Universität Potsdam
Institut für Informatik
Lehrstuhl Maschinelles Lernen

Models, Data, Learning Problems

Tobias Scheffer

Overview

- Types of learning problems:
  - Supervised Learning (Classification, Regression, Ordinal Regression, Recommendations, Sequences und Structures)
  - Unsupervised Learning
  - Reinforcement-Learning (Exploration vs. Exploitation)
- Models
- Regularized empirical risk minimization
  - Loss functions,
  - Regularizer
- Evaluation

Supervised Learning: Basic Concepts

- Instance: $\mathbf{x} \in X$
  - In statistics: independent variable
  - X could be a vector space over *attributes* ($X = \mathbb{R}^m$)
  - An instance is then an assignment to the attributes.
  - $\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix}$ feature vector
- Target variable: $y \in Y$
  - In Statistics: dependent variable
- A model maps instances to the target variable.

$$\mathbf{x} \xrightarrow{\text{Model}} y$$

Supervised Learning: Classification

- Input: Instance $\mathbf{x} \in X$.
  - e.g., a feature vector

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix}$$

- Output: Class $y \in Y$; finite set Y.
  - The class is also referred to as the target attribute.
  - y is also called the (class) label

$$\mathbf{x} \xrightarrow{\text{Classifier}} y$$

Classification: Example

- Input: Instance $\mathbf{x} \in X$
  - X : the set of all possible combinations of regiment of medication

Attribute	Instance $\mathbf{x}$
Medication #1 included?	$\begin{pmatrix}0\\1\\1\\0\\1\\0\end{pmatrix}$
⋮	
Medication #6 included?	

Attribute values

Feature vector

Medication combination

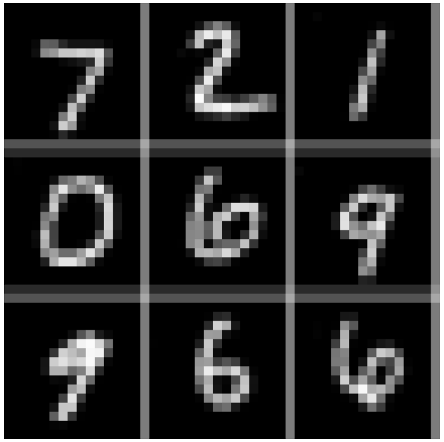
- Output: $y \in Y = \{\text{toxic}, \text{ok}\}$ ☹ / ☺

$\longrightarrow$ **classifier** $\longrightarrow$ ☹

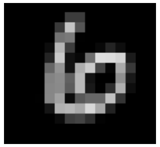
Classification: Example

- Input: Instance $\mathbf{x} \in X$
  - X : the set of all 16×16 pixel bitmaps

$$\begin{array}{ll}\text{Attribute} & \text{Instance } \mathbf{x}\\ \begin{array}{l}\text{Gray value of pixel 1}\\ \\ \\ \vdots\\ \\ \text{Gray value of pixel 256}\end{array} & \left(\begin{array}{c}0.1\\0.3\\0.45\\\vdots\\0.65\\0.87\end{array}\right)\text{256 pixel values}\end{array}$$



- Output: $y \in Y = \{0,1,2,3,4,5,6,7,8,9\}$: recognized digit

 $\longrightarrow$ **classifier** $\longrightarrow$ "6"

Classification: Example

- Input: Instance $\mathbf{x} \in X$
  - X : bag-of-words representation of all possible email texts

Attribute

Word #1 occurs?

⋮

Word #m occurs?

$m \approx 1{,}000{,}000$

Instance $\mathbf{x}$

$$\left(\begin{array}{c}0\\1\\0\\\vdots\\1\\0\end{array}\right)\begin{array}{l}\text{Aardvark}\\\text{Beneficiary}\\\text{Friend}\\\vdots\\\text{Sterling}\\\text{Science}\end{array}$$

Email

Dear Beneficiary,

your Email address has been picked
online in this years MICROSOFT
CONSUMER AWARD as a
Winner of One Hundred and Fifty Five
Thousand
Pounds Sterling…

- Output: $y \in Y = \{\text{spam}, \text{ok}\}$

Dear Beneficiary,

We are pleased to notify you that your Email address
has been picked online in this second quarter's
MICROSOFT CONSUMER AWARD (MCA) as a
Winner of One Hundred and Fifty Five Thousand
Pounds Sterling…

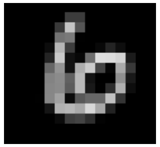
$\longrightarrow$ **classifier** $\longrightarrow$ “Spam“

Classification

- Classifier should be learned from training data.

