STK-IN4300
Statistical Learning Methods in Data Science

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Outline of the lecture

- Linear Methods for Regression
  - Linear Regression Models and Least Squares
  - Subset selection
- Model Assessment and Selection
  - Bias, Variance and Model Complexity
  - The Bias–Variance Decomposition
  - Optimism of the Training Error Rate
  - Estimates of In-Sample Prediction Error
  - The Effective Number of Parameters
  - The Bayesian Approach and BIC

Linear Regression Models and Least Squares: recap

Consider:

- continuous outcome Y, with $Y = f(X) + \epsilon$;
- linear regression $f(X) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$

We know:

- $\hat{\beta} = \text{argmin}_\beta RSS(\beta) = (X^T X)^{-1} X^T y$;
- $\hat{y} = X\hat{\beta} = \underbrace{X(X^T X)^{-1} X^T}_{\text{hat matrix H}} y$;
- $\text{Var}(\hat{\beta}) = (X^T X)^{-1}\sigma^2$
  - $\hat{\sigma}^2 = \frac{1}{N-p-1}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$;

When $\epsilon \sim N(0, \sigma^2)$,

- $\hat{\beta} \sim N(\beta, (X^T X)^{-1}\sigma^2)$;
- $(N-p-1)\hat{\sigma}^2 \sim \sigma^2 \chi^2_{N-p-1}$.

Linear Regression Models and Least Squares: Gauss – Markov theorem

The least square estimator $\hat{\theta} = a^T(X^TX)^{-1}X^Ty$ is the

B est $\leftarrow$ smallest error (MSE)

L inear $\leftarrow \hat{\theta} = a^T\beta$

U nbiased $\leftarrow E[\hat{\theta}] = \theta$

E stimator

Remember the error decomposition,

$$E[(Y - \hat{f}(X))^2] = \underbrace{\sigma^2}_{\text{irreducible error}} + \underbrace{\underbrace{\text{Var}(\hat{f}(X))}_{\text{variance}} + \underbrace{E[\hat{f}(X) - f(X)]^2}_{\text{bias}^2}}_{\text{mean square error (MSE)}};$$

then, any estimator $\tilde{\theta} = c^TY$, s.t. $E[c^TY] = a^T\beta$, has

$$\text{Var}(c^TY) \geqslant \text{Var}(a^T\hat{\beta})$$

Linear Regression Models and Least Squares: hypothesis testing

To test $H_0 : \beta_j = 0$, we use the Z-score statistic,

$$z_j = \frac{\hat{\beta}_j - 0}{sd(\hat{\beta}_j)} = \frac{\hat{\beta}_j}{\hat{\sigma}\sqrt{(X^T X)^{-1}_{[j,j]}}}$$

- When σ^2 is unknown, under H_0,

$$z_j \sim t_{N-p-1},$$

  where t_k is a Student t distribution with k degrees of freedom.
- When σ^2 is known, under H_0,

$$z_j \sim N(0; 1).$$

To test $H_0 : \beta_j, \beta_k = 0$,

$$F = \frac{(RSS_0 - RSS_1)/(p_1 - p_0)}{RSS_1/(N - p - 1)},$$

where $_1$ and $_0$ refer to the larger and smaller models, respectively.

Subset selection: variable selection

Why choosing a sparser (less variables) model?

- prediction accuracy (smaller variance);
- interpretability (easier to understand the model);
- portability (easier to use in practice).

Classical approaches:

- forward selection;
- backward elimination;
- stepwise and stepback selection;
- best subset technique.
- stagewise selection.

Subset selection: classical approaches

Forward selection:

- start with the null model, $Y = \beta_0 + \epsilon$;
- among a set of possible variables, add that which reduces the unexplained variability the most
  - e.g.: after the first step, $Y = \beta_0 + \beta_2 X_2 + \epsilon$;
- repeat iteratively until a certain stopping criterion (p-value larger than a threshold α, increasing AIC, ...) is met.

Backward elimination:

- start with the full model, $Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \epsilon$;
- remove the variable that contributes the least in explaining the outcome variability
  - e.g.: after the first step, $Y = \beta_0 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon$;
- repeat iteratively until a stopping criterion (p-value of all remaining variable smaller than α, increasing AIC, ...) is met.

Subset selection: classical approaches

Stepwise and stepback selection:

- mixture of forward and backward selection;
- allow both adding and removing variables at each step;
  - starting from the null model: stepwise selection;
  - starting from the full model: stepback selection.

