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Machine learning, big data and artificial intelligence – Block 1

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November 2022

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This weeks lectures

- Regularization
- Model Selection and Assement
- Cross-Validation
- Evaluate classification models

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Section 1

Model Predictive Performance

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Previous Model Evaluation

In the past, we have used a large number of tools for assessing models, e.g.:

- Various plots
- Residuals
- Leverage, Cook's distance
- p-values
- R^2

That is, they only tell us how well the model fits the data, and diagnose the model.

The focus is usually *estimation* or *attribution*.

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Predictive Performance

- We are interested in how our model work when predicting a new observation
- Models can be overly optimistic – the model can have a good fit but be poor at making predictions for new data[1], a phenomenon known as overfitting.

[1] See e.g. Picard, R.R., Cook, R.D. (1984). Cross-validation of regression models. *Journal of the American Statistical Association*, **79(387)**, 575–583.

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Loss Functions (again)

- To assess the performance we use the loss function for a new unseen observation y_0, and the prediction of that observation $\hat{y}$

$$L(y_0, \hat{y}_0)$$

- This is quite general and we choose based L based on what we want the model performe well on.
- Examples:
  - Regression problems:

$$L(y_0, \hat{y}_0) =$$

  - Language models: Perplexity, Glue, Human annotation

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Confusion Matrix

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Accuracy

$$\text{Accuracy} = \frac{(\text{TP}+\text{TN})}{(\text{TP}+\text{FP}+\text{FN}+\text{TN})}$$

What is the problem with Accuracy?

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Precision and Recall

$$\text{Precision} = \frac{(\text{TP})}{(\text{TP}+\text{FP})}$$

Of the predicted positives, how many are actually positive?

$$\text{Recall} = \text{Sensitivity} = \frac{(\text{TP})}{(\text{TP}+\text{FN})}$$

Of all positives, how many are predicted correctly?

$$\text{Specificity} = \frac{(\text{TN})}{(\text{TN}+\text{FP})}$$

Of all negative, how many are predicted correctly?

$$\text{F1} = 2 \cdot \frac{(\text{Precision} \cdot \text{Recall})}{(\text{Precision} + \text{Recall})}$$

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Example

Say that we want to classify spam vs. ham.

	$\hat{y} = 0$	$\hat{y} = 1$
$y = 0$	515	91
$y = 1$	85	569

The cell counts yield us estimates of

- Accuracy $P(\hat{y} = y)$: $\frac{515+569}{515+91+85+569} \approx 0.86$

In this example, we let $\hat{y}_i = 1$ whenever $\hat{\pi}_i > 0.5$. What if we choose another cut-off level $\hat{\pi}_i > \alpha$ instead?

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Classification tables

Previous table, with acc. 86 %, sens. 87 % and spec. 85 %:

$\alpha = 0.5$	$\hat{y} = 0$	$\hat{y} = 1$
$y = 0$	515	91
$y = 1$	85	569

Now let $\alpha = 0.3$ instead, so that we are more prone to say that $\hat{y} = 1$:

$\alpha = 0.3$	$\hat{y} = 0$	$\hat{y} = 1$
$y = 0$	462	144
$y = 1$	38	616

Accuracy: 86 %, sensitivity: 94 %, specificity: 76 %.

The sensitivity has increased, but the sensitivity has decreased...

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A more reasonable example

Previous table, highly unbalanced. 1001 ham and 17 spam.

Our new classifier: Everything is ham!

	$\hat{y} = 0$	$\hat{y} = 1$
$y = 0$	1001	0
$y = 1$	17	0

Accuracy: 98 %! and sensitivity: 100 %, specificity: 0 %.

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Cross-Entropy Loss

- When we have probabilities $\hat{p} = \hat{y}_0$:

$$L(y_0, \hat{p}) = -(y_0 \log \hat{p}) + ((1 - y_0) \log (1 - \hat{p}))$$

  Question: Do you recognize the loss function?
- Maximizing the likelihood is the same as minimizing the cross-entropy.
- Multi class generalization over M classes

$$L(\mathbf{y}_0, \hat{\mathbf{p}}) = -\sum_{j=1}^{M} y_{0,j} \log \hat{p}_j$$

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Section 2

Test error

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Test Error

- The main error of interest - *generalization error*
- Conditional Test Error
  (Model performance for the *training* data):

$$\mathrm{Err}_{\mathcal{T}} = \mathbb{E}_{Y,X}(L(Y, \hat{Y}(X)|\mathcal{T})$$

- Expected Test Error
  (Model performance over *different* data):

$$\mathrm{Err} = \mathbb{E}_{\mathcal{T}}(\mathbb{E}_{Y,X}(L(Y, \hat{Y}(X)))$$

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Training Error

- The Error the algorithm try to minimize
- Error over the training sample:

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

- Can be seen as a Monte Carlo Appraximation over data

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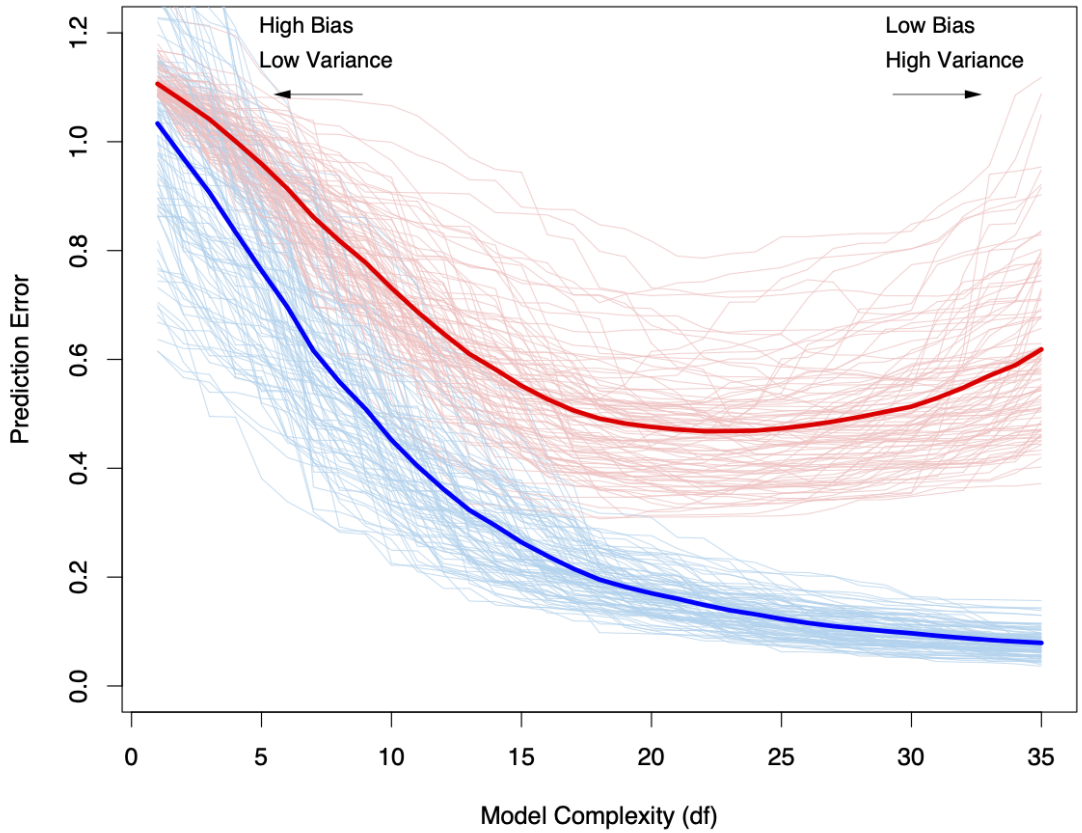
How are training and test error related?

Figure: Test, training, and model complexity (Hastie et al, 2009, Figure 7)



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How to estimate the Test Error: Model Assesment

- We set aside a *test set* from the data
- Use as the last step to *estimate* the test error
- Should only be used *ONCE*
- Size of testset:
  - Common suggestion 10%
  - A statistical estimation problem

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Multiple Use of Test Set for Model Assesment

- Say that we have $\hat{L}(\mathcal{T})$ an estimate of the loss on the test set given a training set
- Lets say that we have $i \in \{1, ..., M\}$ be models trained on M independent training sets $\mathcal{T}_i$ but they all have the same underlying error L^*
- Then we can assume that

$$\hat{L}_i(\mathcal{T}_i) \sim N(L^*, \sigma)$$

- What happens if we use the test set to pick the model?