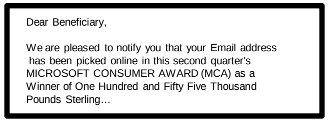
Classifier

☹



Classifier

"6"



Dear Beneficiary,

We are pleased to notify you that your Email address has been picked online in this second quarter's MICROSOFT CONSUMER AWARD (MCA) as a Winner of One Hundred and Fifty Five Thousand Pounds Sterling…

Classifier

“Spam“

Classifier Learning

- Input to the Learner: Training data T_n.
  - $$\mathbf{X} = \begin{array}{cc} \begin{pmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nm} \end{pmatrix} & \begin{array}{c} \text{💊} \\ \\ \text{💊} \end{array} \end{array}$$
  - $$\mathbf{y} = \begin{array}{cc} \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} & \begin{array}{c} \text{🙂} \\ \\ \text{☹} \end{array} \end{array}$$

- Output: a Model
  - 💊 ↦ ☹
    $y_\theta : X \to Y$
  - for example:
    $$y_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{cases} \text{☹} & \text{if } \mathbf{x}^{\mathrm{T}}\boldsymbol{\theta} \geq 0 \\ \text{🙂} & otherwise \end{cases}$$

Linear classifier with parameter vector $\boldsymbol{\theta}$.

- Training Data: $T_n = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$

Classifier Learning

- Input to the Learner: Training data T_n.
  - $\mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nm} \end{pmatrix}$

  - $\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$ ☺ ☹
- Training Data: $T_n = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$
- Output: a model
  - $\mapsto$ ☹

    $y_\theta : X \to Y$
- Model classes
  - (Generalized) linear model
  - Decision tree
  - Ensemble classifier
  - …

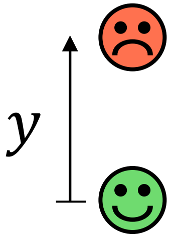
Supervised Learning: Regression

- Input: Instance $\mathbf{x} \in X$.
  - e.g., feature vector

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix}$$

How toxic is a combination?

- Output: continuous (real) value, $y \in \mathbb{R}$
  - e.g., *toxicity*.



Regressor Learning

- Input to the Learner: Training data T_n.
  - $$\mathbf{X} = \left(\begin{array}{ccc} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nm} \end{array}\right)\begin{array}{c} 💊 \\ \\ 💊 \end{array}$$
  - $$\mathbf{y} = \left(\begin{array}{c} y_1 \\ \vdots \\ y_n \end{array}\right)\begin{array}{c} ☺ \uparrow ☹ \\ \\ ☺ \uparrow ☹ \end{array}$$
- Training Data: $T_n = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$

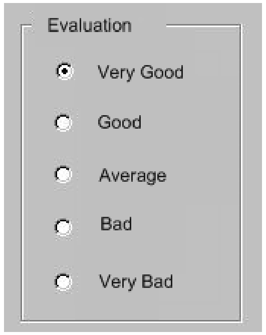
- Output: a model
  - 💊 ↦ ☹
    $y_\theta : X \to Y$
  - For example
    $y_{\boldsymbol{\theta}}(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\boldsymbol{\theta}$

Generalized linear model with parameter vector $\boldsymbol{\theta}$.

Supervised Learning: Ordinal Regression

- Input: Instance $\mathbf{x} \in X$.
- Output: discrete value $y \in Y$ like classification, but there is an ordering on the elements of Y.
- A large discrepancy between the model‘s prediction and the true value is worse than a small one.

$\longmapsto$



Evaluation

● Very Good

○ Good

○ Average

○ Bad

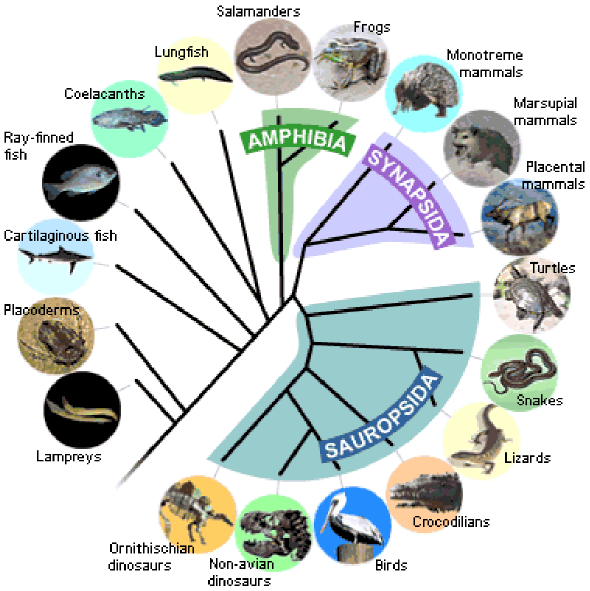
○ Very Bad

Satisfied with the outcome?