Best subset:

- compute all the 2^p possible models (each variable in/out);
- choose the model which minimizes a loss function (e.g., AIC).

Stagewise selection:

- similar to the forward selection;
- at each step, the specific regression coefficient is updated only using the information related to the corresponding variable;
  - slow to converge in low-dimensions;
  - turned out to be effective in high-dimensional settings.

Model Assessment and Selection: introduction

- **Model Assessment:** evaluate the performance (e.g., in terms of prediction) of a selected model.
- **Model Selection:** select the best model for the task (e.g., best for prediction).
- **Generalization:** a (prediction) model must be valid in broad generality, not specific for a specific dataset.

Bias, Variance and Model Complexity: definitions

Define:

- Y = target variable;
- X = input matrix;
- $\hat{f}(X)$ = prediction rule, trained on a training set $\mathcal{T}$.

The error is measured through a loss function

$$L(Y, \hat{f}(X))$$

which penalizes differences between Y and $\hat{f}(X)$.

Typical choices for continuous outcomes are:

- $L(Y, \hat{f}(X)) = (Y - \hat{f}(X))^2$, the quadratic loss;
- $L(Y, \hat{f}(X)) = |Y - \hat{f}(X)|$, the absolute loss.

Bias, Variance and Model Complexity: categorical variables

Similar story for the categorical variables:

- $G =$ target variable $\rightarrow$ takes K values in $\mathcal{G}$;

Typical choices for the loss function in this case are:

- $L(Y, \hat{f}(X)) = \mathbb{1}(G \neq \hat{G}(X))$, the 0-1 loss;
- $L(Y, \hat{f}(X)) = -2 \log \hat{p}_G(X)$, the deviance.

- $\log \hat{p}_G(X) = \ell(\hat{f}(X))$ is general and can be use for every kind of outcome (binomial, Gamma, Poisson, log-normal, ...)
- the factor -2 is added to make the loss function equal to the squared loss in the Gaussian case,

$$L(\hat{f}(X)) = \frac{1}{\sqrt{2\pi 1}} \exp\left\{-\frac{1}{2 \cdot 1}(Y - \hat{f}(X))^2\right\}$$

$$\ell(\hat{f}(X)) = -\frac{1}{2}(Y - \hat{f}(X))^2$$

Bias, Variance and Model Complexity: test error

The test error (or generalization error) is the prediction error over an independent test sample

$$\text{Err}_{\mathcal{T}} = E[L(Y, \hat{f}(X))|\mathcal{T}]$$

where both X and Y are drawn randomly from their joint distribution.

The specific training set $\mathcal{T}$ used to derive the prediction rule is fixed $\rightarrow$ the test error refers to the error for this specific $\mathcal{T}$.

In general, we would like to minimize the expected prediction error (expected test error),

$$\text{Err} = E[L(Y, \hat{f}(X))] = E[\text{Err}_{\mathcal{T}}].$$

Bias, Variance and Model Complexity: training error

- We would like to get Err, but we only have information on the single training set (we will see later how to solve this issue);
- our goal, therefore, is to estimate $\text{Err}_{\mathcal{T}}$.

