When Models Meet Data

Data, Models, and Learning Empirical Risk Minimization

Section 8.1 and 8.2 from Mathematics for Machine Learning



INDEX

1. Data, models and learning

- 1.1. Data as vectors
- 1.2. Models as functions
- 1.3. Models as probability distributions
- 1.4. Finding parameters

2. Empirical risk minimization

- 2.1. Hypothesis Class of Functions
- 2.2. Empirical Risk Minimization
- 2.3. Loss Function for Training
- 2.4. Regularization to Reduce Overfitting
- 2.5. Cross-Validation to Assess the Generalization Performance

DATA, MODELS AND LEARNING

- → DATA AS VECTORS
- → MODELS AS FUNCTIONS
- → MODELS AS PROBABILITY DISTRIBUTIONS
- → FINDING PARAMETERS

Introduction: what is a good model?

3 components of a machine learning system:

- DATA: unprocessed value, text, picture, sound...
 - Training data: initial data we use to train our model.
- **MODELS**: file that has been trained to recognize certain types of patterns
- LEARNING

A good model should perform well on unseen data.

→ **Performance metrics**: measure the performance of a model.



Our computer should be able to read our data → TABULAR DATA

Each column = particular feature ; Each row = particular example

Even thought machine learning can be applied in other types of data (ex. Genomic sequences), we will focus on tabular data.

... Our tabular data is not yet prepared.

Company B

CTCTGGGCATCGTCAGTCTGGAAAACATCCTGGTTATCCTGGCCGTGGTCAGGAACGG CAACCTGCACTCCCGATGTACTTCTTTCTCTGCAGCCTGGCGGTGGCCGACATGCTGGTA AGTGTGTCCAATGCCCTGGAGACCATCATGATCGCCATCGTCCACAGGGACTACCTGACCT TCGAGGACCAGTTTATCCAGCACATGGACAACATCTTCGACTCCATGATCTGCATCTCCCT GGTGGCCTCCATCTGCAACCTCCTGGCCATCGCCGTCGACAGGTACGTCACCATCTTTTAC GCGCTCCGCTACCACAGCATCATGACCGTGAGGAAGGCCCTCACCT GGGTCTGCTGCGGCGTCTGTGGCGTGTTCATCGTCTACTCGGAGAGCAAAATGGTCAT TGTGTGCCTCATCACCATGTTCTTCGCCATGATGCTCCTCATGGGCACCCTCTACGTGCAC ATGTTCCTCTTTGCGCGGCTGCACGTCAAGCGCATAGCAGCACTGCCACCTGCCGACGGGG TGGCCCCACAGCAACACTCATGCATGAAGGGGGCAGTCACCATCACCATTCTCCTGGGCGT GTTCATCTTCTGCTGGGCCCCCTTCTTCCTCCACCTGGTCCTCATCATCACCTGCCCCACC ACTCCGTCATCGACCCACTCATCTACGCTTTCCGGAGCCTGGAATTGCGCAACACCTTTAG GGAGATTCTCTGTGGCTGCAACGGCATGAACTTGGGATAGgatgcagggccatggaaatga gtttacaaagccttttaaaggggaaaattggtgaacaacagattctctgaaaggattccaa gatgggtaagtcacaaactctgatttcccaaatagtcactgggagaaatcagcgaaggctt ctctgcatgctctctgcactcatttccaaacacccagggtgtgcgacgcctgtctgctcat ctgctccacacccacgtcttcatgctccaggccagaccagactgaaggattctcatgaaca ataagggtggttcagatctcttgcaagcaaacctgttacagctacgacctcctgctgccag ctacacggagagatagctttgcacttataactccgtaggagactgagttctactctattat totatttacagttagacaattgtototttqtgaaaggaggaatgctatgccgttttcccct tttcttacccccatatcccttcagttgtccccacccccaaaggtagcatgaggatgtaacc

cacttctattttttctggtggtg

| Owner | Country | File_Date | IPC_Class 8 H05H13 | |
|-----------|---------|------------|---------------------|--|
| Company A | US | 6/18/2008 | | |
| Company A | EP | 1/30/1998 | A61N5 | |
| Company A | EP | 1/30/1998 | A61N5 | |
| Company A | EP | 1/30/1998 | A61N5 | |
| Company A | JP | 8/28/1997 | A61N5 | |
| Company A | JP | 10/4/2002 | A61N5 | |
| Company A | JP | 1/27/2003 | A61N5 | |
| Company A | JP | 4/14/2003 | A61N5 | |
| Company A | JP | 5/13/2011 | A61N5 | |
| Company B | JP | 4/2/1998 | G12B13 | |
| Company B | JP | 4/2/1998 | G12B13 | |
| Company B | JP | 5/28/1997 | A61N5 | |
| Company B | JP | 11/12/1997 | A61N5 | |
| Company B | JP | 2/29/2000 | A61N5 | |
| | | | | |

