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Machine learning – Block 1(b)

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Section 1

Predictive Performance

Previous Model Evaluation

- In the past, tools for assessing models, e.g.:
  - Residuals
  - Leverage, Cook's distance
  - p-values
  - R^2
  - AIC
  - (LOO-CV)
- Model diagnoses and how well the model fits the data.

Previous Model Evaluation

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- Model diagnoses and how well the model fits the data.
- Statistics: estimation and attribution
- Supervised learning: predictive performance

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Predictive Performance

How well our model $\hat{f}_{\mathcal{T}}$ trained on

$$\mathcal{T} = \{(y_i, x_i), i = 1, ..., n\}$$

work when predicting a new observation (y_0, x_0) from the data generating process $P_{y,x}$.

$$\mathbb{E}\left[L(y_0, \hat{f}_{\mathcal{T}}(x_0))\right] = \int L(y_0, \hat{f}_{\mathcal{T}}(x_0)) P_{(y,x)} d(y_0, x_0)$$

where $L(y, x)$ is a loss function (e.g. $L(x, y) = (x - y)^2$)

Predictive Performance

- The ability to perform well on previously unobserved inputs is called generalization
- $\mathbb{E}\left[L(y_0, \hat{f}_{\mathcal{T}}(x_0))\right]$ is the generalization error

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- Models can underfit
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- Predictive Performance
- Measuring Performance
- Test and training error
- Estimating the test error
- Bias and Variance
- Cross-validation

Section 2

Measuring Performance

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Loss Functions

- To assess the performance we use the loss function for a new unseen observation y_0 and the prediction of that observation $\hat{f}(x_0)$

$$L(y_0, \hat{f}(x_0))$$

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- Examples:
  - Regression problems (squared loss/error):

$$L(y_0, \hat{f}(x_0)) = (y_0 - \hat{f}(x_0))^2$$

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  - Classification (0-1 loss)

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- Examples:
  - Regression problems (squared loss/error):
  $$L(y_0, \hat{f}(x_0)) = (y_0 - \hat{f}(x_0))^2$$
  - Classification (0-1 loss)
  $$L(y_0, \hat{f}(x_0)) = I(y_0 = \hat{f}(x_0))$$
  - In general: The negative log likelihood is a good loss function

Cross-Entropy Loss

- When we predict probabilities $\hat{f}(x_0) = \hat{p}$:

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

Question: Do you recognize the (cross-entropy) loss function?

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Question: Do you recognize the (cross-entropy) loss function?

- Maximizing the likelihood is the same as minimizing the cross-entropy.
- Multi class cross-entroy 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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The Confusion Matrix

- A common way to present performance in classification is the confusion matrix:

	Prediction	
Actual	Positive	Negative
Positive	True Positive (TP)	False Negative (FN)
Negative	False Positive (FP)	True Negative ((TN)

The Confusion Matrix: Multi-class

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	Prediction		
Actual	a	b	c
a	T_a	F_{ab}	F_{ac}
b	F_{ba}	T_b	F_{bc}
c	F_{ca}	F_{cb}	T_c

and

	Prediction		
Actual	TP	FP	FN
a	T_a	$F_{ba} + F_{ca}$	$F_{ab} + F_{ac}$
...	...	...	...

and N is the sum over all cells.

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Accuracy

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

or

$$\text{Accuracy} = \frac{T_a + T_b + T_c}{N}$$

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or

$$\text{Accuracy} = \frac{T_a + T_b + T_c}{N}$$

Question: Can you see a problem with Accuracy?

Precision

Of all the predicted positives, how many are actually positive?

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

or

$$\text{Precision}_a = \frac{(T_a)}{T_a + F_{ba} + F_{ca})}$$

All predicted a: $T_a + F_{ba} + F_{ca}$

If we want one precision estimate for all classes:

1. Macro-average $(\text{Precision}_a, ..., \text{Precision}_c)$
2. Micro-average (use Table 2)

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Recall

Of all positives, how many are predicted correctly (recalled)?

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Recall

Of all positives, how many are predicted correctly (recalled)?