Supervised Learning: Taxonomy Classification

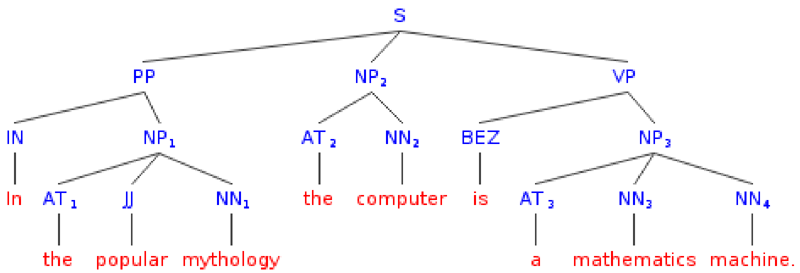
- Input: Instance $\mathbf{x} \in X$.
- Output: discrete value $y \in Y$ like classification, but there is a tree-based ordering on the elements of Y.
- The prediction is worse the farhter apart the predicted and actual nodes are apart.

$\longmapsto$

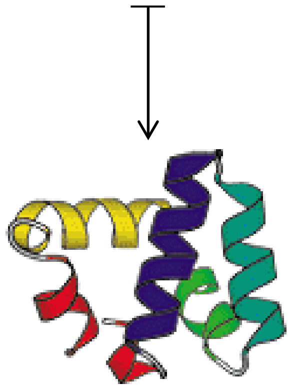


Supervised Learning: Sequence and Structure Prediction

- Input: Instance $\mathbf{x} \in X$.
- Output: Sequence, Tree or Graph $y \in Y$.
- Example applications:
    - Parse natural languages
    - Protein folding

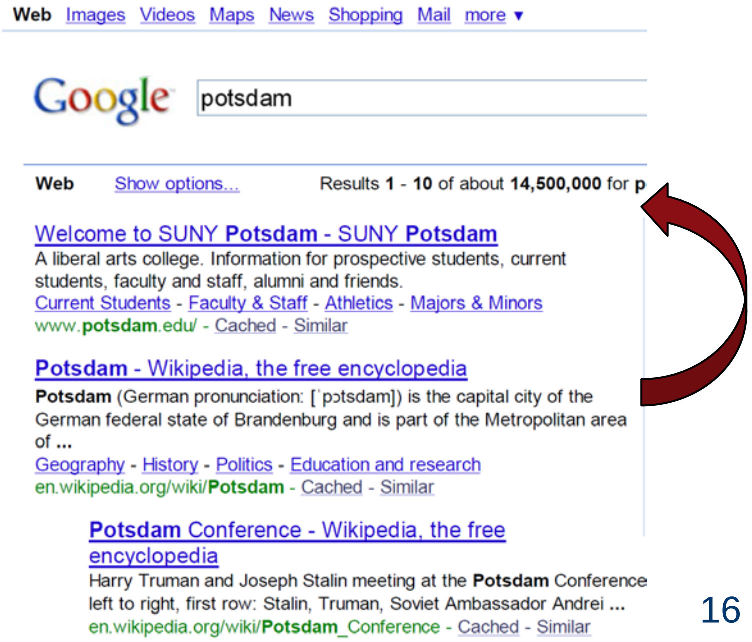


…AAGCTTGCACTGCCGT…



Supervised Learning: Rankings

- Input: query q and list of items $I_1, \ldots, I_n$.
- Output: a sorting of the items
- Training data: user clicks on I_j after querying with q:
  - The selected item should be ranked higher than those listed higher that were not clicked.



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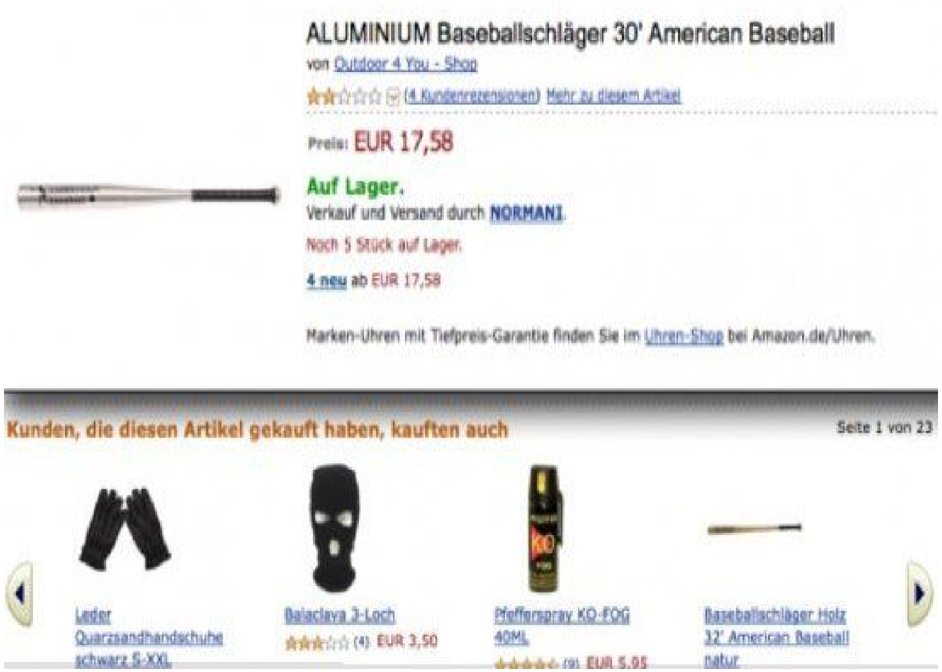
Supervised Learning: Recommendations

- Input: users, items, contextual information.
- Output: How much will a user like a recommendation?
- Training data: ratings, sales, page views.



