixed covariate.
- We consider a set of iid **random variables** $(X_1, Y_1), \dots, (X_n, Y_n)$, whose realization is $(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_n, y_n)$. This time, the covariates are **random**.
- The main assumption is that these pairs are **iid**, namely:

$$(X_i, Y_i) \overset{\text{iid}}{\sim} \mathcal{P}, \quad i = 1, \dots, n.$$

- Conditionally on $X_i = \boldsymbol{x}_i$, in **regression problems** we let as before

$$Y_i = f(\boldsymbol{x}_i) + \epsilon_i, \quad i = 1, \dots, n,$$

where ϵ_i are iid "**error**" terms with $\mathbb{E}(\epsilon_i) = 0$ and $\text{var}(\epsilon_i) = \sigma^2$.

Expected prediction error

- In this setting with random covariates, we want to minimize the **expected prediction error**:

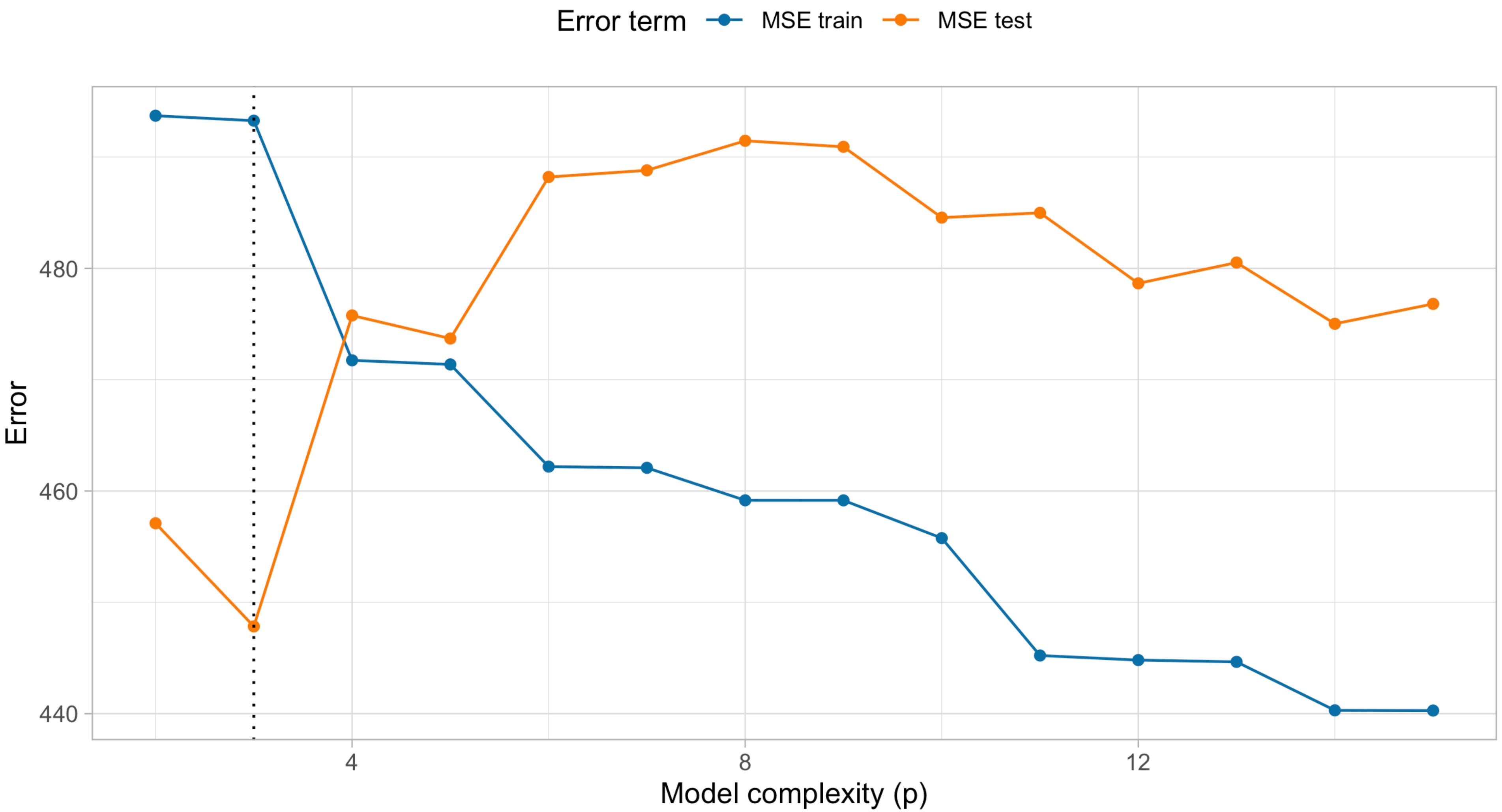
  $$\mathrm{Err} = \mathbb{E}\left[\mathscr{L}\{\tilde{Y}; \hat{f}(\tilde{X})\}\right],$$