The training error

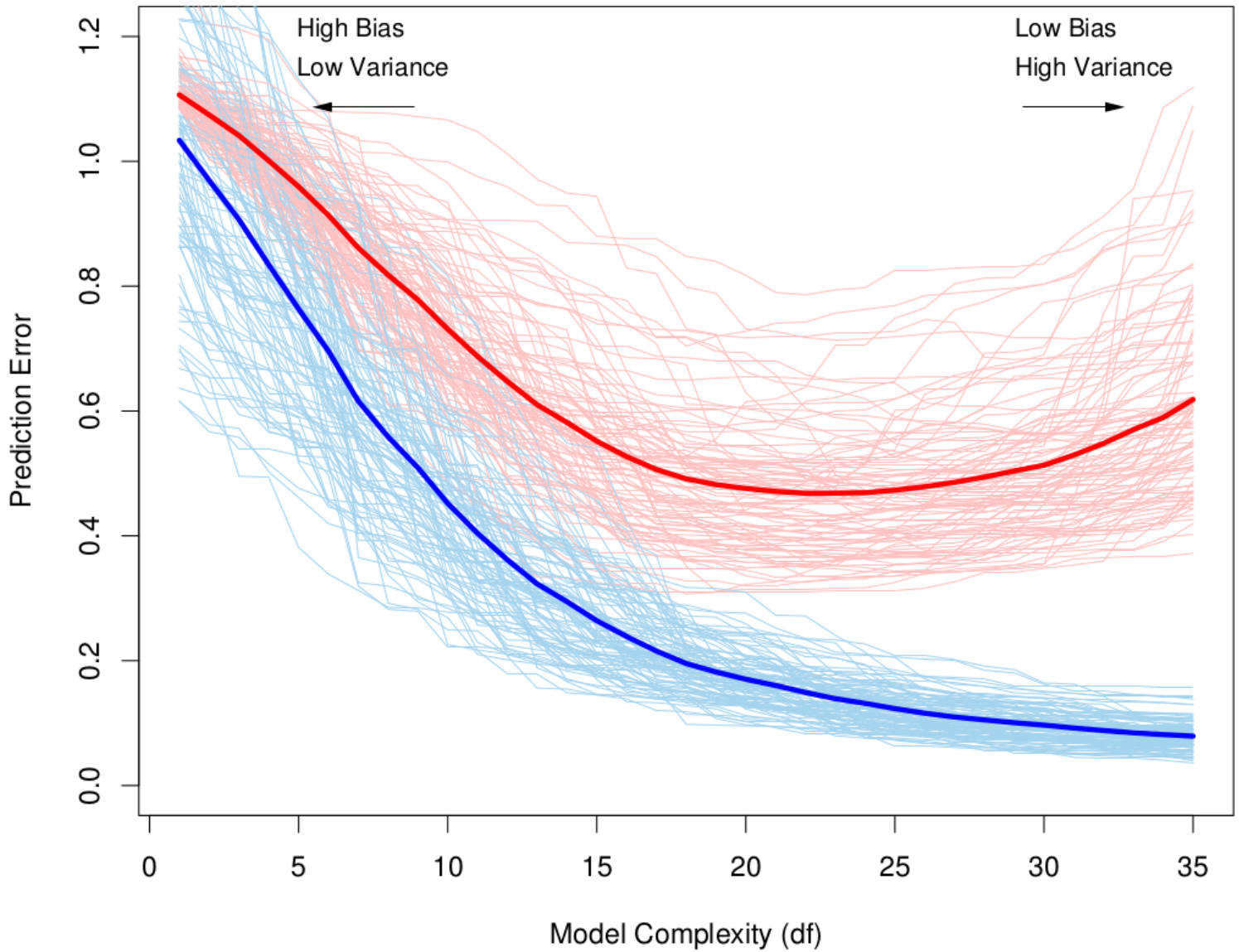
$$\overline{\text{err}} = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}(x_i)),$$

is **NOT** a good estimator of $\text{Err}_{\mathcal{T}}$.

We do not want to minimize the training error:

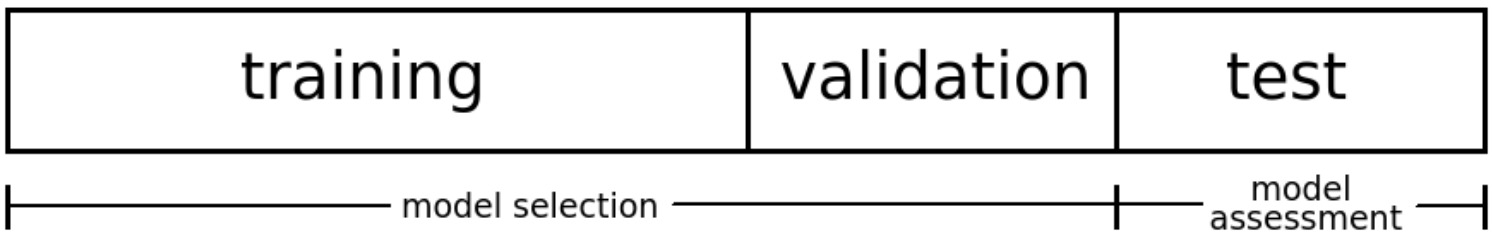
- increasing the model complexity, we can always decrease it;
- overfitting issues:
  - model specific for the training data;
  - generalize very poorly.

Bias, Variance and Model Complexity: prediction error



Bias, Variance and Model Complexity: data split

In an ideal (= a lot of data) situation, the best option is **randomly** splitting the data in three **independent** sets,



- **training set:** data used to fit the model(s);
- **validation set:** data used to identify the best model;
- **test set:** data used to assess the performance of the best model (must be completely ignored during model selection).