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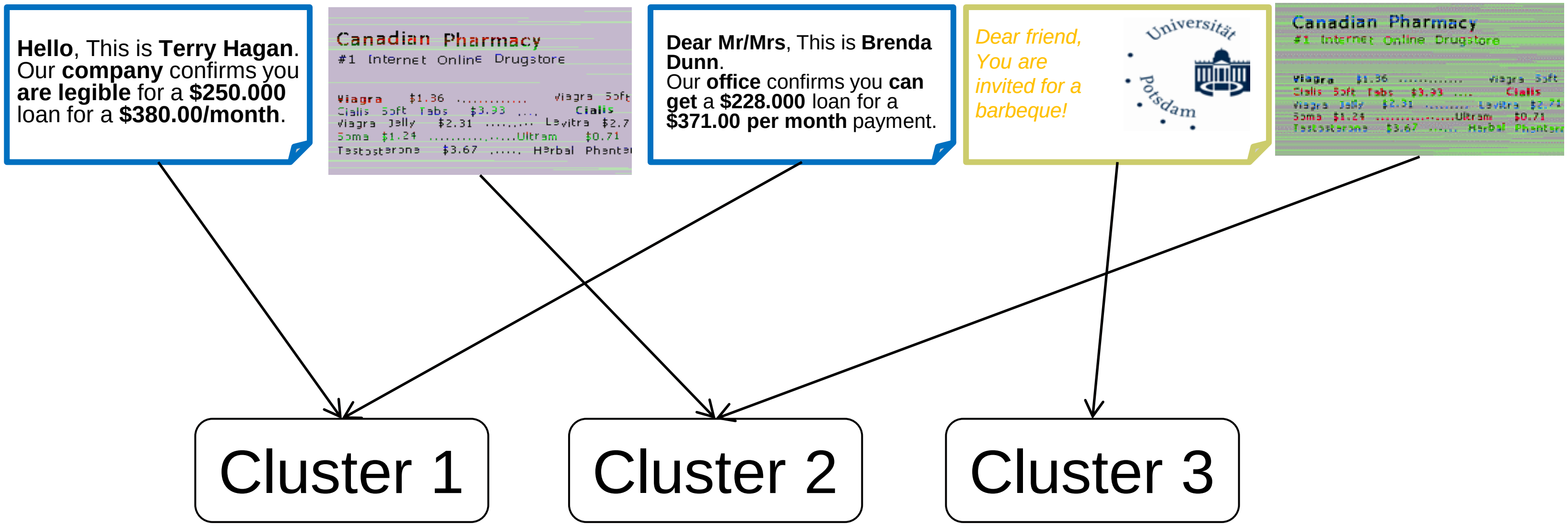
Baseballschläger Holz 32' American Baseball natur

Unsupervised Learning

- Training data for unsupervised learning: Set of instances $\mathbf{x} \in X$.
- Additional assumptions about the data formation process; for example, independence of random variables.
- The goal is the detection of structure in the data:
  - For example, find the most likely grouping into clusters of instances that share certain properties, which were not directly observable in the data.

Cluster Analysis: Email Campaign Example

- Input: a stream of emails.
- Output: a partitioning into subsets that belong to the same email campaign.



Hello, This is **Terry Hagan**. Our **company** confirms you **are legible** for a **$250.000** loan for a **$380.00/month**.

Dear Mr/Mrs, This is **Brenda Dunn**. Our **office** confirms you **can get** a **$228.000** loan for a **$371.00 per month** payment.

Dear friend, You are invited for a barbeque!

Canadian Pharmacy
#1 Internet Online Drugstore
Viagra $1.36 .... Viagra Soft
Cialis Soft Tabs $3.93 .... Cialis
Viagra Jelly $2.31 .... Levitra $2.7
Soma $1.24 ....Ultram $0.71
Testosterone $3.67 ...... Herbal Phenter
Universität Potsdam
Canadian Pharmacy
#1 Internet Online Drugstore
Viagra $1.36 .... Viagra Soft
Cialis Soft Tabs $3.93 .... Cialis
Viagra Jelly $2.31 .... Levitra $2.71
Soma $1.24 ....Ultram $0.71
Testosterone $3.67 ...... Herbal Phenter