  where $(\tilde{X}, \tilde{Y}) \sim \mathcal{P}$ is a **new data point** and $\hat{f}$ is an estimate using n observations.
- We can **randomly** split the original set of data $\{1, \dots, n\}$ into two groups V_{train} and V_{test}.
- We call $\hat{f}_{\text{train}}$ the estimate based on the data in V_{train}.
- Then, we obtain a (slightly biased) estimate of Err by using the empirical quantity:

  $$\widehat{\mathrm{Err}} = \frac{1}{|V_{\text{test}}|}\sum_{i \in V_{\text{test}}} \mathscr{L}\{\tilde{y}_i; \hat{f}_{\text{train}}(\boldsymbol{x}_i)\}.$$

- The data-splitting strategy we used before is an effective tool for assessing the error. However, its **interpretation** is changed: we are now estimating Err and not ErrF.

MSE on training and test (cholesterol data)

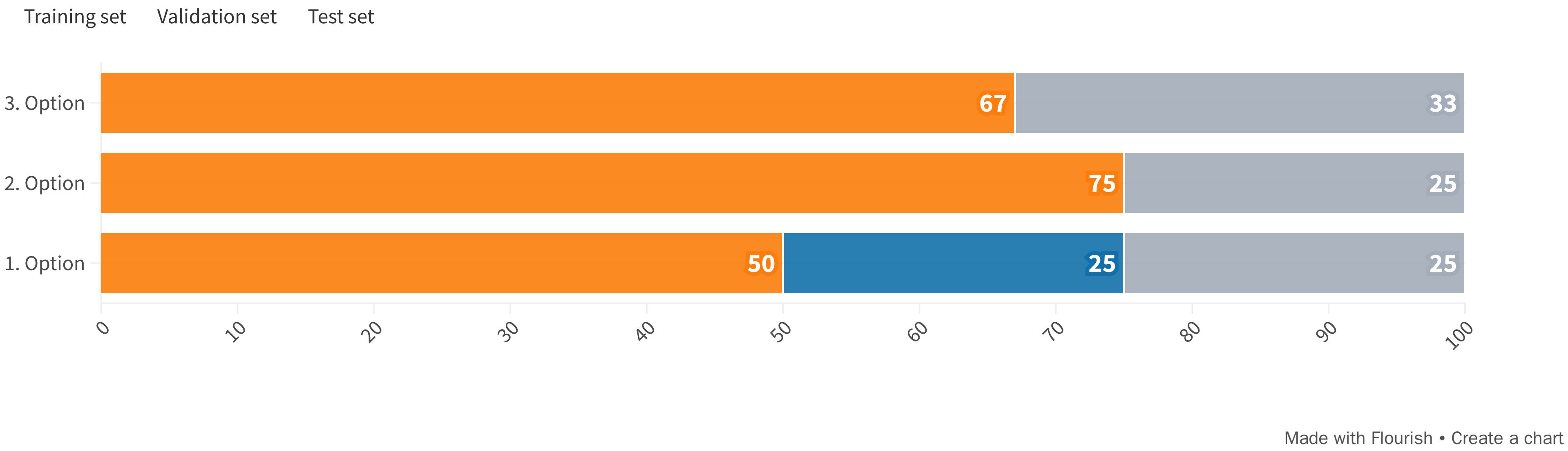


Training, validation, and test I

- On many occasions, we may need to select several complexity parameters and compare hundreds of models.
- If the same test set is used for such a task, the final assessment of the error is somewhat biased and **too optimistic**, because we are "learning" from the test set.
- If we are in a data-rich situation, the best approach is to divide the dataset into three parts randomly:
  - a **training set**, used for **fitting** the models;
  - a **validation set**, used to estimate prediction error and perform **model selection**;
  - a **test set**, for **assessment of the error** of the final chosen model.
- Ideally, the test set should be kept in a "vault" and be brought out only at the end of the data analysis.

Training, validation, and test II

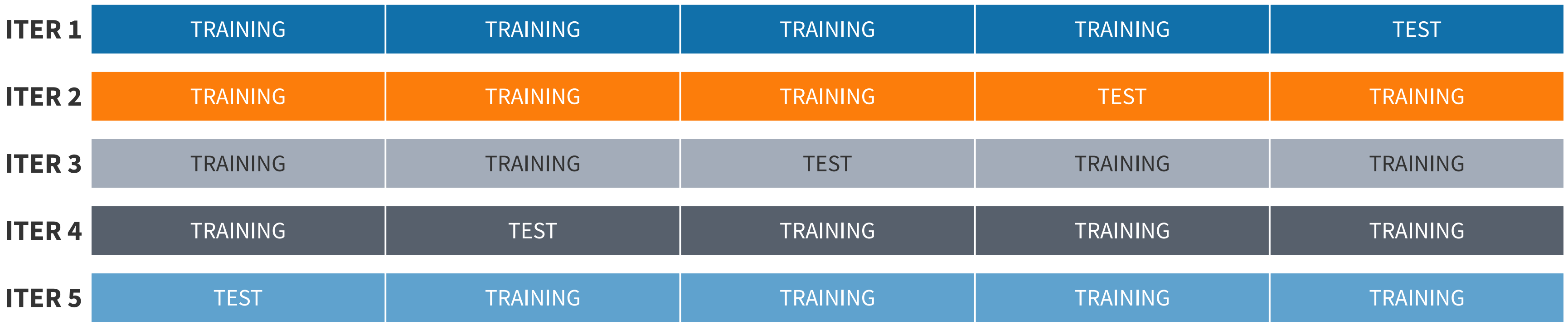
- There is no precise rule on how to select the size of these sets; a rule of thumb is given in the picture below.