Example of data represented as rows and columns

4/30/2002

A61N5

Data as vectors: Transforming tabular data

| Name | Gender | Degree | Postcode | Age | Annual salary |
|-----------|--------|--------------|--------------|--------|----------------|
| Aditya | M | MSc | W21BG | 36 | 89563 |
| Bob | M | PhD | EC1A1BA | 47 | 123543 |
| Chloé | F | BEcon | SW1A1BH | 26 | 23989 |
| Daisuke | M | BSc | SE207AT | 68 | 138769 |
| Elisabeth | F | MBA | SE10AA | 33 | 113888 |
| | | | \ | | |
| Gender ID | Degree | Latitude | Longitude | Age | Annual Salary |
| | | (in degrees) | (in degrees) | 100000 | (in thousands) |
| -1 | 2 | 51.5073 | 0.1290 | 36 | 89.563 |
| -1 | 3 | 51.5074 | 0.1275 | 47 | 123.543 |
| +1 | 1 | 51.5071 | 0.1278 | 26 | 23.989 |
| -1 | 1 | 51.5075 | 0.1281 | 68 | 138.769 |
| +1 | 2 | 51.5074 | 0.1278 | 33 | 113.888 |



Data as vectors: Transforming tabular data into vector representation

Each input (x_n) is a D-dimensional vector of real numbers, called:

- **Features**: individual measurable properties (ex. height)
- Attributes: features of each data point (ex. 170cm)
- Covariants: independent variables

Examples

Notation:

- N= number of examples in dataset
- n= index of the examples (n=1,...,n=N)
- Each row = one example xn
- Each column = one feature (d=1,...,d=D)

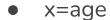
Features

| Gender ID | Degree | Latitude (in degrees) | Longitude (in degrees) | Age | Annual Salary (in thousands) |
|-----------|--------|-----------------------|------------------------|-----|------------------------------|
| -1 | 2 | 51.5073 | 0.1290 | 36 | 89.563 |
| -1 | 3 | 51.5074 | 0.1275 | 47 | 123.543 |
| +1 | 1 | 51.5071 | 0.1278 | 26 | 23.989 |
| -1 | 1 | 51.5075 | 0.1281 | 68 | 138.769 |
| +1 | 2 | 51.5074 | 0.1278 | 33 | 113.888 |

Example: predicting annual salary from age

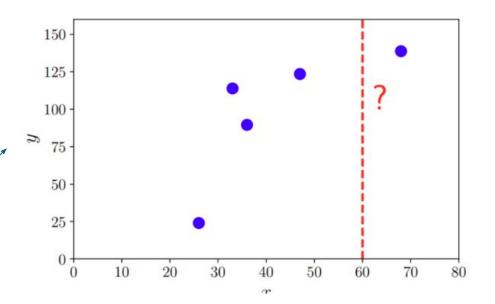
We want to know the salary of a person of age 60:

Notation



• y= salary





Models as function

INPUT: vector of D dimensions → Features

$$f: R \stackrel{D}{\rightarrow} R$$



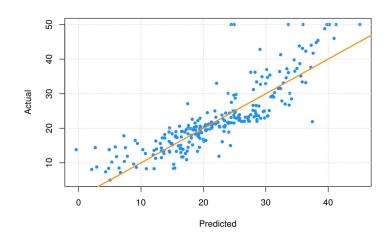
| Gender ID | Degree | Latitude (in degrees) | Longitude (in degrees) | Age | Annual Salary (in thousands) |
|-----------|--------|-----------------------|------------------------|-----|------------------------------|
| -1 | 2 | 51.5073 | 0.1290 | 36 | 89.563 |
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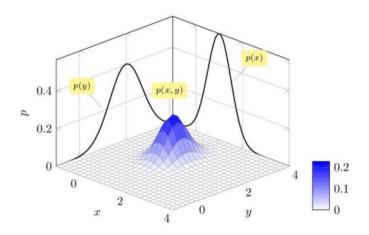


Models as probability distributions

- NOISY OBSERVATIONS!!