NB: it is extremely important to use the sets fully independently!

Bias, Variance and Model Complexity: data split

Example with k-nearest neighbour:

- in the **training set:** fit kNN with different values of k;
- in the **validation set:** select the model with best performance (choose k);
- in the **test set:** evaluate the prediction error of the model with the selected k.

Bias, Variance and Model Complexity: data split

How to split the data in three set? There is not a general rule.
The book's suggestion:

- **training set:** 50%;
- **validation set:** 25%;
- **test set:** 25%.

We will see later what to do when there are no enough data;

- difficult to say when the data are "enough".

The Bias–Variance Decomposition: computations

Consider $Y = f(X) + \epsilon$, $E[\epsilon] = 0$, $\text{Var}[\epsilon] = \sigma^2$. Then

$$\begin{aligned}
\text{Err}(x_0) &= E[(Y - \hat{f}(X))^2 | X = x_0] \\
&= E[Y^2] + E[\hat{f}(x_0)^2] - 2E[Y\hat{f}(x_0))] \\
&= \text{Var}[Y] + f(x_0)^2 + \text{Var}[\hat{f}(x_0)] + E[\hat{f}(x_0)]^2 - 2f(x_0)E[\hat{f}(x_0)] \\
&= \sigma^2 + \text{bias}^2(\hat{f}(x_0)) + \text{Var}[\hat{f}(x_0)] \\
&= \text{irreducible error} + \text{bias}^2 + \text{variance}
\end{aligned}$$

Remember that:

- $E[Y] = E[f(X) + \epsilon] = E[f(X)] + E[\epsilon] = f(X) + 0 = f(X)$;
- $E[Y^2] = \text{Var}[Y] + E[Y]^2 = \sigma^2 + f(X)^2$;
- $\hat{f}(X)$ and ϵ are uncorrelated.

The Bias–Variance Decomposition: k-nearest neighbours

For the kNN regression:

$$\begin{aligned}\text{Err}(x_0) &= E_Y[(Y - \hat{f}_k(x_0))^2 | X = x_0] \\ &= \sigma_\epsilon^2 + \left[f(x_0) - \frac{1}{k} \sum_{\ell=1}^{k} f(x_\ell) \right]^2 + \frac{\sigma_\epsilon^2}{k}\end{aligned}$$

Note:

- the number of neighbour is inversely related to the complexity;
- smaller k $\rightarrow$ smaller bias, larger variance;
- larger k $\rightarrow$ larger bias, smaller variance.

The Bias–Variance Decomposition: linear regression

For linear regression, with a p-dimensional β (regression coefficients) estimated by least squares,

$$\begin{aligned}\text{Err}(x_0) &= E_Y[(Y - \hat{f}_p(x_0))^2 | X = x_0] \\ &= \sigma_\epsilon^2 + [f(x_0) - E[f_p(x_0)]]^2 + ||h(x_0)||^2 \sigma_\epsilon^2\end{aligned}$$