- The training, validation, and test setup **reduces** the **number of observations** we can use to fit the models. It could be problematic if the sample size is relatively small.

Cross-validation I

- A way to partially overcome the loss of efficiency of the training / test paradigm consists in **randomly splitting the data** $\{1, \dots, n\}$ in equal parts, say $V_1, \dots, V_K$.
- In the **K-fold cross-validation** method we use the observations $i \notin V_k$ to train the model and the remaining observations $i \in V_k$ to perform model selection.
- In the following scheme, we let $K = 5$.



ITER 1	TRAINING	TRAINING	TRAINING	TRAINING	TEST
ITER 2	TRAINING	TRAINING	TRAINING	TEST	TRAINING
ITER 3	TRAINING	TRAINING	TEST	TRAINING	TRAINING
ITER 4	TRAINING	TEST	TRAINING	TRAINING	TRAINING
ITER 5	TEST	TRAINING	TRAINING	TRAINING	TRAINING

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Cross-validation II

- In the **K-fold cross validation** we compute for each fold k we fit a model $\hat{f}_{-V_k}(\boldsymbol{x})$ without using the observations of V_k.
- Hence, the model must be estimated **K times**, which could be computationally challenging.
- The error of each on the kth folds is computed as

$$\widehat{\mathrm{Err}}_{V_k} = \frac{1}{|V_k|}\sum_{i \in V_k} \mathscr{L}\{y_i; \hat{f}_{-V_k}(\boldsymbol{x}_i)\},$$

  where $|V_k|$ is the cardinality of V_k, i.e. $V_k \approx n/K$.
- We summarize the above errors using the mean, obtaining the following **estimate** for the **expected prediction error**:

$$\widehat{\mathrm{Err}} = \frac{1}{K}\sum_{k=1}^{K}\widehat{\mathrm{Err}}_{V_k} = \frac{1}{K}\sum_{k=1}^{K}\left[\frac{1}{|V_k|}\sum_{i \in V_k} \mathscr{L}\{y_i; \hat{f}_{-V_k}(\boldsymbol{x}_i)\}\right].$$

Cross-validation III

- An advantage of CV is that **variance** of the Monte Carlo estimate $\widehat{\mathrm{Err}}$ can be quantified.
- Let us define cross-validated "**residuals**" of our procedure as follows