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Section 4

Model Selection

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Model Selection

- We want to select a model based on performance.
- Important when using hyperparameters (as in regularization)

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Bias and Variance

Assume we have the following data generating process:

$$Y = f(X) + \epsilon\,,$$

where $\mathbb{E}(\epsilon) = 0$ and $V(\epsilon) = \sigma_\epsilon$.

$$\begin{aligned}
\text{Err}(x_0) &= \mathbb{E}_Y\{(Y - \hat{f}(x_0))^2 | X = x_0\} \\
&= \sigma_\epsilon^2 + \{\mathbb{E}_Y(\hat{f}(x_0)) - f(x_0)\}^2 + \mathbb{E}\{\hat{f}(x_0) - \mathbb{E}_Y(\hat{f}(x_0))\}^2 \\
&= \sigma_\epsilon^2 + \text{Bias}^2(\hat{f}(x_0)) + V(\hat{f}(x_0))
\end{aligned}$$

- *Bias*: How close can we get to the true model
- *Variance*: The variability of the predictions
- *Irreducible error*: The best (theoretically) possible model

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Bias and Variance: Linear regression

In linear regression we have:

$$\hat{f}(x_i) = \hat{\beta} x_i$$

This give us the following error decomposition:

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

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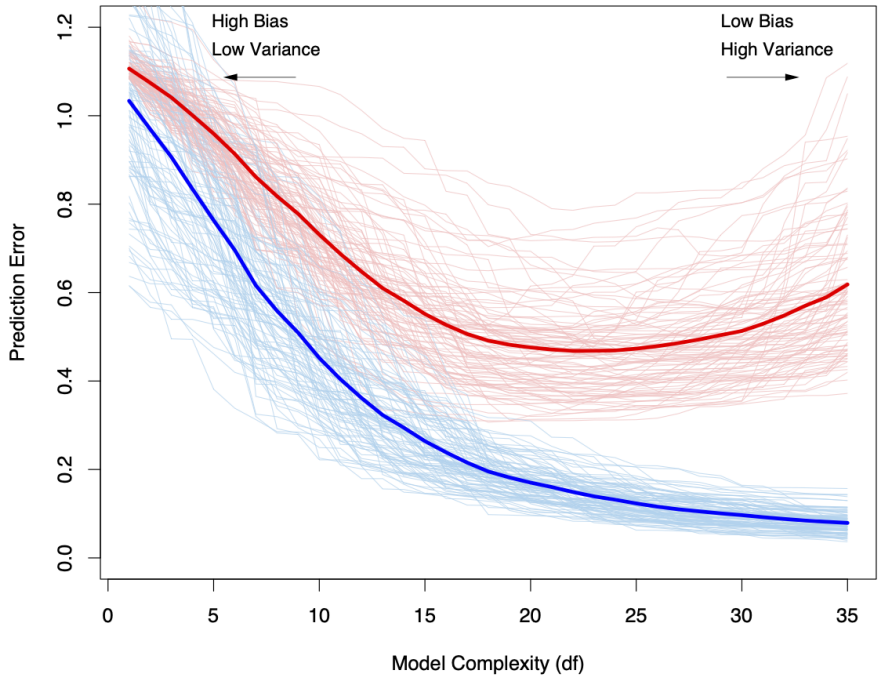
Bias and Variance

Figure: Test, training, and model complexity (Hastie et al, 2009, Figure 7)



- High Bias: Underfit
- High Variance: Overfit
- High Irreducible error: No model is good

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Optimism of Training Error

The in-sample test error:

$$\text{Err}_{\text{in}} = \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}_{Y^0}\{L(Y_i^0, \hat{f}(x_i))|\mathcal{T}\},$$

where $Y_{0,i}$ is a new response variable condition on x_i.

We have that

$$\mathbb{E}_{\mathbf{y}}(\text{Err}_{\text{in}}) = \mathbb{E}_{\mathbf{y}}(\overline{\text{err}}) + \underbrace{\frac{2}{N}\sum_{i=1}^{N}\text{Cov}(\hat{y}_i, y_i)}_{\text{optimism}},$$

where $\overline{\text{err}}$ is the training error.

How could we create an optimistic classifier for the training data?

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Estimating Optimism

- Under certain conditions we can estimate this optimism.
- AIC, BIC etc are examples of this – asymptotic predictive performance.