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

and

$$\text{Recall}_a = \frac{(T_a)}{T_a + F_{ab} + F_{ac})}$$

All true/actual a: $T_a + F_{ab} + F_{ac}$

If we want one precision estimate for all classes:

1. Macro-average (Recall$_a$, ..., Recall$_c$)
2. Micro-average (use Table 2)

Sensitivity and specificity

$$\text{Sensitivity} = \text{Recall of positive class} = \frac{\text{TP}}{\text{TP}+\text{FN}}$$

and

$$\text{Specificity} = \text{Recall of negative class} = \frac{\text{TN}}{\text{TN}+\text{FP}}$$

F1-score

Harmonic mean of Precision and Recall.

$$F_1 = \frac{2}{\text{Precision}^{-1} + \text{Recall}^{-1}} = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$$

Question: What happens if Precision or Recalls goes toward zero/one?

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Question: What happens if Precision or Recalls goes toward zero/one? Very common performance measurement in practice.

If we want one precision estimate for all classes:

1. Macro-average $(F_{1a}, ..., F_{1c})$
2. Micro-average (use Table 2)

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Example

Say that we want to classify spam vs. ham.

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Example

Say that we want to classify spam vs. ham.

	$\hat{f}(x) = 1$	$\hat{f}(x) = 0$
$y = 1$	515	91
$y = 0$	85	569

The cell counts yield us estimates of

1. Accuracy: $\frac{515+569}{515+91+85+569} \approx 0.86$
2. Precision: $\frac{515}{515+85} \approx 0.86$
3. Recall: $\frac{515}{515+91} \approx 0.85$
4. F_1: $\frac{2 \cdot 0.85 \cdot 0.86}{0.85+0.86} \approx 0.855$

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3. Recall: $\frac{515}{515+91} \approx 0.85$
4. F_1: $\frac{2 \cdot 0.85 \cdot 0.86}{0.85+0.86} \approx 0.855$

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

$\alpha = 0.5$	$\hat{f}(x) = 1$	$\hat{f}(x) = 0$
$y = 0$	515	91
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Classification tables

$\alpha = 0.5$	$\hat{f}(x) = 1$	$\hat{f}(x) = 0$
$y = 0$	515	91
$y = 1$	85	569

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

$\alpha = 0.3$	$\hat{f}(x) = 1$	$\hat{f}(x) = 0$
$y = 1$	462	144
$y = 0$	38	616

The cell counts yield us estimates of

1. Accuracy: $\frac{462+616}{462+38+144+616} \approx 0.86$
2. Precision: $\frac{462}{462+38} \approx 0.92$
3. Recall: $\frac{462}{462+144} \approx 0.76$
4. F_1: $\frac{2 \cdot 0.92 \cdot 0.76}{0.92+0.76} \approx 0.83$

The Precision has increased, but the Recall has decreased...

A more problematic example

A highly unbalanced example. 1001 ham and 17 spam.

Our new classifier: Everything is ham!

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A more problematic example

A highly unbalanced example. 1001 ham and 17 spam.

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	$\hat{f}(x) = 1$	$\hat{f}(x) = 0$
$y = 1$	1001	0
$y = 0$	17	0

A more problematic example

A highly unbalanced example. 1001 ham and 17 spam.

Our new classifier: Everything is ham!

	$\hat{f}(x) = 1$	$\hat{f}(x) = 0$
$y = 1$	1001	0
$y = 0$	17	0

The cell counts yield us estimates of

1. Accuracy: $\frac{1001}{1001+17} \approx 0.99$
2. Precision: $\frac{1001}{1001+0} \approx 1.0$
3. Recall: $\frac{1001}{1001+17} \approx 0.99$
4. F_1: $\frac{2 \cdot 1 \cdot 0.99}{0.99+1} \approx 0.99$

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The cell counts yield us estimates of

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2. Precision: $\frac{1001}{1001+0} \approx 1.0$
3. Recall: $\frac{1001}{1001+17} \approx 0.99$
4. F_1: $\frac{2 \cdot 1 \cdot 0.99}{0.99+1} \approx 0.99$
5. F_1 for negative class: $\frac{2 \cdot 0 \cdot 0}{0+0}$ Not defined, but 0 in the limit as Precision and Recall goes to 0.
6. And Specificity is 0!

Questions?

Questions?