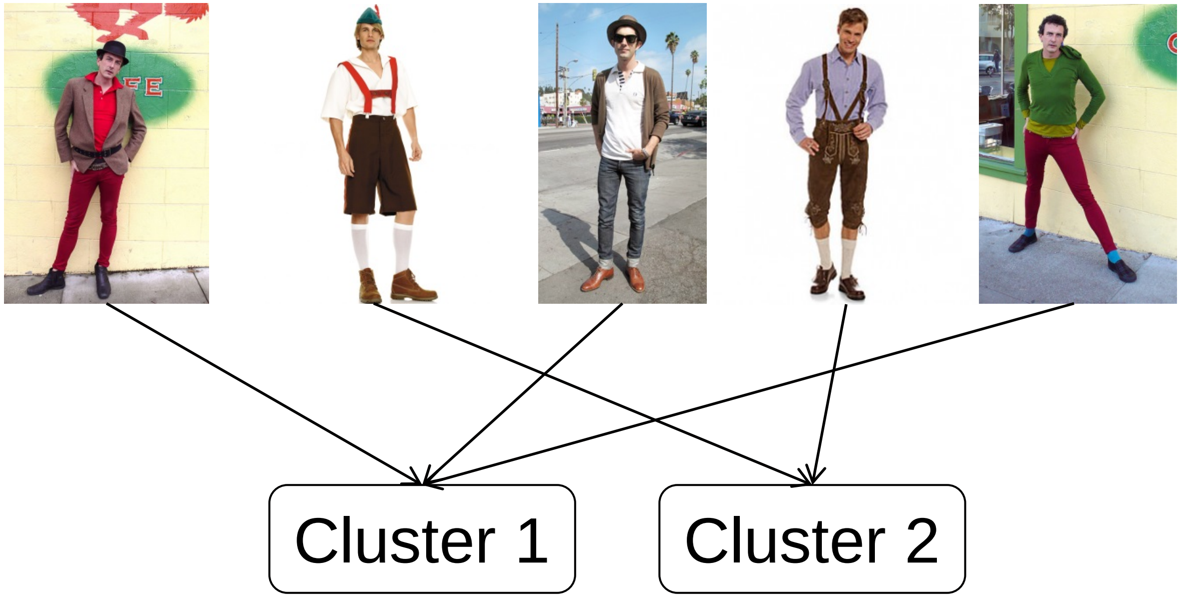
Cluster 1

Cluster 2

Cluster 3

Cluster Analysis: Market Segmentation Example

- Input: data over customer behavior.
- Output: a partitioning into clusters of customers who have similar product preferences.



Cluster 1

Cluster 2

Reinforcement Learning: Learning to Control a System

- Suppose there is a system with control parameters.
- A utility function describes the desired system behavior.
- Changes of the control parameters may have time-lagging effects.
- The Learner must experiment with the system to find a model that achieves the desired behavior (Exploration).
- At the same time, the system should be kept in the best state that is possible (Exploitation).

Reinforcement Learning:
Learning to Control a System: Example

- Advertisement (Ad) placement.
- To learn which ads the user clicks, the learner must experiment.
- However, when the learner experiments with using ads other than the most popular verwenden, sales are lost.

BLACKBERRY
The always-on email solution for Attention Deficit Disorder
www.valleyofthegeeks.com
half.com by ebay
The lowest prices on stolen goods!
go
www.valleyofthegeeks.com
ANDERSEN
Creative Accounting Solutions
www.valleyofthegeeks.com

Taxonomy of Learning Problems

- Supervised: Training data contain values for variable that model has to predict
  - Classification: categorial variable
  - Regression: continuous variable
  - Ordinal regression, finite, ordered set of values
  - Rankings: ordering of elements
  - Structured prediction: sequence, tree, graph, …
  - Recommendation: Item-by-user matrix

Taxonomy of Learning Problems

- Unsupervised: discover structural properties of data
  - Clustering
  - Unsupervised feature learning: find attributes that can be used to describe the data well
- Control / reinforcement learning: learning to control a dynamical system

Overview

- Types of learning problems:
  - Supervised Learning (Classification, Regression, Ordinal Regression, Recommendations, Sequences und Structures)
  - Unsupervised Learning
  - Reinforcement-Learning (Exploration vs. Exploitation)
- Models
- Regularized empirical risk minimization
  - Loss functions,
  - Regularizer
- Evaluation

Classifier Learning

- Input to the Learner: Training data T_n.
  - $\mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nm} \end{pmatrix}$

  - $\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$ ☺ ☹
- Training Data: $T_n = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$

- Output: a classifier
  - $\mapsto$ ☹

    $y_\theta : X \to Y$
- How can a learning algorithm learn a model (classifier) from the training data?
- This is a search problem in the space of all models.

Model or Parameter Space

- Model space, parameter or hypothesis space Θ:
  - The classifier has parameters $\boldsymbol{\theta} \in \Theta$.
  - Θ is a set of models (classifiers), which are suitable for a learning method.
  - The model space is one of the degrees of freedom for maschine learning; there are many commonly used spaces.
  - Also called *Language Bias*
- Example:
  - Linear models

$$y_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{cases} \text{☹} & \text{if } \sum_{j=1}^{m} x_j \theta_j \geq \theta_0 \\ \text{☺} & otherwise \end{cases}$$

Loss Function, Optimization Criterion

- Learning problems will be formulated as optimization problems.
  - The *loss function* measures the goodness-of-fit a model has to the observed training data.
  - The *regularization function* measures, whether the model is *likely* according to our prior knowledge.
  - The *optimization criterion* is a (weighted) sum of the losses for the training data and the regularizer.
  - We seek the model that minimizes the optimization criterion.