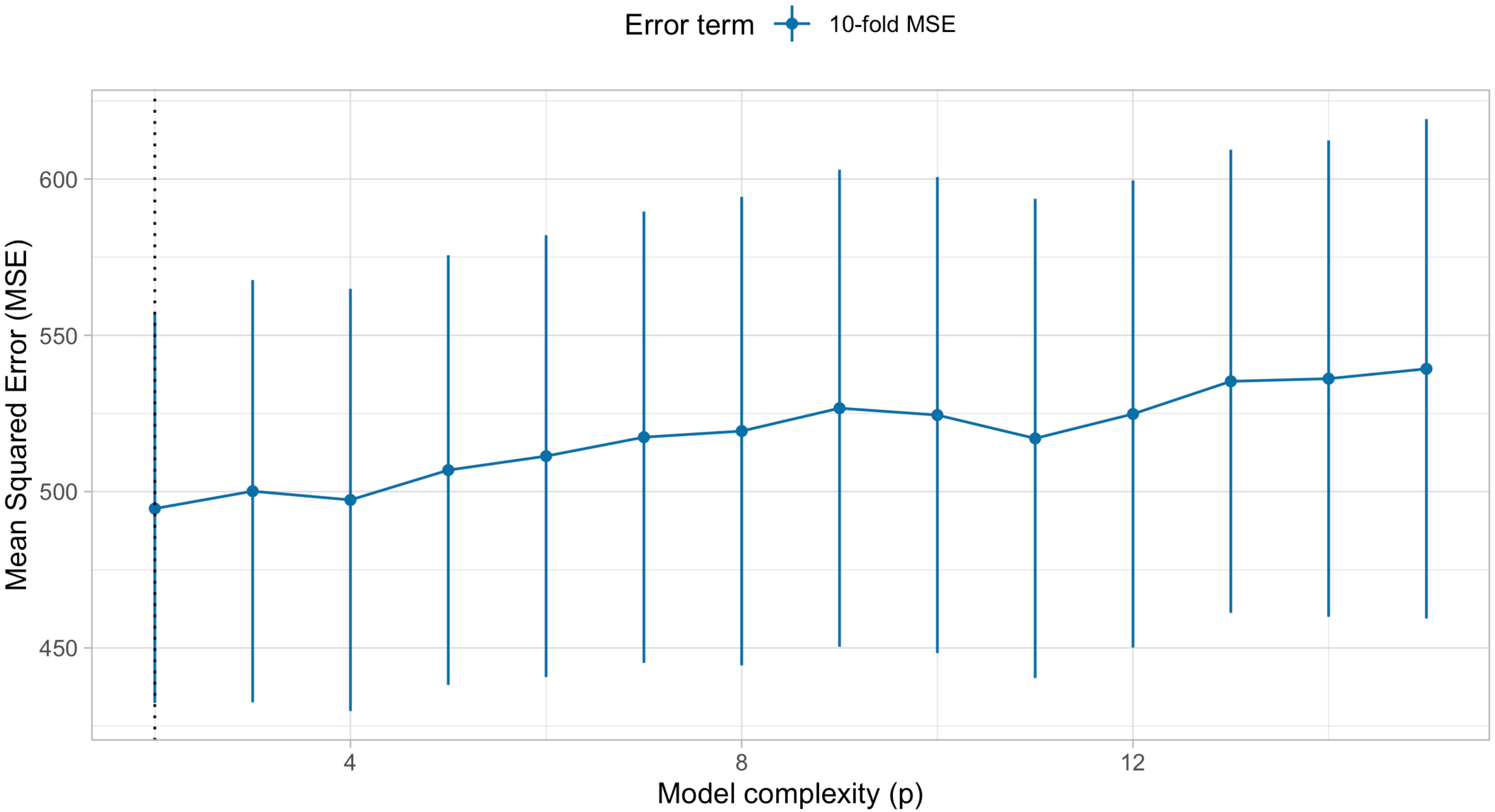
  $$r_i = \mathscr{L}\{y_i; \hat{f}_{-V_k}(\boldsymbol{x}_i)\}, \qquad i = 1, \dots, n.$$

  so that $\widehat{\mathrm{Err}} = \bar{r}$. Does it coincide with the estimate $\widehat{\mathrm{Err}}$ presented in the previous slide? Recall that $V_k \approx n/K$...
- Then, a simple estimate for the standard error of $\widehat{\mathrm{Err}}$ is

  $$\widehat{\mathrm{se}} = \frac{1}{\sqrt{n}}\mathrm{sd}(r) = \frac{1}{\sqrt{n}}\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(r_i - \bar{r})^2}.$$

- The above formula is often criticized for producing intervals that are **too narrow**!
- Indeed, the estimate $\widehat{\mathrm{se}}$ of the standard deviation of $\widehat{\mathrm{Err}}$ assumes that the observed errors $r_1, \dots, r_n$ are independent, but this is false!

Cross-validation IV (cholesterol data)



Leave-one-out cross-validation

- The maximum possible value for K is n, the **leave-one-out** cross-validation (LOO-CV).
- The LOO-CV is hard to implement because it requires the estimation of n different models.
- However, in **ordinary least squares** there is a brilliant **computational shortcut**.

LOO-CV (Ordinary least squares)

Let $\hat{y}_{-i} = \boldsymbol{x}_i^T \hat{\beta}_{-i}$ be the leave-one-out predictions of a **linear model** and let $h_i = [\boldsymbol{H}]_{ii}$ and $\hat{y}_i$ be the leverages and the predictions of the full model. Then:

$$y_i - \hat{y}_{-i} = \frac{y_i - \hat{y}_i}{1 - h_i}, \qquad i = 1, \dots, n.$$

Therefore, the leave-one-out mean squared error is

$$\widehat{\mathrm{Err}} = \frac{1}{n}\sum_{i=1}^{n} \widehat{\mathrm{Err}}_{V_i} = \frac{1}{n}\sum_{i=1}^{n} \left(\frac{y_i - \hat{y}_i}{1 - h_i}\right)^2.$$

Generalized cross-validation

- An alternative to LOO-CV is the so-called **generalized cross validation** (GCV), defined as

$$\text{GCV} = \widehat{\text{Err}} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - p/n}\right)^2.$$

- The GCV is an approximate LOO-CV for **ordinary least squares**, in which the leverages h_i are replaced by their mean:

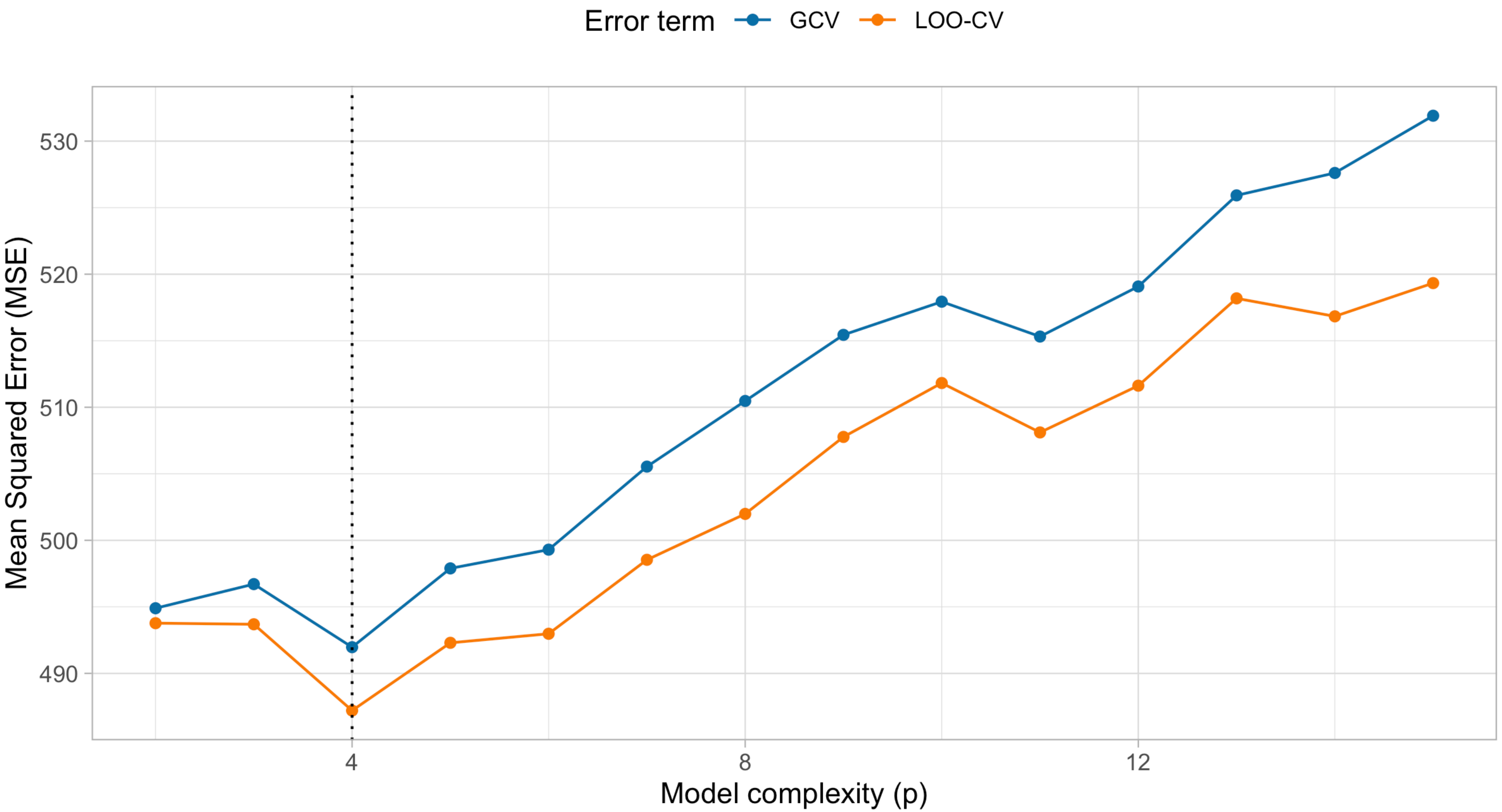
$$\frac{1}{n}\sum_{i=1}^{n} h_i = \frac{p}{n}.$$

- For small $x > 0$ it holds that $(1-x)^{-2} \approx 1 + 2x$. Then, we will write

$$\text{GCV} \approx \frac{1}{n}\sum_{i=1}^{n}\{y_i - f(\boldsymbol{x}_i; \hat{\beta})\}^2 + \frac{2\hat{\sigma}^2 p}{n}, \qquad \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}\{y_i - f(\boldsymbol{x}_i; \hat{\beta})\}^2,$$

revealing a sharp connection with the C_p of Mallows.

LOO-CV and GCV (cholesterol data)



On the choice of K

- Common choices are $K = 5$ or $K = 10$. It is quite evident that a **larger K** requires more **computations**.
- A K-fold CV with $K = 5$ or $K = 10$ is a (upwords) **biased estimate** of Err because it uses less observations than those available (either $4/5$ or $9/10$).
- The LOO-CV has a very **small bias**, since each fit uses $n - 1$ observations, but it has **high variance**, being the average of n highly positively correlated quantities.
- Indeed, the estimates $\hat{f}_{-i}$ and $\hat{f}_{-i'}$ have $n - 2$ observations in common. Recall that the variance of the sum is:

$$\mathrm{var}(X + Y) = \mathrm{var}(X) + \mathrm{var}(Y) + 2\mathrm{cov}(X, Y).$$

- Overall, the choice is very much context-dependent.