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Section 3

Test and training error

Test Error

- The main error of interest - *generalization error*
- Conditional Test Error
  (Performance for the model trained on actual training data):

$$\mathrm{Err}_{\mathcal{T}} = \mathbb{E}_{p(X_0,Y_0)}(L(Y_0, \hat{f}(X_0)|\mathcal{T})$$

- Expected Test Error
  (Model performance over different training datasets):

$$\mathrm{Err} = \mathbb{E}_{p(X,Y)}(L(Y_0, \hat{f}(X_0)))$$

- Sometimes refered to as generalization error.
- Conditional Test Error is more difficult to estimate than the Expected Test Error (Bates, Hastie, and Tibshiriani, 2021)

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Training Error

- Training error: The loss the algorithm try to minimize
- The Error in the training data:

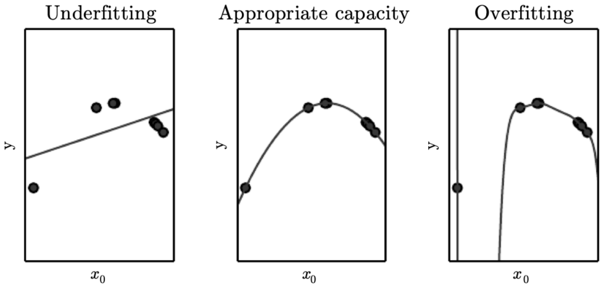
$$\overline{\text{err}} = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}(x_i))$$

where $L(y, x)$ is the loss function.

Model complexity/capacity

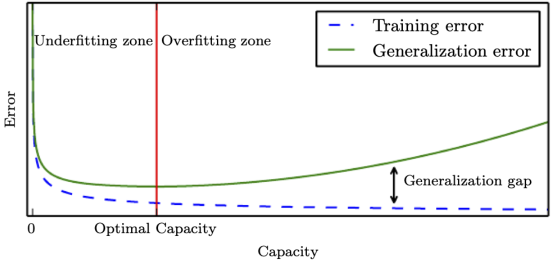
- Model complexity/capacity: The flexibility of the model.
- Underfitting: Too low capacity of model
- Overfitting: Too high capacity of model
- Example: Polynomial regression with higher order terms

Figure: Model complexity (Goodfellow et al, 2017, Figure 5.2)



Training, test, and complexity

Figure: Test, training, and model complexity (Goodfellow et al, 2017, Figure 5.3)



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 generalization error
- Should only be used ONCE (or a few times)

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- We set aside a test set from the data
- Use as the last step to estimate the generalization error
- Should only be used ONCE (or a few times)
- Size of testset:
  - Common suggestion is 10%, but
  - It is a statistical estimation problem (choice of sampling size)

Multiple Use of Test Set for Model Assesment

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

Questions?

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Questions?

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Section 5

Bias and Variance

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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 $V(\epsilon) = \sigma_\epsilon$.

We have an estimated model $\hat{f}$ and want to predict a new, unseen, observation x_0. The error can then be decomposed into:

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

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- *Bias*: How close can $\hat{f}$ get to the true model f
- *Variance*: The variability of the predictions from $\hat{f}$
- *Irreducible/Bayes error*: The minimum possible error

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:

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

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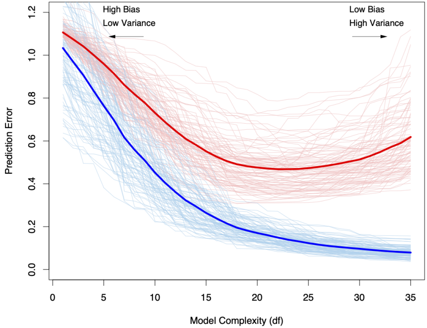
Bias and Variance

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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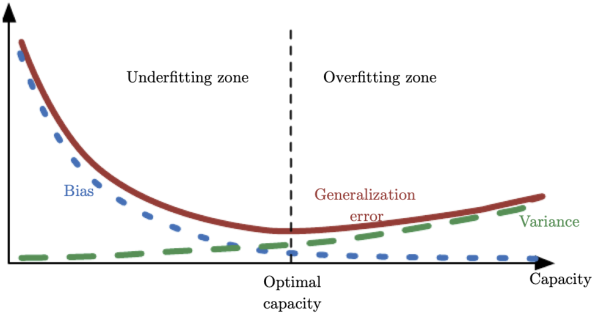
Bias and Variance

Figure: Bias and variance (Goodfellow et al., 2017, Figure 5.6)



Optimism and training error

The in-sample test error:

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

where Y_i^0 is a new variable conditioned on x_i.

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

where Y_i^0 is a new variable conditioned on x_i.

We have that for many loss functions

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

or

$$\mathrm{op} = \mathbb{E}_{\mathbf{y}}(\mathrm{Err_{in}}) - \mathbb{E}_{\mathbf{y}}(\overline{\mathrm{err}})$$

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

As $\hat{f}(x_i) \to y_i$, optimism will increase.

Question: Why?