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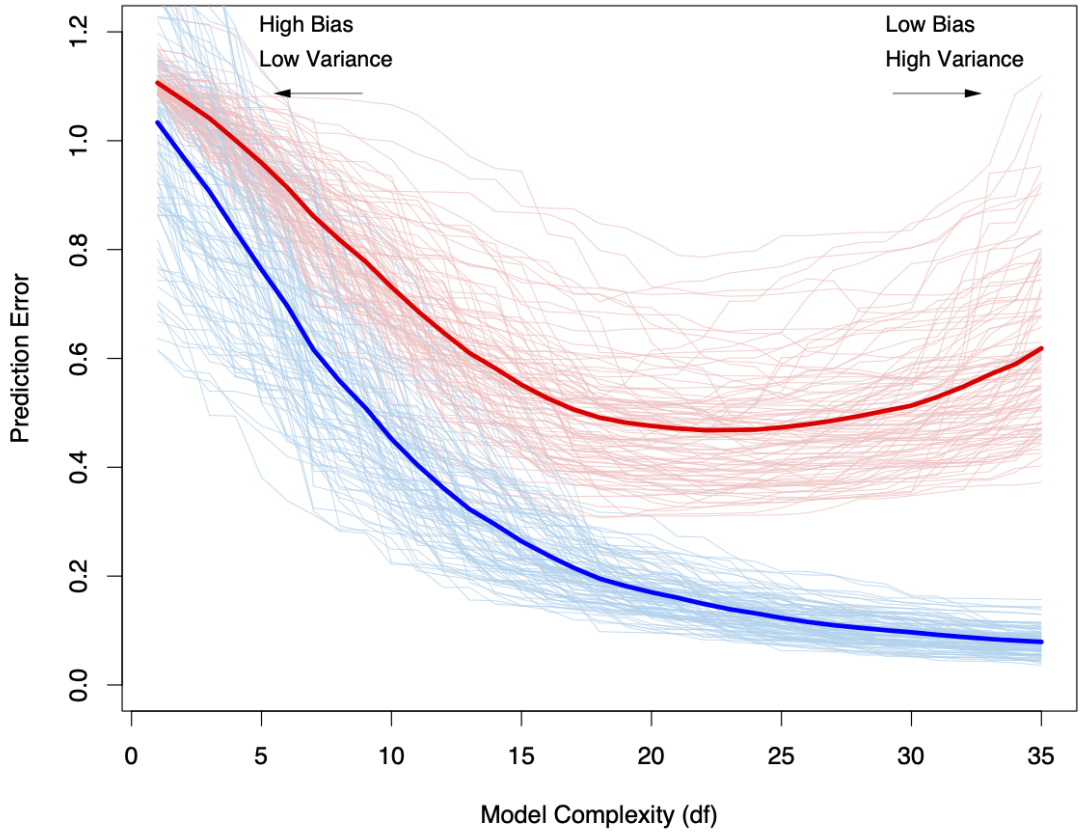
Find the Optimism!

Figure: Test, training, and model complexity (Hastie et al, 2009, Figure 7)



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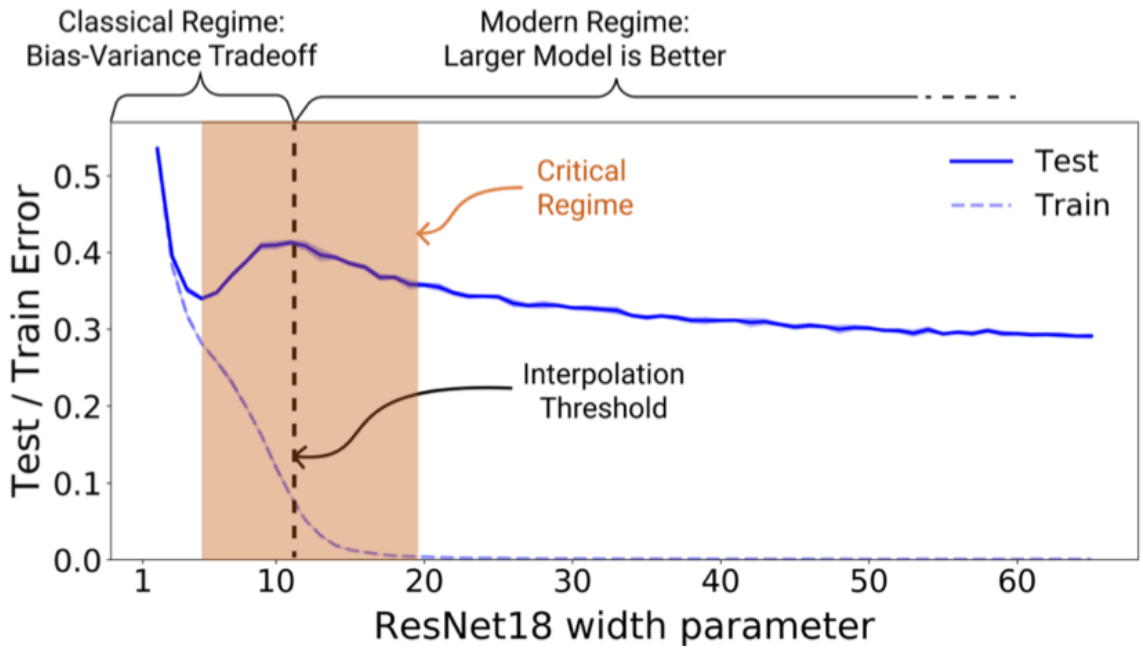
The double descent behaviour of large models

