Machine learning – Block 1(b)

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This weeks lectures

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

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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
- Model diagnoses and how well the model fits the data.
- In statistics: focus on estimation and attribution.

Predictive Performance

- Supervised learning: focus on predictive performance:
- How well our model $\hat{f}$ trained on

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

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

$$\mathbb{E}(L(Y_0, X_0)|\mathcal{T}) = \int L(Y_0, \hat{f}(X_0)) P_{y,x} d(Y_0, X_0)|\mathcal{T}$$

- ability to perform well on previously unobserved inputs is called generalization
- Models can be overly optimistic[1]:
  - explain training data well
  - poor generalizability
- 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.

Section 2

Measuring Performance

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):

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

  - Classification (0-1 loss)

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

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.

Cross-Entropy Loss

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

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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

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

The Confusion Matrix

- Predictive Performance
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- 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

	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	$F_{ba} + F_{ca}$	$F_{ab} + F_{ac}$
...	...	...	...

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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Question: What is the problem with Accuracy?

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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)

Recall

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

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

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

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F1-score

Harmonic mean of Precision and Recall.

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

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)

Example

Say that we want to classify spam vs. ham.

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

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...

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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.

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: $\frac{2 \cdot 1 \cdot 0.99}{0.99+1} \approx 0.99$
5. But Specificity is 0!

Questions?

Questions?

Section 3

Test and training error

Test Error

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

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

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

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

- Sometimes refered to as generalization error.

Training Error

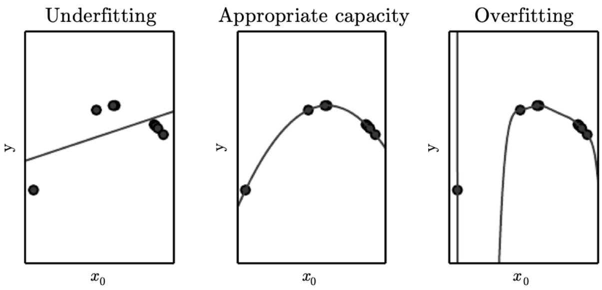
- The loss function the algorithm try to minimize
- The Error in the training data:

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

Model complexity/capacity

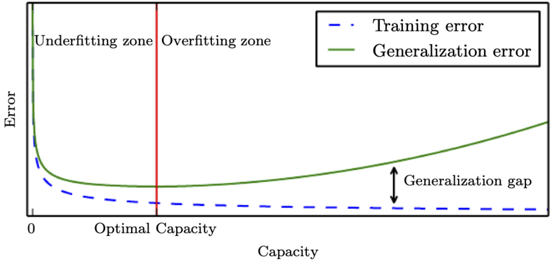
- Model complexity/capacity: The flexibility of the model.
- Underfitting: Too low capacity of model
- Overfitting: Too high capacity of model
- Example: Polynomial regression with higher order terms

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 test error
- Should only be used ONCE

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- We set aside a *test set* from the data
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- Should only be used ONCE
- Size of testset:
  - Common suggestion 10%
  - A statistical estimation problem (choice of samling size)

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Multiple Use of Test Set for Model Assesment

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

Questions?

Questions?

Section 5

Bias and Variance

Bias and Variance

Assume we have the following data generating process:

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

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

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

- *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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- Predictive Performance
- Measuring Performance
- Test and training error
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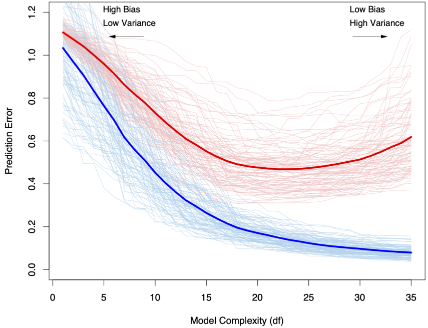
- Bias and Variance
- Cross-validation
- Regularisation

Bias and Variance

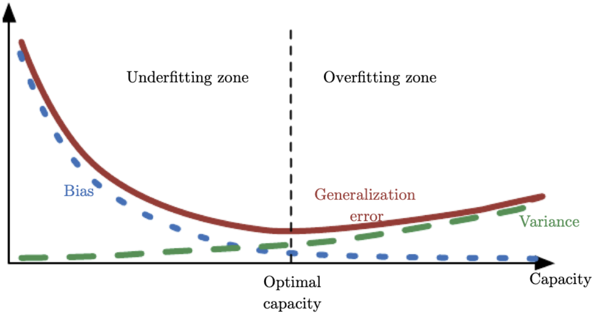
Figure: Test, training, and model complexity (Hastie et al, 2009, Figure 7)



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

Bias and Variance

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



Optimism

The in-sample test error:

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

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

Optimism

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

We have that

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

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

Question: 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 is an example of this – asymptotic predictive performance.
- Find the optimism