- Learning finds the overal most likely model given the training data and prior knowledge.

Loss Function

- Loss function: How bad is it if the model predicts value $y_{\boldsymbol{\theta}}(\mathbf{x}_i)$ when the true value of the target variable is y_i?

$$\ell(y_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i)$$

- We average the loss over the entire training data T_n:
  - Empirical risk $\hat{R}(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i)$
- Example: Binary classification problem with positive class (+1) and negative class (-1). False positives and false negatives are equally bad.
  - Zero-One Loss: $\ell_{0/1}(y_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i) = \begin{cases} 0 & \text{if } y_{\boldsymbol{\theta}}(\mathbf{x}_i) = y_i \\ 1 & otherwise \end{cases}$

Loss Function

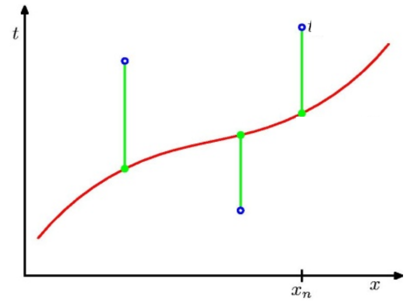
- Example: in diagnostic classification problems, an overlooked illness (false negative) is worse than an incorrectly diagnosed one (false positive).
  - Cost matrix

$$\ell_{c_{FP},c_{FN}}(y_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i) = \left\{ \begin{array}{l|c|c|} & y_i = +1 & y_i = -1 \\ \hline y_{\boldsymbol{\theta}}(\mathbf{x}_i) = +1 & 0 & c_{FP} \\ \hline y_{\boldsymbol{\theta}}(\mathbf{x}_i) = -1 & c_{FN} & 0 \\ \hline \end{array} \right.$$

Loss Function

- Example of a loss function for regression: the prediction should be as close as possible to the actual value of the target attribute.
    - Quadratic error:

$$\ell_2(y_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i) = (y_{\boldsymbol{\theta}}(\mathbf{x}_i) - y_i)^2$$



Loss Function

- How bad is it if the model predicts value y' when the true value of the target variable is y?
  - Loss: $\ell(y', y)$

- The selected loss function is motivated by the particular application.

FNM US $ s ↓ 39.443 -3.597 D 7s N 39.44/39.46 P 4x1 sho
At 10:58 Vol 18,511,558 Op 44 T Hi 44.82 D Lo 36.86 ValTrd 736.584m
Worksheet List
Edit
Options
G 6 - HILO
70
60
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40
30
20
10
50,000
0

FNM shares have broken hard and look like longer term they go to $ 20.00 even if they bounce first. This chart looks eerily similar to TYC before its 60% haircut. Bounces are selling opps.

Search for a Model

- Search for a Classifier of “toxic combinations“.

- Model space:

$$y_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{cases} \text{☹} & \text{if } \sum_{j=1}^{m} x_j \theta_j \geq \theta_0 \\ \text{☺} & \mathit{otherwise} \end{cases}$$

Training data

Medications in the combination

Sample Combinations

	x_1	x_2	x_3	x_4	x_5	x_6	y
$\mathbf{x}_1$	1	1	0	0	1	1	☹
$\mathbf{x}_2$	0	1	1	0	1	1	☹
$\mathbf{x}_3$	1	0	1	0	1	0	☺
$\mathbf{x}_4$	0	1	1	0	0	0	☺

- Approach: empirical risk should be minimal

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \sum_{i=1}^{n} \ell_{0/1}(y_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i)$$

- Is there such a model? Are there many?

Search for a Model

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  of “toxic combinations“.

- Model space:

$$y_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{cases} \text{☹} & \text{if } \sum_{j=1}^{m} x_j\theta_j \geq \theta_0 \\ \text{☺} & otherwise \end{cases}$$

- Models with 0 loss:
  - $y_{\boldsymbol{\theta}}(\mathbf{x}) =$ ☹, if $x_6 \geq 1$
  - $y_{\boldsymbol{\theta}}(\mathbf{x}) =$ ☹, if $x_2 + x_5 \geq 2$
  - $y_{\boldsymbol{\theta}}(\mathbf{x}) =$ ☹, if $2x_4 + x_6 \geq 1$
  - …

Training data

Medications in the combination

Sample Combinations

	x_1	x_2	x_3	x_4	x_5	x_6	y
$\mathbf{x}_1$	1	1	0	0	1	1	☹
$\mathbf{x}_2$	0	1	1	0	1	1	☹
$\mathbf{x}_3$	1	0	1	0	1	0	☺
$\mathbf{x}_4$	0	1	1	0	0	0	☺

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Training data

Medications in the combination

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$\mathbf{x}_3$	1	0	1	0	1	0	☺
$\mathbf{x}_4$	0	1	1	0	0	0	☺

- The models with an empirical risk of 0 form the *version space*.
- The version space is empty for a set of contradictory data.