where $h(x_0) = X(X^T X)^{-1} x_0$,

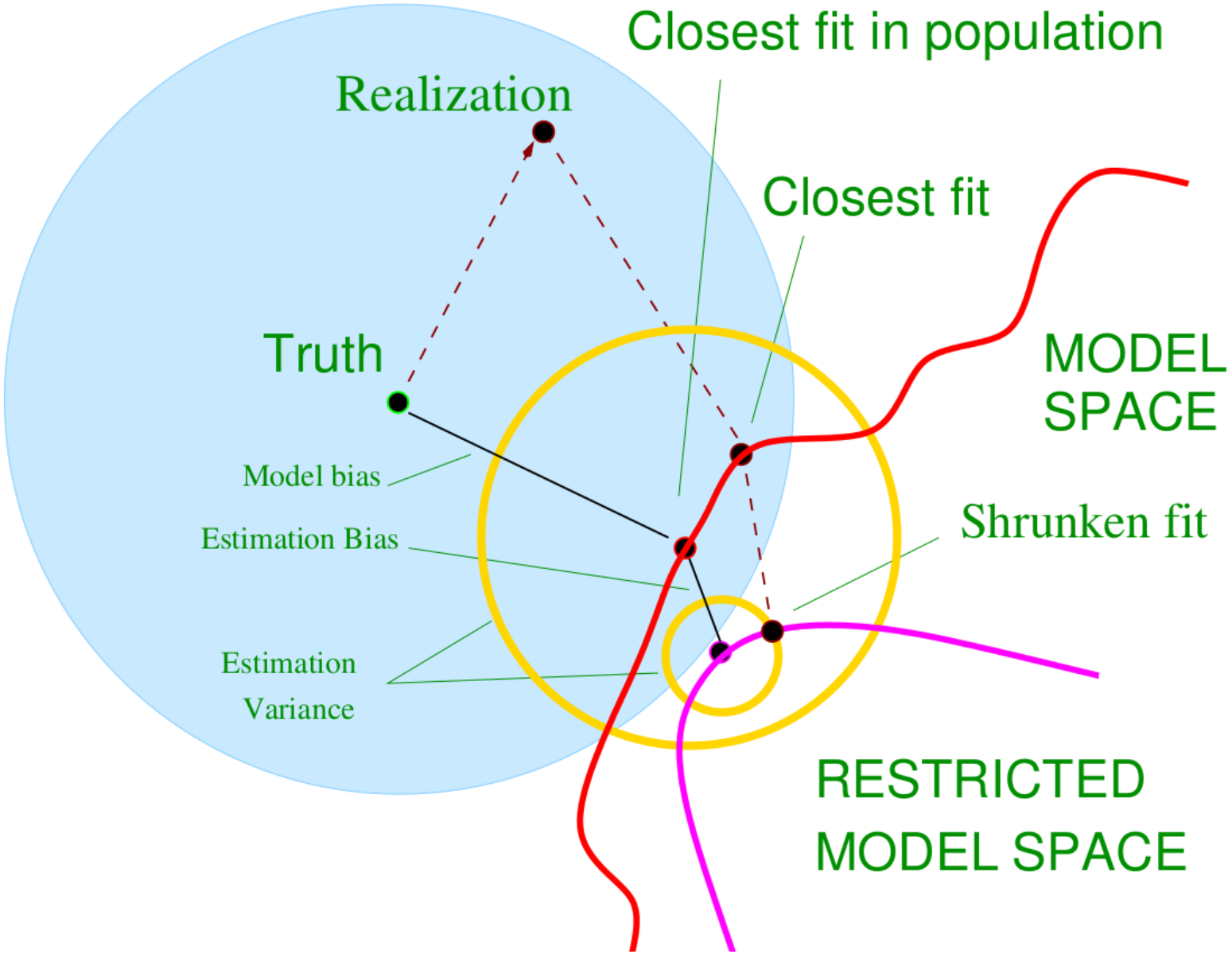
- $\hat{f}_p(x_0) = x_0^T (X^T X)^{-1} X^T y \rightarrow \text{Var}[\hat{f}_p(x_0)] = ||h(x_0)||^2 \sigma_\epsilon^2$.