Figure: The double descent of large models (Nakkiran et al., 2019, Figure 1)



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Section 5

Cross-validation

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Cross-Valdidation

We want to estimate Err for different models and to choose the best model.

Cross-Validation is probably the most popular approach to estimate Err.

- The model is judged only on how well it does predictions for new data.
- No need for rules-of-thumbs to verify that tests and estimators are applicable.
- No need to worry about significance levels, standard errors etc.
- Equally useful for frequentist, Bayesian and algorithmic methods (and these can easily be compared).

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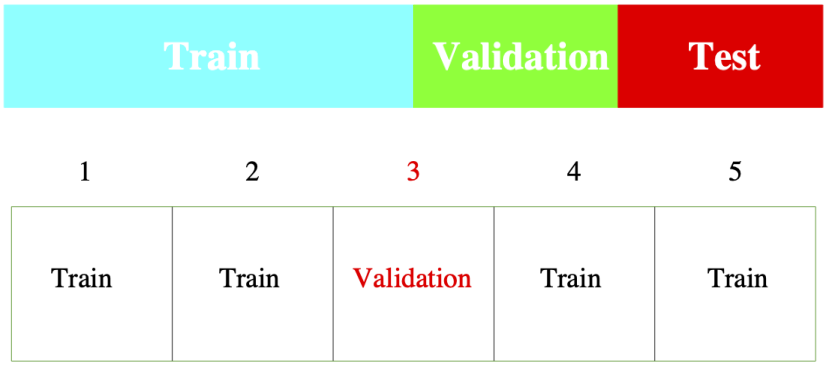
Cross-Valdidation Algorithm

Figure: Cross-Validation (Hastie et al, 2009, p. 222, 242)



1. Split data in K folds
2. For each fold $k = 1, 2, ..., K$
   - 2.1 Use all samples except those in k to build the predictive model
   - 2.2 Use the model and predict the observations in fold k

$$CV(\hat{f}, \alpha) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, \hat{y}_{-\kappa(i)}(x_i, \alpha)$$

