Model selection

Lecture 1e

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Overview

- Model fitting
- Model selection

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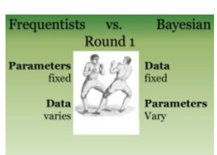
Frequentist vs Bayesian

- Probabilistic Model $p(y, x, w)$
  - **Frequentists**: w is a parameter that should be estimated by model fitting
  - **Bayesians**: w is a random variable that has a prior distribution $p(w)$
    - How to set $p(w)$??



Example: Linear regression, what are parameters here?

$y \sim w_0 + \boldsymbol{wx} + e, e \sim N(0, \sigma^2)$

$y \sim N(w_0 + \boldsymbol{wx}, \sigma^2)$

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An estimator

- $\hat{\boldsymbol{w}} = \delta(D)$ (some function of your data) – an **estimator**
- Optimal parameter values?→there can be many ways to compute them (MLE, shrinkage…)
  - Compare Bayesian: given estimators $\boldsymbol{w}^1$ and $\boldsymbol{w}^2$, we **can** compare them! $p(\boldsymbol{w}^1|\boldsymbol{D}) > \boldsymbol{p}(\boldsymbol{w}^2|\boldsymbol{D})$
  - There is no easy way to compare estimators in frequentist tradition

Example: Linear regression

- Estimator 1: $\boldsymbol{w} = (X^T X)^{-1} X^T Y$ (maximum likelihood)
- Estimator 2: $\boldsymbol{w} = (0, \ldots, 0,1)$
- Which one is better?
  - A comparison strategy is needed!

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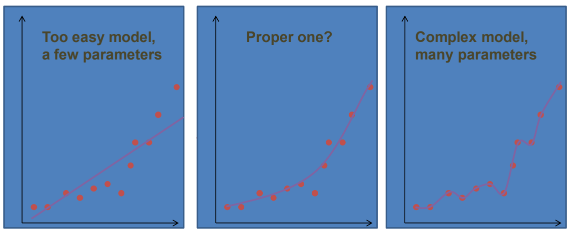
Overfitting

- Complex model can overfit your data



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Overfitting: solutions

- Observed: Maximum likelihood can lead to overfitting.

- Solutions
  - Selecting proper parameter values
    - Regularized risk minimization
  - Selecting proper model type, for ex. number of parameters
    - Houldout method
    - Cross-validation

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Model selection

- Given a model, choose the optimal parameter values
  - Decision theory
- Define loss $L(Y, \hat{y})$
  - How much we loose in guessing true Y incorrectly
- If we know the true distribution $p(y, x|w)$ then we choose $\hat{y}$

$$\min_{f} EL(y, \hat{y}) = \min_{\hat{y}} \int L(y, \hat{y}) p(y, x|w) dx dy$$

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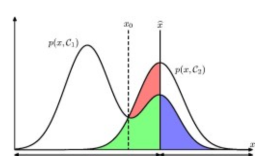
Model selection

Example: Spam classification

- Loss for incorrect classifying mails and spams
  - $L_{12} = 100, L_{21} = 1$



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Loss functions

- How to define loss function?
  - No unique choice, often defined by application
  - **Normal practice: Choose the loss related to minus loglikelihood**

Example: Predicting the amount of the product at the storage:

$$L(Y,\hat{y}) = \begin{cases} 10 + \frac{\hat{y}}{Y}, \hat{y} \geq Y \\ 1000, \hat{y} < Y \end{cases}$$

Example: Compute loss function related to
- Normal distribution

Guess why such loss function was chosen

Loss functions

- Classification problems
  - Common loss function $L(Y,\hat{y}) = \begin{cases} 0, Y = \hat{y} \\ 1, Y \neq \hat{y} \end{cases}$
  - When minimizing the loss, equivalent to misclassification rate

Model selection

- **Problem**: true model and true $\boldsymbol{w}$ are unknown→can not compute expected loss!
- How to find an optimal model?
  - Consider what expected loss (**risk**) depends on

$$R(Y,\hat{y}) = E[L(Y,\hat{y}(X,D))]$$

- Random factors:
  - D – **training set**
  - Y, X – data to be predicted **(validation set)**

Holdout method

- Simplify the risk estimation:
  - Fix D as a particular training set T
  - Fix Y,X as a particular validation set V
- Risk becomes (**empirical risk**)

$$\hat{R}(y,\hat{y}) = \frac{1}{|V|} \sum_{(X,Y) \in V} L(Y,\hat{y}(X,T))$$

  - Estimator is fit by Maximum Likelihood using training set
  - Risk estimated by using validation set
  - Model with minimum empirical risk is selected

General model selection strategy

- Given data $D = \{\boldsymbol{X}_i, Y_i, i = 1 \dots n\}$

Decide models
$Y \sim M(x, w, \alpha_1)$
$Y \sim M(x, w, \alpha_2)$
…

Learning step

Fit models
$Y \sim M(x, \widehat{w}, \alpha_1)$
$Y \sim M(x, \widehat{w}, \alpha_2)$

Decision step

Select model
..that minimizes the risk

- When fitting data, Maximum Likelihood is usually used
- α_i can be different things:
  - Type of distribution
  - Number of variables in the model
  - Regulatization parameter value
  - …

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Holdout method

Divide into training, validation and test sets

Training	Validation	Test

- Choose proportions in some way

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Holdout method

- Given: training, validation, test sets and models to select between

M1(?,?) M2(?,?,?) M3(?,?,?,?,?)