In average,

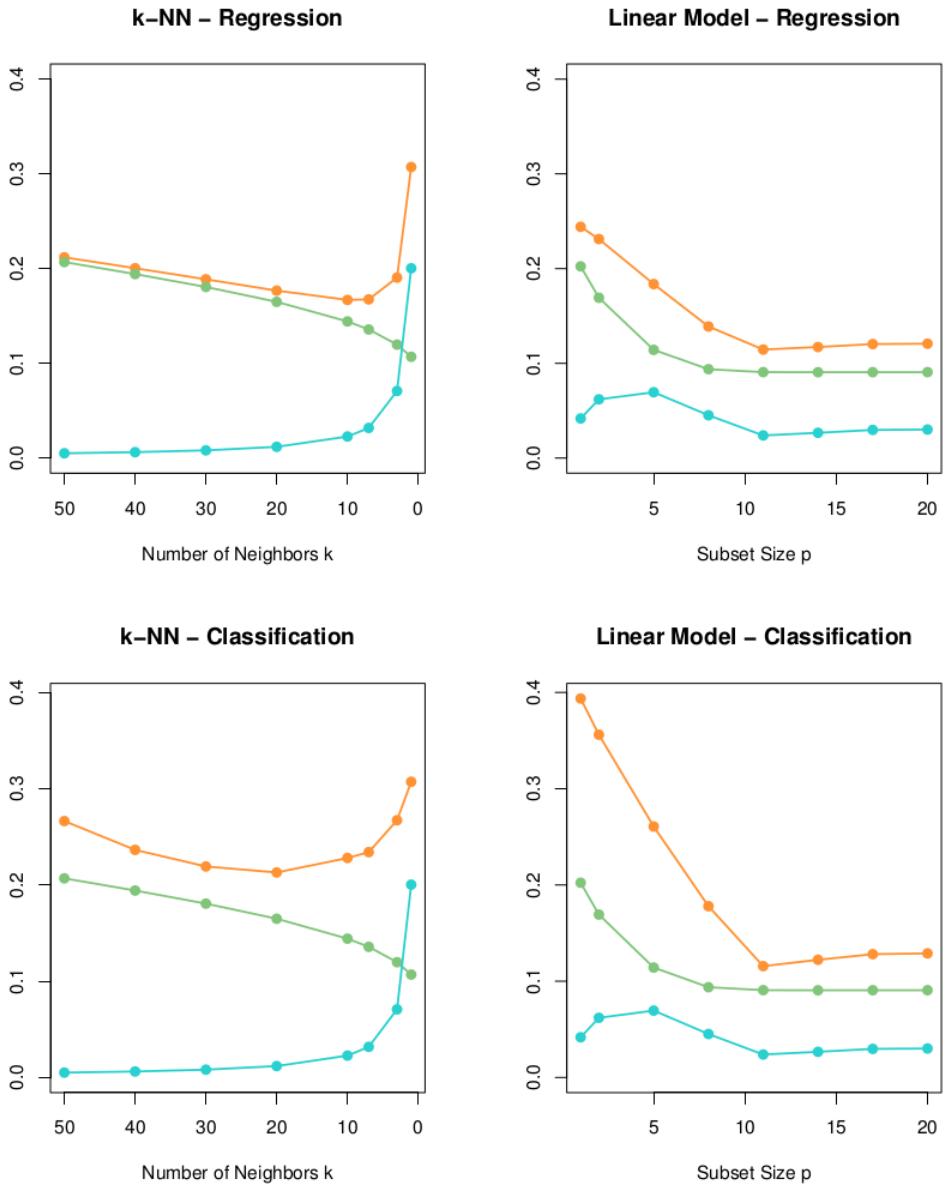
$$\frac{1}{N} \sum_{i=1}^{N} \text{Err}(x_i) = \sigma_\epsilon^2 + \frac{1}{N} \sum_{i=1}^{N} [f(x_i) - E[f_p(x_i)]]^2 + \frac{p}{N} \sigma_\epsilon^2,$$

so the model complexity is directly related to p.

The Bias–Variance Decomposition:



The Bias–Variance Decomposition: example



Optimism of the Training Error Rate: definitions

Being a little bit more formal,

$$\text{Err}_{\mathcal{T}} = E_{X_0,Y_0}[L(Y_0, \hat{f}(X_0))|\mathcal{T}]$$

where:

- (X_0, Y_0) are from the new test set;
- $\mathcal{T} = \{(x_1, y_1) \dots (x_n, y_n)\}$ is fixed.

Taking the expected value over $\mathcal{T}$, we obtain the expected error

$$\text{Err} = E_{\mathcal{T}}\left[E_{X_0,Y_0}[L(Y_0, \hat{f}(X_0))|\mathcal{T}]\right].$$

Optimism of the Training Error Rate: definitions

We said that the training error,

$$\overline{\text{err}} = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}(x_i)),$$

is **NOT** a good estimator of $\text{Err}_{\mathcal{T}}$:

- same data used both for training and test;
- a fitting method tends to adapt to the specific dataset;
- the result is a too optimistic evaluation of the error.

How to measure this optimism?

Optimism of the Training Error Rate: optimism and average optimism

Let us define the in-sample error,

$$\text{Err}_{\text{in}} = \sum_{i=1}^{N} E_{Y_0}[L(Y_{i0}, \hat{f}(x_i))|\mathcal{T}],$$

i.e., the error computed w.r.t. new values of the outcome on the same values of the training points $x_i, i = 1, \ldots, N$.

We define optimism the difference between Err_{in} and $\overline{\text{err}}$,

$$\text{op} := \text{Err}_{\text{in}} - \overline{\text{err}}.$$

and the average optimism its expectation,

$$\omega := E_Y[\text{op}].$$

NB: as the training points are fixed, the expected value is taken w.r.t. their outcomes.