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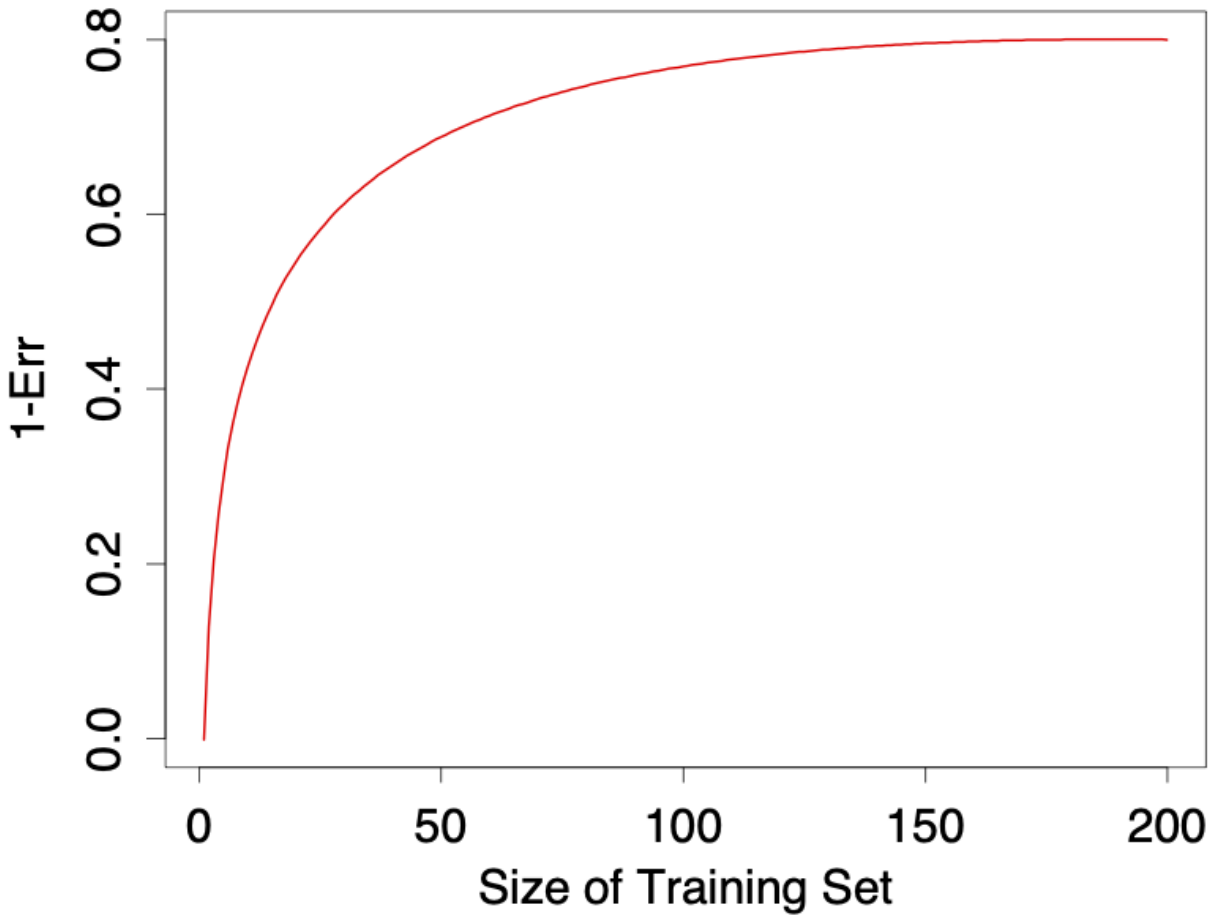
The Bias of Cross-Valdidaton

Figure: Cross-Validation Bias (Hastie et al, 2009, Fig. 7.8)



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Leave-One-Out Cross Validation

- We set $K = N$
- Benefits
  - Almost unbiased estimate of Err
  - Can be less computationally costly is some situations
- Drawbacks
  - Higher Variance
  - Can be more computationally costly (naive implementation)