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- Predictive Performance
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- Test and training error
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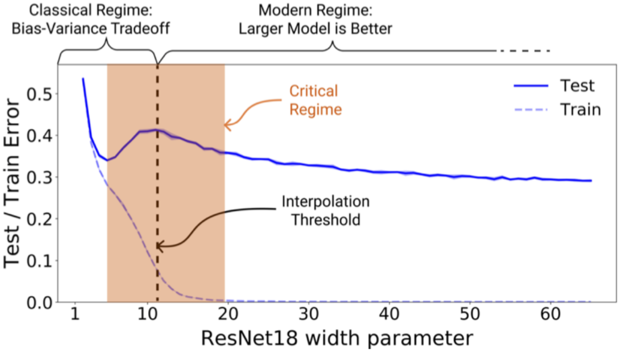
- Regularisation

The double descent of large models

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



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Questions?

Questions?

Section 6

Cross-validation

Cross-Valdidation

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

$$\begin{aligned} \text{Err} &= \mathbb{E}_{\mathcal{T}}(\text{Err}_{\mathcal{T}}) \\ &= \mathbb{E}_{\mathcal{T}}(\mathbb{E}(L(Y_0, X_0)|\mathcal{T})) \\ &= \int (\int L(Y_0, \hat{f}(X_0)) P_{y,x} d(Y_0, X_0)|\mathcal{T}) d\mathcal{T} \end{aligned}$$

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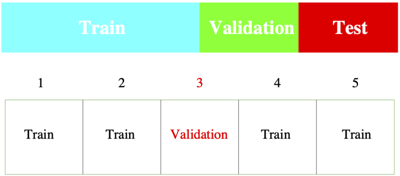
  3. No need for rules-of-thumbs to verify that it is applicable
  4. Equally useful for many different type of models
  5. Flexible for the use case at hand
- Common approach to learn hyper parameters (that is a model choice)

Cross-Valdidation Algorithm

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



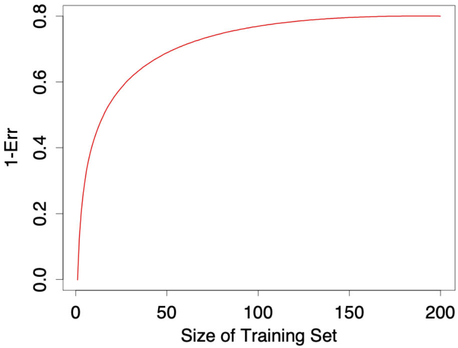
1. Split data in K folds
2. For each fold $k = 1, 2, ..., K$
   2.1 Use all samples except those in k to build $\hat{f}(x)$
   2.2 Use the model and predict the observations in fold k

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

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

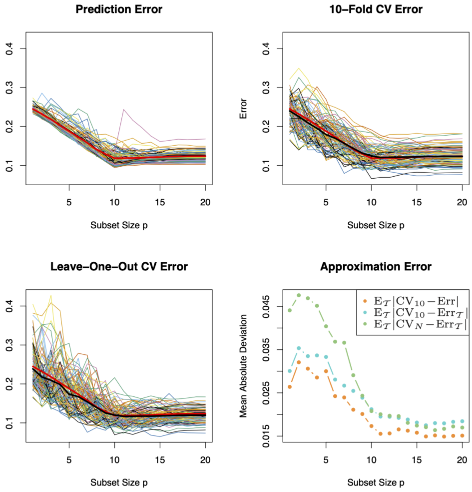
- Common K are: $K = \{2, 5, 10\}$
- Smaller K gives larger bias
- Larger K is computationally more costly
- $K = 10$ is a common approach

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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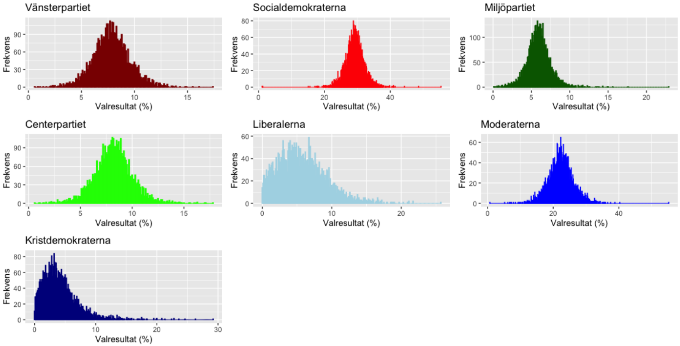
Example: Election prediction

- 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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Questions?

Questions?

Section 7

Regularisation

Regression and GLM

- Linear regression and logistic regression are examples of generalised linear models, GLMs.

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

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  - 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.

Regularised regression models

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

Connection to Bayesian estimation

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

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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 $p(\beta)$!

Inference and invariance

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    - 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.

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- Regularised regression models are however very useful for predictive modelling.

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L_q-penalties

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

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

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$\lambda \geq 0$ 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.

Ridge regression

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

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Examples in R

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

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  - 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).