Information criteria

Goodness of fit with a penalty term

- The main statistical method for estimating unknown parameters of a model is the **maximize the log-likelihood** $\ell(\theta) = \ell(\theta; y_1, \dots, y_n)$.
- However, we cannot pick the value of p that maximizes the log-likelihood (why not?)
- We must consider the different number of parameters, introducing a **penalty**:

$$\mathrm{IC}(p) = -2\ell(\hat{\theta}) + \mathrm{penalty}(p),$$

- The IC is called an **information criterion**. We select the number of parameters minimizing the IC.
- The choice of the specific penalty identifies a particular criterion.
- An advantage of IC is that they are based on the full dataset.

The Akaike information criterion I

- Akaike suggested minimizing over p the **expectation** of the **Kullback-Leibler divergence**:

$$\mathrm{KL}(p(\cdot;\theta_0)\,||\,p(\cdot;\hat\theta)) = \int p(\tilde{\boldsymbol{Y}};\theta_0)\log p(\tilde{\boldsymbol{Y}};\theta_0)\mathrm{d}\tilde{\boldsymbol{Y}} - \int p(\tilde{\boldsymbol{Y}};\theta_0)\log p(\tilde{\boldsymbol{Y}};\hat\theta)\mathrm{d}\tilde{\boldsymbol{Y}},$$

  between the "true" model $p(\boldsymbol{Y};\theta_0)$ with parameter θ_0 and the estimated model $p(\boldsymbol{Y};\hat\theta)$.

- In the above Kullback-Leibler, for any fixed p, the parameter θ is replaced with its **maximum likelihood estimator** $\hat\theta = \hat\theta(\boldsymbol{Y})$, using the data $\boldsymbol{Y} = (Y_1,\dots,Y_n)$.
- **Equivalently**, we can select p such that the expectation w.r.t. $p(\boldsymbol{Y};\theta_0)$

$$\begin{aligned}\Delta(p) &= 2\,\mathbb{E}_{\theta_0}\left[\mathrm{KL}(p(\cdot;\theta_0)\,||\,p(\cdot;\hat\theta))\right] - \underbrace{2\int p(\tilde{\boldsymbol{Y}};\theta_0)\log p(\tilde{\boldsymbol{Y}};\theta_0)\mathrm{d}\tilde{\boldsymbol{Y}}}_{\text{Does not depend on } p}\\ &= -2\,\mathbb{E}_{\theta_0}\left[\int p(\tilde{\boldsymbol{Y}};\theta_0)\log p(\tilde{\boldsymbol{Y}};\hat\theta)\mathrm{d}\tilde{\boldsymbol{Y}}\right]\end{aligned}$$

  is **minimized**. Unfortunately, we cannot compute nor minimize $\Delta(p)$ because θ_0 is unknown.

The Akaike information criterion II

- The theoretical quantity $\Delta(p)$ cannot be obtained. However, the quantity

  $$\mathrm{AIC} = -2\ell(\hat{\theta}) + 2p,$$

  namely the **Akaike information criterion**, is a good estimator of $\Delta(p)$.
- More formally, it can be proved that under technical conditions:

  $$\mathbb{E}_{\theta_0}(\mathrm{AIC}) + o(1) = \Delta(p),$$

  for $n \to \infty$.
- In practice, we will select the value of p minimizing the AIC, which is typically quite easy.
- The factor 2 is just a **convention**, introduced to match the quantities of the usual asymptotic theory.

The AIC for Gaussian linear models

- Let us assume that σ^2 is **known**. Then the AIC for a Gaussian linear model is

$$\begin{aligned}\mathrm{AIC} = -2\ell(\hat{\beta}) + 2p &= -2\left\{-\frac{n}{2}\log\left(2\pi\sigma^2\right) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i^T\hat{\beta})^2\right\} + 2p\\ &= n\log\left(2\pi\sigma^2\right) + \frac{n}{\sigma^2}\left\{\frac{1}{n}\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i^T\hat{\beta})^2 + \frac{2p\sigma^2}{n}\right\}\\ &= n\log\left(2\pi\sigma^2\right) + \frac{n}{\sigma^2}C_p,\end{aligned}$$

  implying that for fixed values σ^2 the C_p of Mallows and the Akaike's AIC are **equivalent**, i.e. they lead to the same **minimum**.

- When σ^2 is unknown, then it is estimated, and the C_p and AIC may be slightly different.