Optimism of the Training Error Rate: optimism and average optimism

For a reasonable number of loss functions, including 0-1 loss and squared error, it can be shown that

$$\omega = \frac{2}{N}\sum_{i=1}^{N} \text{Cov}(\hat{y}_i, y_i),$$

where:

- Cov stands for covariance;
- $\hat{y}_i$ is the prediction, $\hat{y}_i = \hat{f}(x_i)$;
- y_i is the actual value.

Therefore:

- optimism depends on how much y_i affects its own prediction;
- the "harder" we fit the data, the larger the value of $\text{Cov}(\hat{y}_i, y)$ $\longrightarrow$ the larger the optimism.

Optimism of the Training Error Rate: optimism and average optimism

As a consequence,

$$E_Y[\mathsf{Err}_{\mathsf{in}}] = E_Y[\overline{\mathsf{err}}] + \frac{2}{N}\sum_{i=1}^{N}\mathsf{Cov}(\hat{y}_i, y_i).$$

When $\hat{y}_i$ is obtained by a linear fit of d inputs the expression simplifies. For the linear additive model $Y = f(X) + \epsilon$,

$$\sum_{i=1}^{N}\mathsf{Cov}(\hat{y}_i, y_i) = d\sigma_\epsilon^2,$$

and

$$E_Y[\mathsf{Err}_{\mathsf{in}}] = E_Y[\overline{\mathsf{err}}] + 2\frac{d}{N}\sigma_\epsilon^2. \quad (1)$$

Therefore:

- optimism increases linearly with the number of predictors;
- it decreases linearly with the training sample size.

Optimism of the Training Error Rate: estimation

Methods we will see:

- C_p, AIC, BIC estimate the optimism and add it to the training error (work when estimates are linear in their parameters);
- cross-validation and bootstrap directly estimate the expected error (work in general).

Further notes:

- in-sample error is in general NOT of interest;
- when doing model selection/find the right model complexity, we are more interested in the relative difference in error rather than the absolute one.

Estimates of In-Sample Prediction Error: C_p

Consider the general form of the in-sample estimates,

$$\widehat{\mathsf{Err}}_{\mathsf{in}} = \overline{\mathsf{err}} + \hat{\omega}.$$

Equation (1),

$$E_Y[\mathsf{Err}_{\mathsf{in}}] = E_Y[\overline{\mathsf{err}}] + 2\frac{d}{N}\sigma_\epsilon^2,$$

in the case of linearity and square errors, leads to the C_p statistics,

$$C_p = \overline{\mathsf{err}} + 2\frac{d}{N}\hat{\sigma}_\epsilon^2,$$

where:

- $\overline{\mathsf{err}}$ is the training error computed by the square loss;
- d is the number of parameters (e.g., regression coefficients);
- $\hat{\sigma}_\epsilon^2$ is an estimate of the noise variance (computed on the full model, i.e., that having the smallest bias).

Estimates of In-Sample Prediction Error: AIC

Similar idea for AIC (Akaike Information Criterion):

- we start from equation (1);
- more general by using a log-likelihood approach,

$$-2E[\log p_{\hat{\theta}}(Y)] \approx -\frac{2}{N} E\left[\sum_{i=1}^{N} \log p_{\hat{\theta}}(y_i)\right] + 2\frac{d}{N}$$

Note that:

- the result holds asymptotically (i.e., $N \to \infty$);
- $p_{\hat{\theta}}(Y)$ is the family of densities of Y, indexed by θ;
- $\sum_{i=1}^{N} \log p_{\hat{\theta}}(y_i) = \ell(\hat{\theta})$, the maximum likelihood estimate.

Examples:

- logistic regression, AIC $= -\frac{2}{N}\ell(\hat{\theta}) + 2\frac{d}{N}$;
- linear regression, AIC $\propto$ C_p.

Estimates of In-Sample Prediction Error: AIC

To find the best model, we choose that with the smallest AIC:

- straightforward in the simplest cases (e.g., linear models);
- more attention must be devoted in more complex situations
  - issue of finding a reasonable measure for the model complexity;

Usually minimizing the AIC is not the best solution to find the value of the tuning parameter

- cross-validation works better in this case.

The Effective Number of Parameters

Generalize the concept of number of predictors to extend the previous approaches to more complex situations.
Let

- $y = (y_1, \ldots, y_n)$ be the outcome;
- $\hat{y} = (\hat{y}_1, \ldots, \hat{y}_n)$ be the prediction.