Search for a Model

- Search for a Classifier of “toxic combinations“.

- Model space:

$$y_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{cases} \text{☹} & \text{if } \sum_{j=1}^{m} x_j\theta_j \geq \theta_0 \\ \text{☺} & \textit{otherwise} \end{cases}$$

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  - $y_{\boldsymbol{\theta}}(\mathbf{x}) =$ ☹, if $2x_4 + x_6 \geq 1$
  - …

Training data

Medications in the combination

Sample Combinations

	x_1	x_2	x_3	x_4	x_5	x_6	y
$\mathbf{x}_1$	1	1	0	0	1	1	☹
$\mathbf{x}_2$	0	1	1	0	1	1	☹
$\mathbf{x}_3$	1	0	1	0	1	0	☺
$\mathbf{x}_4$	0	1	1	0	0	0	☺

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$$y_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{cases} \text{☹} & \text{if } \sum_{j=1}^{m} x_j\theta_j \geq \theta_0 \\ \text{☺} & \textit{otherwise} \end{cases}$$

- Models with 0 loss:
  - $y_{\boldsymbol{\theta}}(\mathbf{x}) =$ ☹, if $x_6 \geq 1$
  - $y_{\boldsymbol{\theta}}(\mathbf{x}) =$ ☹, if $x_2 + x_5 \geq 2$
  - $y_{\boldsymbol{\theta}}(\mathbf{x}) =$ ☹, if $2x_4 + x_6 \geq 1$
  - …

Training data

Medications in the combination

Sample Combinations

	x_1	x_2	x_3	x_4	x_5	x_6	y
$\mathbf{x}_1$	1	1	0	0	1	1	☹
$\mathbf{x}_2$	0	1	1	0	1	1	☹
$\mathbf{x}_3$	1	0	1	0	1	0	☺
$\mathbf{x}_4$	0	1	1	0	0	0	☺

- The models of the version space differ in their predictions of some instances, which do not appear in the training set.
- Which is the correct one?

Uncertainty

- In practice, one can never be certain whether a correct model has been found.
- Data can be contradictory (e.g. due to measurement errors)
- Many different models may achieve a small loss.
- The correct model perhaps may not even lie in the model space.

- Learning as an *optimization problem*
  - Loss function: Degree of consistency with the training data
  - Regularizer: a priori probablity of a model

Regularizer

- Loss function expresses how good the model fits the data.
- Regularisierer $\Omega(\boldsymbol{\theta})$:
    - Expresses assumptions about whether the model $\boldsymbol{\theta}$ is *a priori* probable.
    - Ω is independent from the training data.
    - The higher the regularization term is for a model, the less likely the model is.
- Often the assumptions express that few attributes should be sufficient for a suitable model.
    - Count of the non-zero attributes, L_0-Regularization
    - Sum of the attribute weights, L_1-Regularization
    - Sum of the squared attribute weights, L_2-Regularization.

Regularizer

- Candidates: $(\theta_0, \theta_1, \theta_2, \theta_3, \theta_4, \theta_5, \theta_6\,)$
  - $y_{\boldsymbol{\theta}}(\mathbf{x}) =$ ☹ , if $x_6 \geq 1$ $\quad \boldsymbol{\theta}_1 = (1,0,0,0,0,0,1)^{\mathrm{T}}$
  - $y_{\boldsymbol{\theta}}(\mathbf{x}) =$ ☹ , if $x_2 + x_5 \geq 2$ $\quad \boldsymbol{\theta}_2 = (2,0,1,0,0,1,0)^{\mathrm{T}}$
  - $y_{\boldsymbol{\theta}}(\mathbf{x}) =$ ☹ , if $2x_4 + x_6 \geq 1$ $\quad \boldsymbol{\theta}_3 = (1,0,0,0,2,0,1)^{\mathrm{T}}$
- Regularizer:

L_0-Regularisierung	L_1-Regularisierung	L_2-Regularisierung
$\Omega_0(\boldsymbol{\theta}_1) = 2$	$\Omega_1(\boldsymbol{\theta}_1) = 2$	$\Omega_2(\boldsymbol{\theta}_1) = 2$
$\Omega_0(\boldsymbol{\theta}_2) = 3$	$\Omega_1(\boldsymbol{\theta}_2) = 4$	$\Omega_2(\boldsymbol{\theta}_2) = 6$
$\Omega_0(\boldsymbol{\theta}_3) = 3$	$\Omega_1(\boldsymbol{\theta}_3) = 4$	$\Omega_2(\boldsymbol{\theta}_3) = 6$

Optimization Criterion

- Regularized empirical risk: Trade-off between average loss and regularizer

$$\frac{1}{n}\sum_{i=1}^{n}\ell(y_{\boldsymbol{\theta}}(\mathbf{x}_i),y_i)+\lambda\Omega(\boldsymbol{\theta})$$

- The parameter $\lambda > 0$ controls the trade-off between loss and the regularizer.