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Estimating Optimism

- Under certain conditions we can estimate this optimism.
- AIC is an example of this – asymptotic predictive performance.

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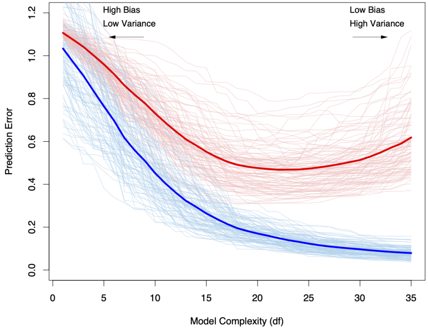
Estimating Optimism

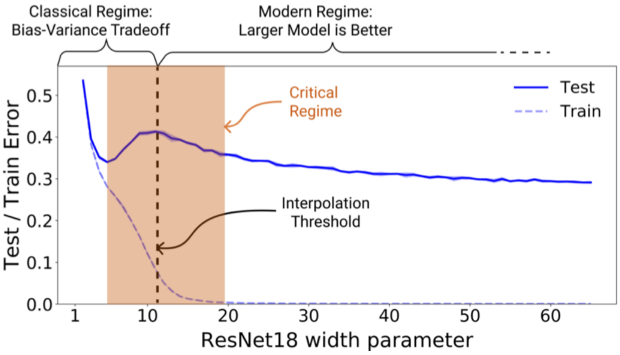
- Under certain conditions we can estimate this optimism.
- AIC is an example of this – asymptotic predictive performance.
- Question: What is the optimism in the Figure below?

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



The double descent of large models

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



Questions?

Questions?

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Section 6

Cross-validation

Cross-Valdidation

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

$$\begin{aligned}\text{Err} &= \mathbb{E}_{p(X,Y)}(\text{Err}_{\mathcal{T}}) \\ &= \mathbb{E}_{p(X,Y)}(\mathbb{E}_{p(X_0,Y_0)}(L(Y_0,X_0)|\mathcal{T}))\end{aligned}$$

- Cross-Validation is probably the most popular approach to estimate Err and choose between models because it is:
  1. Conceptually easy to understand
  2. Easy to implement
  3. No need for rules-of-thumbs to verify that it is applicable
  4. Equally useful for many different type of models
  5. Flexible for the use case at hand

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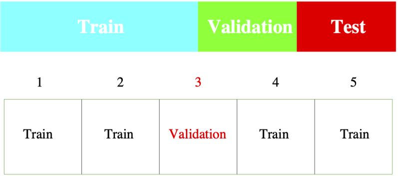
  3. No need for rules-of-thumbs to verify that it is applicable
  4. Equally useful for many different type of models
  5. Flexible for the use case at hand
- Common approach to learn hyper parameters (that is a model choice)

The 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 train $\hat{f}(x)$
    2.2 Use the model and predict the observations in fold k

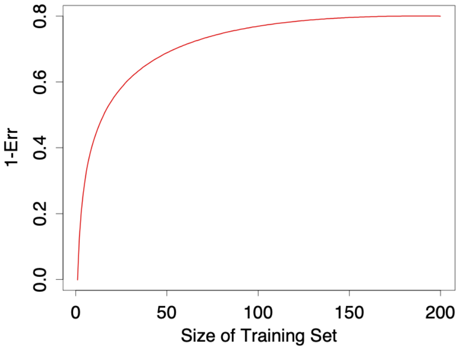
$$\widehat{\mathrm{Err}}_{CV}(\hat{f}) = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}_{\kappa(i)}(x))$$

where $\kappa(i)$ is the set of observations where i is held-out.

The Bias of Cross-Valdidaton

- Cross-validation estimation of Err will be biased
- The training data size is smaller than the full data

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



K-fold Cross Validation

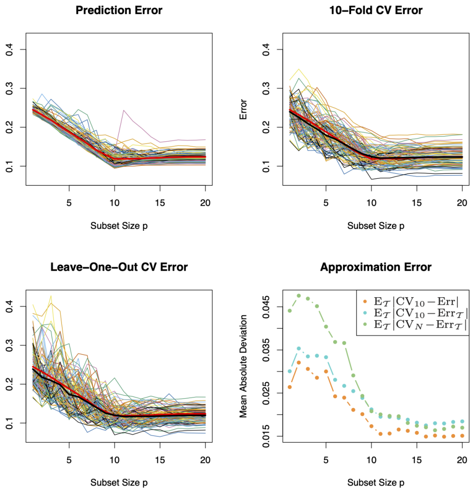
- Common K are: $K = \{2, 5, 10\}$
- Smaller K gives larger bias
- Larger K is computationally more costly
- $K = 10$ is a common approach