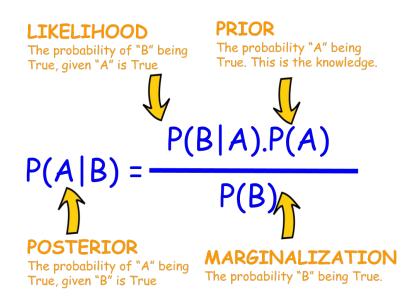
 Distribution of possible functions and multivariate probability distributions!!





Finding parameters

- Prediction / inference
- Training or parameter estimation
 - Quality
 - Bayesian inference
- Hyperparameter turning or models selection.



EMPIRICAL RISK MINIMIZATION

- → HYPOTHESIS CLASS OF FUNCTIONS
- → EMPIRICAL RISK MINIMIZATION
- → LOSS FUNCTION FOR TRAINING
- → REGULARIZATION TO REDUCE OVERFITTING
- → CROSS-VALIDATION TO ASSES THE GENERALIZATION PERFORMANCE

Hypothesis Class of Functions

PROBLEM: Separating spam from legitimate emails

- N examples where emails are labelled 0 or 1
 - -0 → spam
 - $1 \rightarrow \text{not spam}$ $(x1, y1), \dots, (xn, yn)$



PREDICTOR (θ)

 $f(oldsymbol{x}_n,oldsymbol{ heta}^*)pprox y_n\quad ext{for all}\quad n=1,\ldots,N$

Empirical Risk Minimization

ERM: provides bounds to the performance of a family of learning algorithms finding a function that minimizes the empirical risk between predicted output and the actual output 100 WHITE CATS Cats and dogs are different 200 because of its colour 100 BROWN DOGS GOAL: find a reliable predictor How well does the predictor fit the data?

Loss Function for Training

LOSS FUNCTIONS define what a valid prediction is and isn't

INPUT: Truth label and the prediction → positive number (LOSS)

→ Represents how much error we have made on one particular prediction

GOAL: find a parameter vector to minimize the average loss on the set of N examples

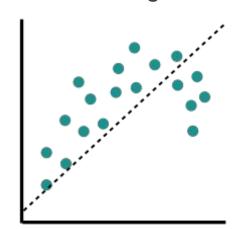
-How should we change our training procedure to generalize well?

-How do we estimate expected risk from (finite) data?

REAL OBJECTIVE: gain a predictor that also performs well (has low risk) on unseen test data

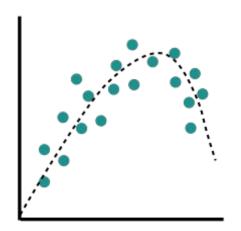
Regularization to Reduce Overfitting: What is overfitting?

Under-fitting



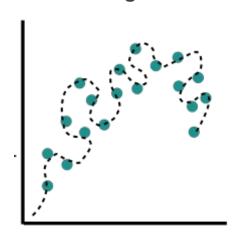
The model does not fit enough points, losing important information

Appropriate-fitting



The model fits the correct amount of data and generalizes without losing important information

Overfitting



The model doesn't generalize well. A lot of irrelevant data points. More possibilities of overfitting when the model has lots of features to learn

Regularization to Reduce Overfitting

Ways to reduce overfitting:

- Reduce the number of variables in a model → increase in the degrees of freedom → loss of relevant information X
- Regularization → keeps all the features and reduces the magnitude of the features available → trade-off between accuracy and generalizability

Cross-Validation to Assess the Generalization Performance

DATA → train machine learning methods and test them

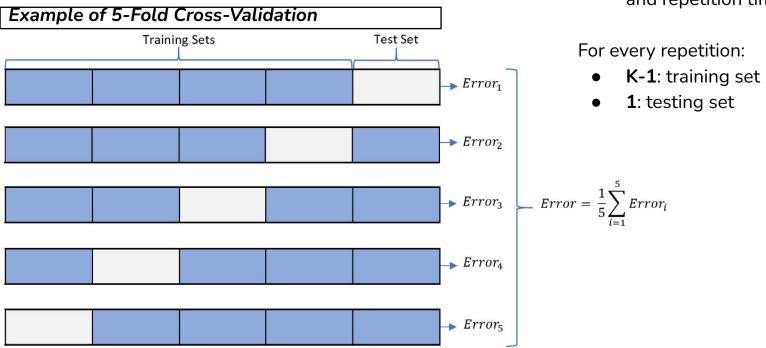
Same data to train and test → how does the model work with unseen data? → **PROBLEM**: we don't have unseen data

SOLUTION → divide the data (different for training and testing) → **HOW**?

Cross-Validation → compare different machine learning methods and get a sense of how they will work in practice

K-Fold Cross-Validation

→ K: divisions of the data and repetition times



THE END

Any questions?