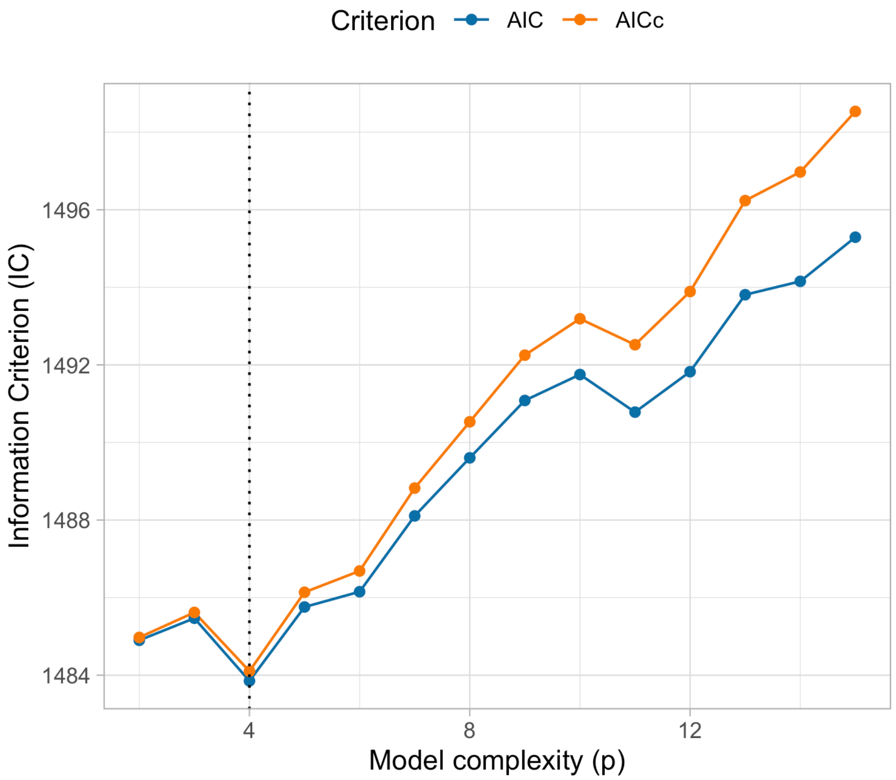
AIC, AICc, BIC

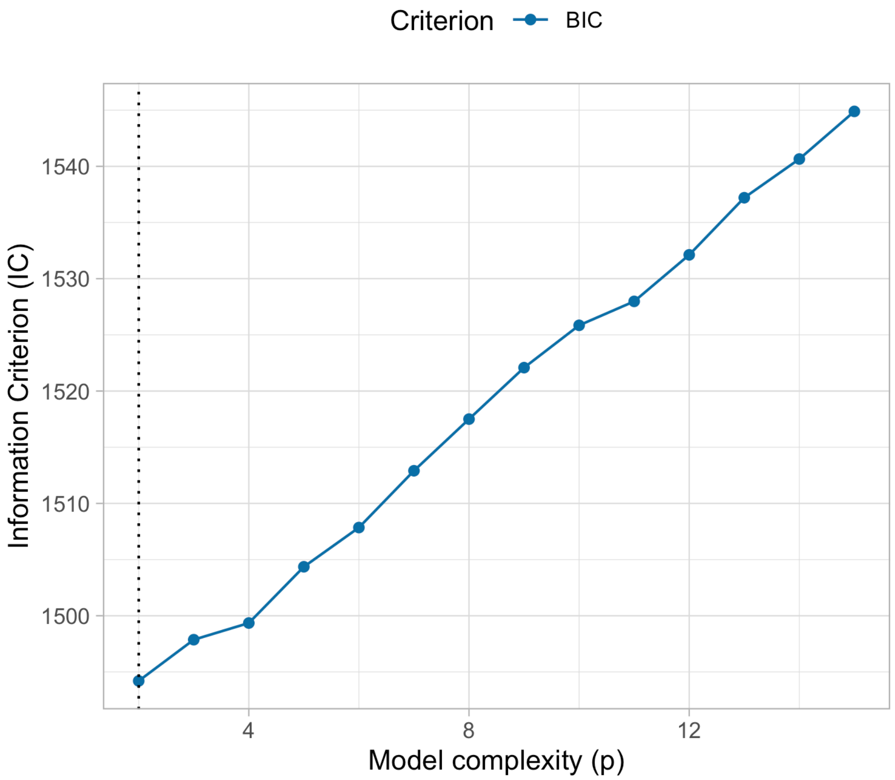
- Several other proposals followed Akaike's original work, differing in their assumptions and the way they approximate certain quantities.

Criterion	Author	Penalty
AIC	Akaike	$2p$
AIC_c	Sugiura, Hurvich-Tsay	$2p + \frac{2p(p+1)}{n-(p+1)}$
BIC	Akaike, Schwarz	$p \log n$

- The AIC_c is an **higher order correction** of the AIC and the differences tend to be negligible for high values of n.
- The justification of BIC is comes from **Bayesian statistics**.
- Since $\log n > 2$ for any $n > 7$, it means that the BIC **penalty** is typically **stronger** than the one of AIC and it favors more parsimonious models.