Leave-One-Out Cross Validation

- When $K = N$
- Benefits
  - Almost unbiased estimate of Err
  - Sometimes we only need to train our model once
- Drawbacks
  - Higher Variance in estimate of Err
  - Can be more computationally very costly (naive implementation)
  - Can be unstable/less robust in some settings

Leave-One-Out Cross Validation

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



The role of the data generating process

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

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

- The (naive) assumption: independence
- Things that can go wrong:
    - temporal leak/concept drift
    - duplicated observations
    - non-randomized data

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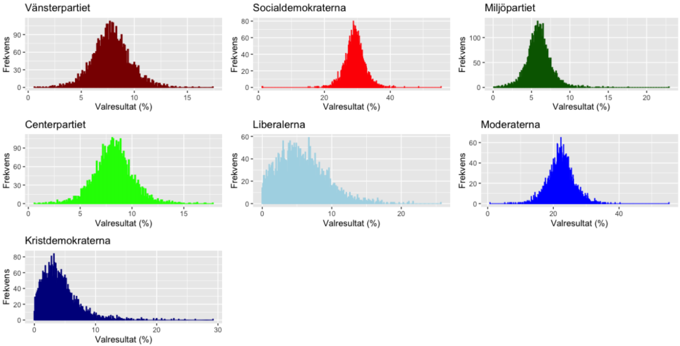
Example: Election prediction

- We want to predict the next election
- We know that there are "concept drift"
- Solution in Frölander and Uddhammar (2021) and Olsson and Ölfvingsson (2021)
  1. LOO-CV on the elections 1973-2014
  2. The elections 2018 as the final validation set

Figure: Predictive distr. (Olsson and Ölfvingsson, 2021, Fig. 6)



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- Predictive Performance
- Measuring Performance
- Test and training error
- Estimating the test error
- Bias and Variance
- Cross-validation

What is CV estimating?

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

1. What do we want CV to estimate, Err or $\mathrm{Err}_{\mathcal{T}}$?

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1. What do we want CV to estimate, Err or $\mathrm{Err}_{\mathcal{T}}$?
2. What is CV estimating?

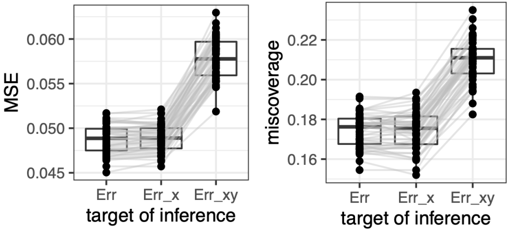
What is CV estimating?

Let $\text{Err}_{XY} = \text{Err}_{\mathcal{T}}$. Further, assume the true model is

$$y_i = \mathbf{x}^T\theta + \epsilon_i$$

where $\epsilon_i \sim N(0, \sigma^2)$.

Figure: MSE and missclassification ($\alpha = 10\%$, Bates et al, 2022)



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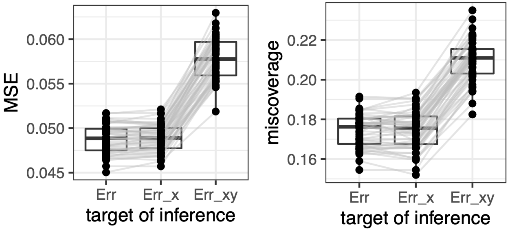

Two take-aways:

1. CV is estimating Err (see Bates et al, 2022)

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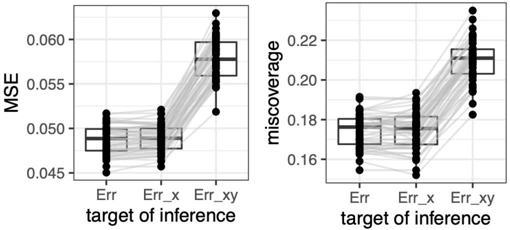

Two take-aways:

1. CV is estimating Err (see Bates et al, 2022)
2. Naive SE of CV estimators underestimate the true SE (see Bengio and Goodfellow, 2004)

Test error and (cross-)validation error?

1. What is the difference between the validation and test error?

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Test error and (cross-)validation error?

1. What is the difference between the validation and test error?
2. Why use cross-validation instead of holding out one validation fold?

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Questions?

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