For linear methods,

$$\hat{y} = Sy$$

where S is a $N \times N$ matrix which

- depend on X
- does NOT depend on y.

The Effective Number of Parameters

The effective number of parameters (or effective degrees of freedom) is defined as

$$\text{df}(S) := \text{trace}(S);$$

- $\text{trace}(S)$ is the sum of the diagonal elements of S;
- we should replace d with $\text{trace}(S)$ to obtain the correct value of the criteria seen before;
- if $y = f(X) + \epsilon$, with $\text{Var}(\epsilon) = \sigma_\epsilon^2$, then $\sum_{i=1}^N \text{Cov}(\hat{y}_i, y_i) = \text{trace}(S)\sigma_\epsilon^2$, which motivates

$$\text{df}(\hat{y}) = \frac{\sum_{i=1}^N \text{Cov}(\hat{y}_i, y_i)}{\sigma_\epsilon^2}.$$

The Bayesian Approach and BIC: BIC

The BIC (Bayesian Information Criterion) is an alternative criterion to AIC,

$$\frac{1}{N}\text{BIC} = -\frac{2}{N}\ell(\hat{\theta}) + \log N \frac{d}{N}$$

- similar to AIC, with $\log N$ instead of 2;
- if $N > e^2 \approx 7.4$, BIC tends to favor simpler models than AIC.

- For the Gaussian model,

$$\text{BIC} = \frac{N}{\sigma_\epsilon^2}\left[\overline{\text{err}} + (\log N)\frac{d}{N}\sigma_\epsilon^2\right].$$

The Bayesian Approach and BIC: motivations

Despite similarities, AIC and BIC come from different ideas. In particular, BIC comes form the Bayesian model selection approach. Suppose

- $\mathcal{M}_m$, $m = 1, \ldots, M$ be a set of candidate models;
- θ_m be their correspondent parameters;
- $Z = (x_1, y_1), \ldots, (x_N, y_N)$ be the training data.

Given the prior distribution $Pr(\theta_m|\mathcal{M}_m)$ for all θ_m, the posterior is

$$Pr(\mathcal{M}_m|z) \propto Pr(\mathcal{M}_m) \cdot Pr(Z|\mathcal{M}_m)$$
$$\propto Pr(\mathcal{M}_m) \cdot \int_{\Theta_m} Pr(Z|\mathcal{M}_m, \theta_m) \cdot Pr(\theta_m|\mathcal{M}_m)\, d\theta_m.$$

The Bayesian Approach and BIC: motivations

To choose between two models, we compare their posterior distributions,

$$\frac{Pr(\mathcal{M}_m|z)}{Pr(\mathcal{M}_\ell|z)} = \underbrace{\frac{Pr(\mathcal{M}_m)}{Pr(\mathcal{M}_\ell)}}_{\text{prior preference}} \cdot \underbrace{\frac{Pr(Z|\mathcal{M}_m)}{Pr(Z|\mathcal{M}_\ell)}}_{\text{Bayes factor}}$$

- usually the first term on the right hand side is equal to 1 (same prior probability for the two models);
- the choice between the models is based on the Bayes factor.

Using some algebra (including the Lapalce approximation), we find

$$\log Pr(Z|\mathcal{M}_m) = \log Pr(Z|\hat{\theta}_m, \mathcal{M}_m) - \frac{d_m}{2}\log N + O(1).$$

where:

- $\hat{\theta}_m$ is the maximum likelihood estimate of θ_m;
- d_m is the number of free parameters in the model $\mathcal{M}_m$.

The Bayesian Approach and BIC: motivations

Note:

- If the loss function is $-2\log Pr(Z|\hat{\theta}_m, \mathcal{M}_m)$, we find again the expression of BIC;

- selecting the model with smallest BIC corresponds to selecting the model with the highest posterior probability;
- in particular, note that,

$$\frac{e^{-\frac{1}{2}BIC_m}}{\sum_{\ell=1}^{M} e^{-\frac{1}{2}BIC_\ell}}$$

is the probability of selecting the model m (out of M models).

The Bayesian Approach and BIC: AIC versus BIC

For model selection, what to choose between AIC and BIC?

- there is no clear winner;
- BIC leads to a sparser model;
- AIC tends to be better for prediction;
- BIC is consistent ($N \to \infty$, Pr(select the true model) $= 1$);
- for finite sample sizes, BIC tends to select a model which is too sparse.