AIC and BIC (cholesterol data)

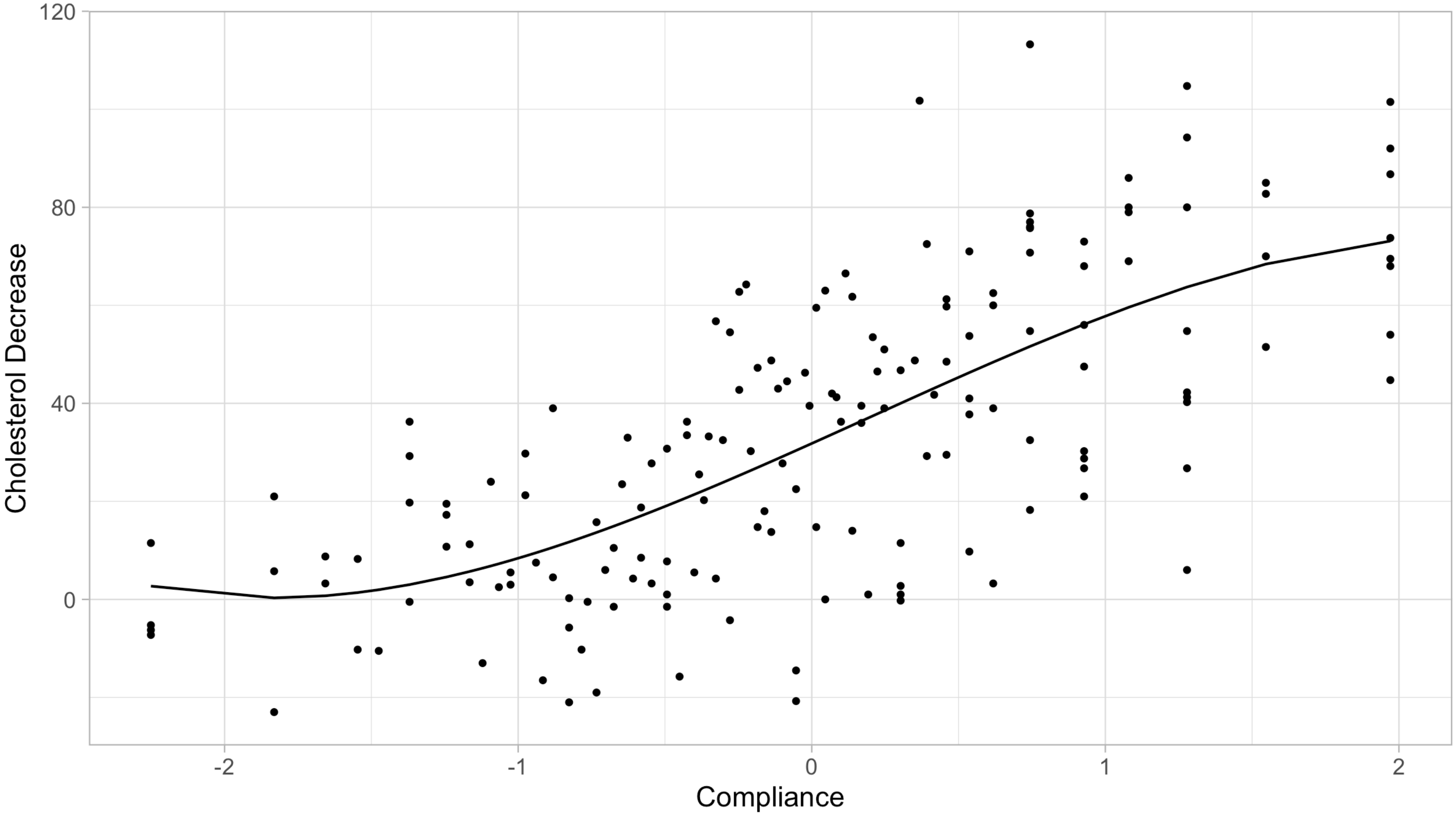




An optimistic summary

- In the `cholesterol` dataset, the various indices produced **different results**!
  - The BIC and and the $10-$fold cross-validation selected $p = 2$ (linear model);
  - The training/test split suggested $p = 3$ (quadratic model);
  - All the others (LOO-CV, GCV, AIC and AIC_c) concluded that $p = 4$ (cubic model).
- The good news is that all the above methods produced **similar findings**. For example, we are sure we should choose $p \le 6$.
- On the other hand, there is some **uncertainty**, which is quite a common situation.
- In this specific case, we may prefer $p = 4$, since it is based on the less-biased estimates of Err, such as the LOO-CV.
- However, this choice is **debatable**: another statistician may prefer the simpler linear model with $p = 2$.

The cholesterol data: final model ($p = 4$)



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