Optimization Problem

- Is there a reason to use this optimization criterion (a *regularized* empirical risk)?
- There are several justifications and derivations:
  - Most probable (a posteriori) model (*MAP-Model*).
  - One can obtain a smaller upper bound for the error on future data depending on $|\boldsymbol{\theta}|$. (*SRM*).
  - Learning without regularization is an *ill-posed* problem; there is no unique solution or it is strongly influenced by minimal changes of the data.

Regularized Empirical Risk Minimization

- Search for a Classifier of “toxic combinations“.

- Model space:

$$y_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{cases} \text{☹} & \text{if } \sum_{j=1}^{m} x_j\theta_j \geq \theta_0 \\ \text{☺} & \mathit{otherwise} \end{cases}$$

Training data

Medications in the combination

Sample Combinations

	x_1	x_2	x_3	x_4	x_5	x_6	y
$\mathbf{x}_1$	1	1	0	0	1	1	☹
$\mathbf{x}_2$	0	1	1	0	1	1	☹
$\mathbf{x}_3$	1	0	1	0	1	0	☺
$\mathbf{x}_4$	0	1	1	0	0	0	☺

- Regularized empirical risk:

$$\frac{1}{n}\sum_{i=1}^{n} \ell_{0/1}\left(y_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i\right) + 0.1\Omega_0(\boldsymbol{\theta})$$

- Model with minimal regularized empirical risk
  - $y_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{cases} \text{☹} & \text{if } x_2 \geq 1 \\ \text{☺} & \mathit{otherwise} \end{cases}$

Evaluation of Models

- How good will a model function in the future?
- Future instances will be drawn according to an (unknown) probability distribution $p(\mathbf{x}, y)$.
- Risk: expected loss under distribution $p(\mathbf{x}, y)$.

$$R(\boldsymbol{\theta}) = \sum_y \int \ell\big((y_{\boldsymbol{\theta}}(\mathbf{x}), y\ )\big) p(\mathbf{x}, y) d\mathbf{x}$$

- Is the empirical risk on the training data a useful estimator for the risk?

Evaluation of Models

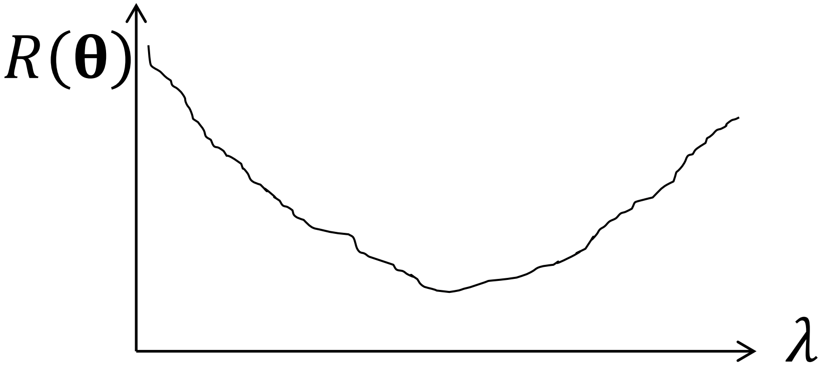
- How good will a model function in the future?
- Future instances will be drawn according to an (unknown) probability distribution $p(\mathbf{x}, y)$.
- Risk: expected loss under distribution $p(\mathbf{x}, y)$.
- Is the empirical risk on the training data a useful estimator for the risk?
  - Problem: All models in the version space have an empirical risk of 0 on the training data.
  - A classifier can achieve 0 empirical risk on the training data by simply storing each training instance in a table and reproducing the stored label when queried.

Evaluation of Models

- How good will a model function in the future?
- Future instances will be drawn according to an (unknown) probability distribution $p(\mathbf{x}, y)$.
- Risk: expected loss under distribution $p(\mathbf{x}, y)$.
- Empirical risk on the training data is an extremely optimistic estimator for the risk.
- Risk is evaluated using that were not used for training.
  - Training and Test datasets.
  - N-fold cross validation.

Optimization Problem

- How should λ be set?
- Divide available data into training and test data.
- Iterate over values of λ
  - Train on training data to find a model
  - Evaluate it on the test data
- Choose the value of λ giving minimal loss
- Train with all data



Data, Models, & Learning Problems

- Supervised Learning: Find the function most likely to have generated the training data.
- Loss function: Measures the agreement between the model‘s predictions and the values of the target variable in the training data.
- Regularizer: Measures the agreement to prior knowledge.
- Unsupervised Learning: with no target variable, discover structure in the data; e.g., by dividing the instances into clusters with common properties.
- Reinforcement Learning: Control of processes.