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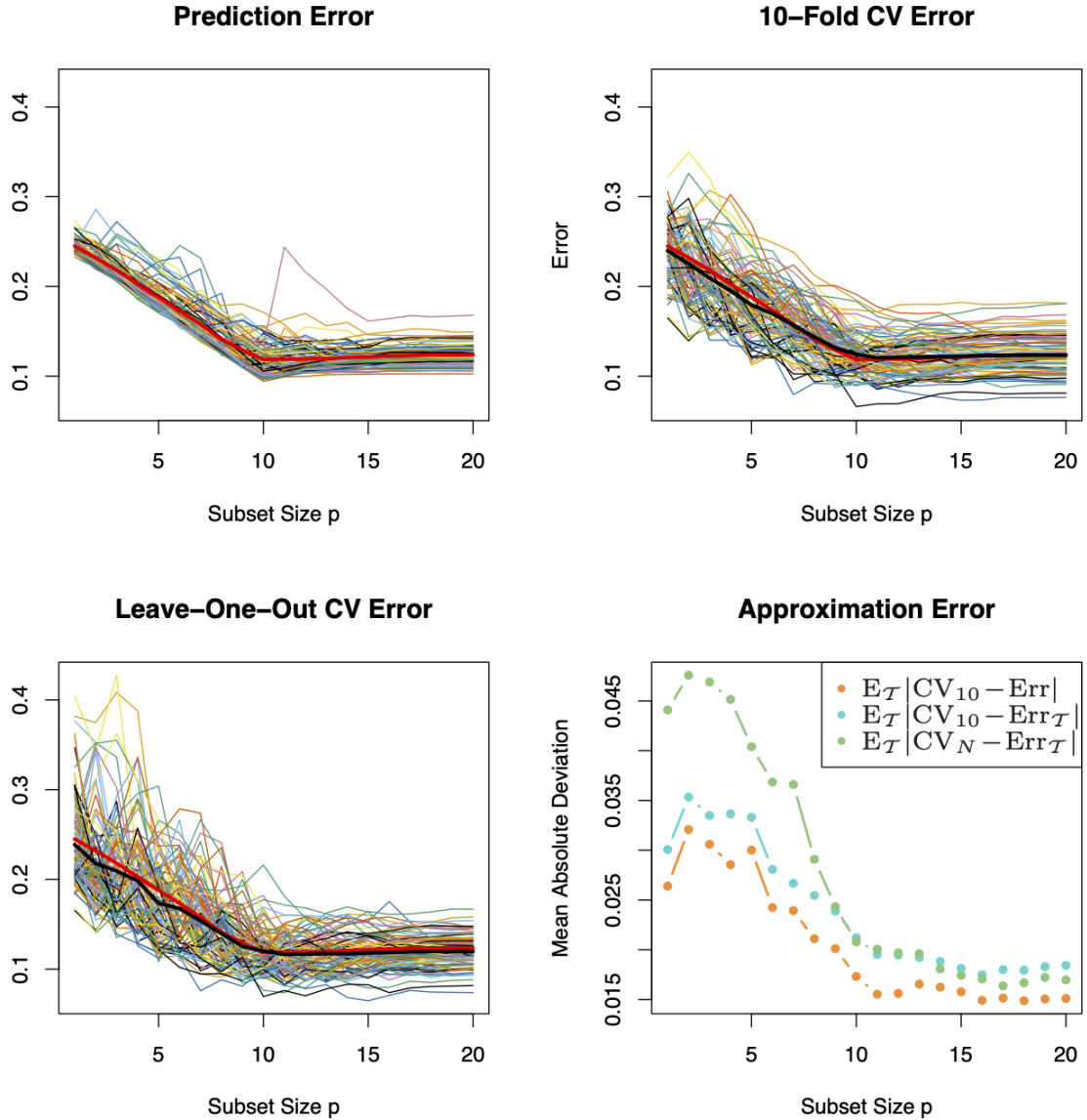
Leave-One-Out Cross Validation

Figure: Cross-Validation Bias (Hastie et al, 2009, Fig. 7.14)



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The role of the data generating process

- we assume that testset and train set are different observations from the same data generating process

$$\mathbf{d} = \{(y_i, \mathbf{x}_i), i = 1, ..., n\} \sim P_{y,x}$$

- Things that can go wrong:
  - temporal leak/concept drift
  - duplicated observations
  - non-randomized data
- Example: Evaluating prediction models for Elections

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Section 6

Regularisation

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Regression and GLM

- Linear regression and logistic regression are examples of generalised linear models, GLMs.
- Both use maximum likelihood estimation for fitting the model, where the likelihood function $L(\beta)$ is maximised.

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Regularised regression models

- In some situations, for instance when the predictors are highly collinear, when there are too many predictors or when there is complete separation in the data, maximum likelihood estimation is unstable.
  - Either the solution is not unique, or minuscule changes in the data can change the solution completely.
  - Such datasets are increasingly common in e.g. genomics, finance, astronomy and image analysis.
- In such cases, regularisation/shrinkage methods can be used instead.
- In a regularized GLM, it is not the likelihood $L(\beta)$ that is maximized, but a regularised function $L(\beta) \cdot p(\beta)$, where p is a penalty function that typically forces the resulting estimates to be closer to 0, which leads to a stable solution.

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Regularised regression models

Regularised linear regression models increase the bias of the estimates, but lowers their variance, thereby potentially decreasing the MSE.

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Connection to Bayesian estimation

In Bayesian estimation, a prior distribution $p(\beta)$ for the parameters β_i is chosen.

The estimates are then computed from the conditional distribution of the β_i given the data, called the posterior distribution.