Training	Validation	Test

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Holdout method

- Training set is to used for fitting models to the dataset by using maximum likelihood

M1(a1,b1) M2(a2,b2,c2) M3(a3,b3,c3,d3,e3)

Training	Validation	Test

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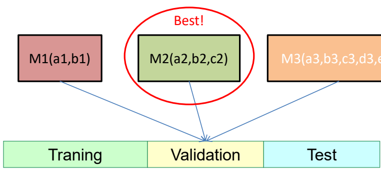
Holdout method

- Validation set is used to choose the best model (lowest risk)



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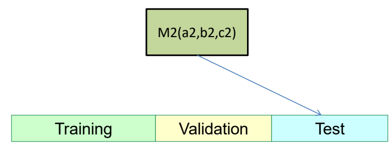
Holdout method

- Test set is used to test a performance on a new data



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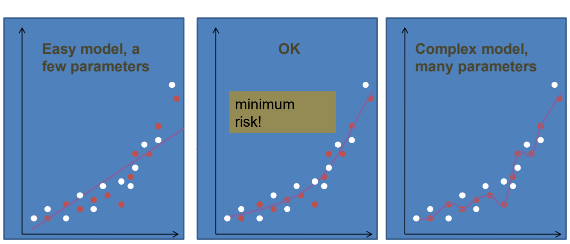
Holdout method



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Holdout in R

- How to partition into train/test?
  - Use set.seed(12345) in the labs to get identical results

```
n=dim(data)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.7))
train=data[id,]
test=data[-id,]
```

- How to partition into train/valid/test?

```
n=dim(data)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.4))
train=data[id,]

id1=setdiff(1:n, id)
set.seed(12345)
id2=sample(id1, floor(n*0.3))
valid=data[id2,]

id3=setdiff(id1,id2)
test=data[id3,]
```


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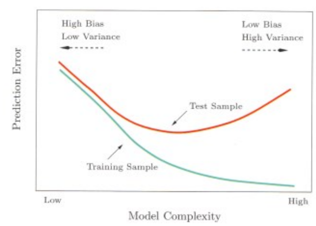
Bias-variance tradeoff

- Bias of an estimator $Bias(\hat{y}\,(x_0)) = E[\hat{y}(x_0) - f(x_0)]$, $f(x_0)$ is expected response
  - If $Bias(\hat{y}(x_0)) = 0$, the estimator is **unbiased**
  - ML estimators are asymptotically unbiased if the model is enough complex
  - However, unbiasedness does not mean a good choice!

Bias-variance tradeoff

- Assume loss is $L(Y, \hat{y}) = (Y - \hat{y})^2$

$$R(Y(x_0), \hat{y}(x_0)) = \sigma^2 + Bias^2(\hat{y}(x_0)) + Var(\hat{y}(x_0))$$



When loss is not quadratic, no such nice formula exist

Cross-validation

- Compared to holdout method:
  - Why do we use only some portion of data for training- can we use more (increase accuracy)?

Cross-validation (Estimates Err)

K-fold cross-validation (rough scheme, show picture):

1. Permute the observations randomly
2. Divide data-set in K roughly equally-sized subsets
3. Remove subset #i and fit the model using remaining data.
4. Predict the function values for subset #i using the fitted model.
5. Repeat steps 3-4 for different i
6. CV= squared difference between observed values and predicted values (another function is possible)

Cross-validation

Cross-validation

1	2	3	4	5
Train	Train	Validation	Train	Train

Note: if $K=N$ then method is *leave-one-out* cross-validation.

$$\kappa : \{1, \dots, N\} \mapsto \{1, \dots, K\}$$

K-fold cross-validation: $CV = \frac{1}{N}\sum_{i=1}^{N} L(Y_i, \hat{y}^{-k(i)}(x_i))$

What to do if N is not a multiple of K?

Cross-validation vs Holdout

- Holdout is easy to do (a few model fits to each data)
- Cross validation is computationally demanding (many model fits)
- Holdout is applicable for large data
  - Otherwise, model selection performs poorly
- Cross validation is more suitable for smaller data

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Analytical methods

- Analytical expressions to select models
  - AIC (Akaike's information criterion)

Idea: Instead of $R(Y, \hat{y}) = E[L(Y, \hat{y}(X, D))]$ consider **in-sample** risk (only *Y* in *D* is random):

$$R_{in}(Y, \hat{y}) = \frac{1}{N}\sum_{i=1}^{N} E_{Y_i}\left[L\left(Y_i, \hat{y}(X, D)\right) | D, X \in D\right]$$

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Analytical methods

- One can show that

$$R_{in}(Y, \hat{y}) \approx R_{train} + \frac{2}{N}\sum_i cov(\hat{y}_i, Y_i)$$

where $R_{train} = \sum_{X_i, Y_i \in T} L(Y_i, \hat{y}_i)$

- Recall, **degrees of freedom** $\mathrm{df(model)} = \frac{1}{\sigma^2}\sum_i cov(\hat{y}_i, Y_i)$
  - When model is linear, *df* is the number of parameters.
- If loss is defined by minus two loglikelihood,

$$AIC \equiv -2loglik(D) + 2df(model)$$

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Model selection

Example Computer Hardware Data Set : performance measured for various processors and also

- Cycle time
- Memory
- Channels
- …

Build model predicting performance

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Cross-validatation

- Try models with different predictor sets

```
data=read.csv("machine.csv", header=F)
library(cvTools)


fit1=lm(V9~V3+V4+V5+V6+V7+V8, data=data)
fit2=lm(V9~V3+V4+V5+V6+V7, data=data)
fit3=lm(V9~V3+V4+V5+V6, data=data)
f1=cvFit(fit1, y=data$V9, data=data,K=10,
foldType="consecutive")
f2=cvFit(fit2, y=data$V9, data=data,K=10,
foldType="consecutive")
f3=cvFit(fit3, y=data$V9, data=data,K=10,
foldType="consecutive")
res=cvSelect(f1,f2,f3)
plot(res)
```