Using Bayes' theorem, we find that

$$P(\beta|\mathbf{x}) \propto L(\beta) \cdot p(\beta),$$

i.e. that the posterior distribution is proportional to the likelihood times the prior.

A special type of Bayesian estimator is the maximum a posteriori (MAP) estimator, which is found by maximizing the above expression (i.e. finding the mode of the posterior).

This is equivalent to the estimates from a regularised frequentist model with penalty function $p(\beta)$!

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Inference and invariance

- Regularised regression models are not invariant under linear rescaling of the predictors.
  - If a predictor is multiplied by a scalar $a \neq 0$, this can change the entire model.
  - A model with measurements in inches might yield completely different results from a model with measurements in cm.
- For this reason, it is widely agreed that the predictors should be standardized to have mean 0 and variance 1 before a regularised model is fitted.
  - With this approach we choose a particular (natural?) scaling, among all possible scalings.
  - All predictors are on the same scale and are therefore treated equally by the penalty function.

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Inference and invariance

- Hypothesis tests are available (e.g. Lockhart et al. (2014), A significance test for the lasso, *Annals of Statistics*), but I advise against using them.
- Note that the hypothesis tests will be conditioned on the choice of scaling.
  - Because of this, regularised models are not appropriate for hypothesis testing – the p-values could change completely if we rescaled the data!
- Regularised regression models are however very useful for predictive modelling.

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L_q-penalties

The most popular penalty terms correspond to common L_q-norms. On a log-scale, the function to be maximized is

$$\ell(\beta) + \lambda \sum_{i=1}^{p} |\beta_i|^q,$$

where $\ell(\beta)$ is the loglikelihood of β and $\sum_{i=1}^{p} |\beta_i|^q$ is the L_q-norm, with $q \geq 0$.

This is equivalent to maximizing $\ell(\beta)$ under the constraint that $\sum_{i=1}^{p} |\beta_i|^q \leq \frac{1}{h(\lambda)}$, for some increasing positive function h.

- Relies on the sparsity assumption that most β are 0.

$\lambda \geq 0$ is a smoothing parameter:

- When $\lambda = 0$, we are back at the standard ML-estimate.
- The $\hat{\beta}$ are forced to be closer to 0 when λ increases.
- λ is usually chosen using cross-validation.

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Ridge regression

When the L_2 penalty is used, the regularised model is called ridge regression, for which we maximize

$$\ell(\beta) + \lambda \sum_{i=1}^{p} \beta_i^2.$$

- Invented and reinvented by several authors, from the 1940's onwards.
- In a linear model, the OLS estimate is $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$, whereas the ridge estimate is $\hat{\beta} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$. The $\lambda\mathbf{I}$ is the 'ridge'.
- The β_i can become very small, but are never pushed all the way down to 0.
- In a Bayesian context, this corresponds to putting a standard normal prior on the β_i.

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Lasso

When the L_1 penalty is used, the regularised model is called the lasso (Least Absolute Shrinkage and Selection Operator), for which we maximize

$$\ell(\beta) + \lambda \sum_{i=1}^{p} |\beta_i|.$$

- Introduced by Robert Tibshirani in 1996.
- As λ increases, more and more β_i become 0.
  - Simultaneously performs estimation and variable selection!
- In a Bayesian context, this corresponds to putting a standard Laplace prior on the β_i.

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Examples in R

Functions for regularised generalized linear models (linear, logistic, Poisson, multinomial, and more) are available e.g. in the `glmnet` package for R.

The syntax used is somewhat different from that for `glm` and `lm`.

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Generalizations

Regularised models have been a hot research topics in the last 20 years. Some additional important models are:

- Elastic net: a compromise between ridge and lasso, in which

$$\ell(\beta) + \lambda_1 \sum_{i=1}^{p} |\beta_i| + \lambda_2 \sum_{i=1}^{p} \beta_i^2$$

  is maximized.
  - Introduced by Zou and Hastie in 2005.
  - Is better than the lasso at handling correlated predictors.
  - Has two smoothing parameters that we need to choose.
  - Available in the `glmnet` package.

- Group lasso: a version of the lasso in which variables can be grouped before fitting the model. The group lasso then selects groups of variables rather than individual variables.
  - Introduced by Yuan and Lin in 2006.
  - Useful e.g. when we have dummies for categorical variables (in contrast, the lasso may choose to only include the dummies for some of the categories).